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Title: Computational Physics and Applied Mathematics Capability Review
June 8-10, 2010
(Binder materials)

Author(s): Various,
Primary Responsible Author, Stephen R. Lee

Intended for: Review Attendees and Committee Members

Los Alamos
NATIONAL LABORATORY
EST 1943

Computational Physics and Applied Mathematics

Capability Review
June 8-10, 2010

Participating Divisions

Chemisry (C)
Computer, Computational, & Statistical Sciences (CCS)
Decision Applications (D)
Earth and Environmental Sciences (EES)
International and Applied Technology (IAT)
International, Space, & Response (ISR)
Materials Sciences and Technology (MST)
Theoretical (T)
Technology Transfer (TT)
Computational Physics (XCP)
Theoretical Design (XTD)

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Agenda

DRAFT Agenda

June 8-10, 2010
Computational Physics and Applied Math Capability Review

Los Alamos National Laboratory, EST. 1943

Participating Organizations/Divisions

Chemistry (C)	International, Space, & Response (ISR)
Computer, Computational, & Statistical Sciences (CCS)	Materials Sciences and Technology (MST)
Decision Applications (D)	Theoretical (T)
Earth and Environmental Sciences (EES)	Technology Transfer (TT)
International and Applied Technology (IAT)	Computational Physics (XCP)

Tuesday, June 8
J. Robert Oppenheimer Study Center, Jemez Room

7:30 - 8:00	Meet at Badge Office	Committee Members Only
8:00 - 8:30	Executive session	Committee Members Only
8:30 - 9:15	Charge to the Computational Physics and Applied Math Capability Review Committee	Duncan McBranch, PADSTE
9:15 - 10:15	Computational Physics and Applied Math Overview	Alan Bishop, ADTSC
10:15 - 10:30	Break	
	Theme Area: Computational Fluid Dynamics	
10:30 - 11:15	Overview of Computational Fluid Dynamics Research at Los Alamos	Rob Lowrie, CCS-2
11:15 - 12:00	Discretizations and Closures for Climate Applications	Todd Ringler, T-3
12:00 - 1:00	Lunch Break	Committee Members Only
1:00 - 1:45	Numerical Methods and Algorithms for High-speed Multimaterial Compressible Hydrodynamics	Misha Shashkov, XCP-4
1:45 - 2:30	LDRD Presentation: Direct Numerical Simulations of Fluid Turbulence	Daniel Livescu, CCS-2
2:30 - 2:45	Break	
	Theme Area: Partial Differential Equations	
2:45 - 3:30	Overview of Partial Differential Equations Theme	Dana Knoll, T-3
3:30 - 4:15	VPIC: Kinetic plasma modeling at the petascale and beyond	Brian Albright, XCP-6
4:15 - 5:00	Newton's Method for SN Transport Applications	Jim Warsa, CCS-2
5:00 - 5:45	On the Slow Dynamics in the Arctic Basin	Beth Wingate, CCS-2
5:45 - 6:30	Break and travel to dinner location	
6:30 - 8:30	Director's Office Hosted Dinner at Ó Eating House, Pueblo of Pojoaque	Committee Members & Invitees Only

Wednesday, June 9 **J. Robert Oppenheimer Study Center, Jemez Room**		
	Theme Area: Monte Carlo Methods	
8:00 - 8:45	Monte Carlo Research at LANL - An Overview	Frank Alexander, Institutes Office
8:45 - 9:30	Hybrid Transport-Diffusion Methods for Implicity Monte Carlo Radiative-Transfer Simulations	Jeff Densmore, CCS-2
9:30 - 10:15	Implicit Monte Carlo on Roadrunner	Tim Kelley, CCS-7
10:15 - 11:00	MCNP	Tim Goorley, XCP-3
11:00 - 12:30	Lunch Break; travel and access to classified session	
Parallel Session	***Theme Area: Integrated Codes (Unclassified)*** **J. Robert Oppenheimer Study Center, Jemez Room**	
12:30 - 2:00	Climate, Ocean and Ice Applications	Phil Jones, T-3
2:00 - 2:30	Break	
Parallel Session	***Theme Area: Integrated Codes (Classified)*** **Powerwall, Strategic Computing Center (SCC)**	
12:30 - 2:00	Nuclear Weapons Applications	Bill Archer, XCP-ASC
2:00 - 2:30	Travel back to Study Center	
	Theme Area: Integrated Codes (Unclassified, Continued)	
2:30 - 3:30	Roles and Opportunities for UQ	Dave Higdon, CCS-6
3:30 - 4:30	Future Directions: capabilities and applications	Andy White, ADTSC
Santa Clara Gallery		
4:30 - 6:30	Poster session and reception	Committee Members & Invitees Only
Thursday, June 10 **J. Robert Oppenheimer Study Center, Jemez Room**		
8:00 - 9:30	Program Manager Roundtable Discussion	Committee Members & Invitees Only
9:30 - 10:30	Postdoc and Early Career Roundtable Discussion	Committee Members & Invitees Only
10:30 - 1:00	Executive session and outbrief preparation Lunch break	Committee Members Only
1:00 - 2:00	Executive Outbrief	Committee Members, Director's Office, & PADSTE Only
2:00 - 2:30	Open Outbrief	Chair

Instructions to Committee

NPAC Self Assessment

Computational Physics and Applied Mathematics (CPAM) Self-Assessment Report

CY2009-2010

CPAM Capability Review

June 8-10, 2010

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Computational Physics and Applied Mathematics Self-Assessment Report

Stephen Lee (CCS), Francis Alexander (IST-OFF), Stephan Eidenbenz (CCS),
Timothy Germann (T), Dana Knoll (T), Robert Lowrie (CCS)
Los Alamos National Laboratory
June 8-10, 2010

1.0 Introduction

Los Alamos National Laboratory will review its Computational Physics and Applied Mathematics (CPAM) capabilities in 2010. The goals of capability reviews are to assess the quality of science, technology, and engineering (STE) performed by the capability, evaluate the integration of this capability across the Laboratory and within the scientific community, examine the relevance of this capability to the Laboratory's programs, and provide advice on the current and future directions of this capability. This is the first such review for CPAM, which has a long and unique history at the Laboratory, starting from the inception of the Laboratory in 1943.

The CPAM capability covers an extremely broad technical area at Los Alamos, encompassing a wide array of disciplines, research topics, and organizations. A vast array of technical disciplines and activities are included in this capability, from general numerical modeling, to coupled multi-physics simulations, to detailed domain science activities in mathematics, methods, and algorithms. The CPAM capability involves over 12 different technical divisions and a majority of our programmatic and scientific activities. To make this large scope tractable, the CPAM capability is broken into the following six technical "themes." These themes represent technical slices through the CPAM capability and collect critical core competencies of the Laboratory, each of which contributes to the capability (and each of which is divided into multiple additional elements in the detailed descriptions of the themes in subsequent sections), as follows.

- *Theme 1: Computational Fluid Dynamics*. This theme speaks to the vast array of scientific capabilities for the simulation of fluids under shocks, low-speed flow, and turbulent conditions – which are key, historical, and fundamental strengths of the Laboratory.
- *Theme 2: Partial Differential Equations*. The technical scope of this theme is the applied mathematics and numerical solution of partial differential equations (broadly defined) in a variety of settings, including particle transport, solvers, and plasma physics.
- *Theme 3: Monte Carlo*. Monte Carlo was invented at Los Alamos. This theme discusses these vitally important methods and their application in everything from particle transport, to condensed matter theory, to biology.
- *Theme 4: Molecular Dynamics*. This theme describes the widespread use of molecular dynamics for a variety of important applications, including nuclear energy, materials science, and biological modeling.
- *Theme 5: Discrete Event Simulation*. The technical scope of this theme represents a class of complex system evolutions governed by the action of discrete events. Examples include network, communication, vehicle traffic, and epidemiology modeling.

- *Theme 6: Integrated Codes*. This theme discusses integrated applications (comprised of all of the supporting science represented in Themes 1-5) that are of *strategic importance* to the Laboratory and the nation. The Laboratory has in approximately 10 *million* source lines of code in over 100 different such strategically important applications.

Of these themes, four of them will be reviewed during the 2010 review cycle: Themes 1, 2, 3, and 6. Because these reviews occur every three years, Themes 4 and 5 will be reviewed in 2013, along with Theme 6 (which will be reviewed during each review, owing to this theme's role as an *integrator* of the supporting science represented by the other five themes). Yearly written status reports will be provided to the CPAM Committee Chair during off-cycle years.

1.1 CPAM Review Challenges and Expectations

CPAM represents a vast array of projects, technology, and technical activities that span the Laboratory. Capabilities included have been built within the confines of individual programs (some since the existence of the Laboratory) and, as such, are typically not strategically planned and managed as integrated and unified capabilities. Integrated codes are built for particular customers for particular purposes, and the supporting science has often been constructed in support of those applications. However, Los Alamos has excelled at applying its broad scientific capabilities to multiple missions and this is obvious when one looks at CPAM. The codes themselves are the integrated product. Figure 1 below is illustrative of our multi-programmatic approach, building from our science base.

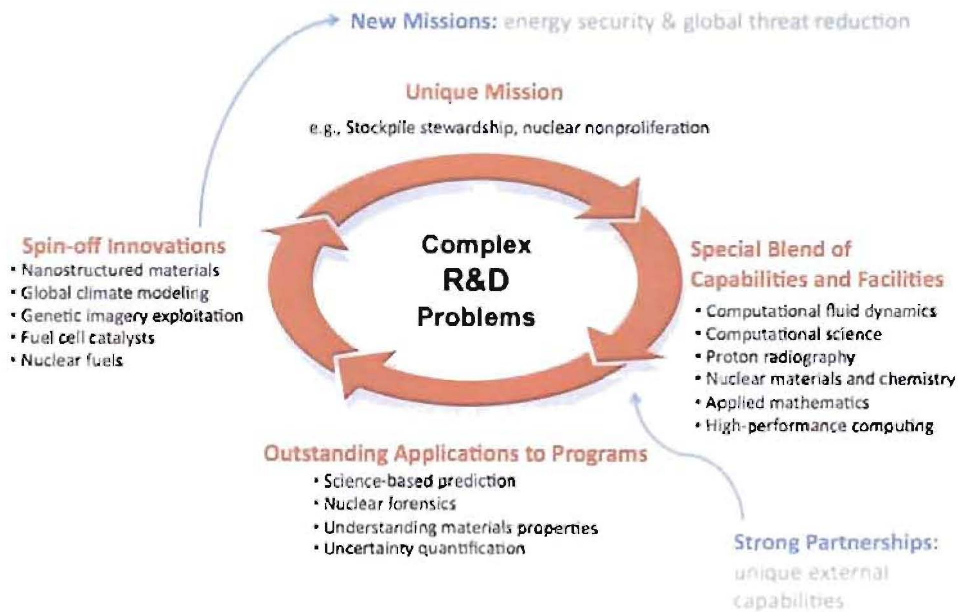


Figure 1. Spin-off innovations based on our core scientific capabilities in support of our unique mission space lead to growth as a capability-based national security laboratory and new mission areas.

The Laboratory seeks the advice of the review committee as we continue to hone our CPAM capabilities as a significant capability at the Laboratory and as a critical element for our future.

1.2 Organization of the Self-Assessment Document

The remainder of this document, with the exception of the general challenges and issues, Section 8, is organized around the six CPAM theme areas. This breakdown is intended to provide an organized assessment of this broad capability. Owing to the report the committee is asked to prepare, this self-assessment addresses, for each theme area, the connection to the goals and mission of the Laboratory, the research breadth and impact, comparison with peers, status of the capability, and challenges and issues.

The themes are completely contained in each major section below, starting with Section 2.0 for Theme 1 and ending with Section 7.0 for Theme 6. Within each of these sections, a subsection exists for each of the assessment areas discussed above with information on each pertaining to that specific theme.

- *Section x.1: Connection to the Goals and Mission of the Laboratory.* Context is provided for how the theme area enables the science required for the mission of the Laboratory, how the theme contributes to our goals, and how the theme leverages growth for the future.
- *Section x.2: Research Breadth and Impact.* The current research portfolio and impact of current and future work at the Laboratory to programs and to the scientific community for the theme area is discussed.
- *Section x.3: Comparison with Peers.* In this section, a brief comparison of work in the theme area is made with similar work conducted by other institutions.
- *Section x.4: Status of the Capabilities.* A snapshot of the current technical challenges and accomplishments is given along with a sense of the sustainability of the capability into the future.
- *Section x.5 Challenges and Issues.* Issues and challenges (technical or otherwise) that specifically pertain to the theme are discussed.

A general section on challenges and issues applying to the entirety of the CPAM capability is presented in Section 8. Section 9 contains references used in this document. A list of acronyms used in this capability, posters, presentations, and other related items are included in the full CPAM Capability Review materials provided separately to committee members at the on-site review.

A separate document provided to review committee members contains selected statistics (publications, presentations, awards, etc.) for this capability.

2.0 Theme 1: Computational Fluid Dynamics

(Theme Leader: Robert Lowrie, CCS Division)

The Computational Fluid Dynamics (CFD) theme is quite broad, spanning multiple projects, technical capabilities, and issues at the Laboratory. As a result, the theme is broken into the following six subject areas for the purposes of this document:

- Discretizations and Closures for Climate Applications
- High-energy Multi-material Compressible Radiation Hydrodynamics
- Direct Numerical Simulations of Fluid Turbulence
- Computational Fluid Dynamics Applications in Astrophysics
- Subsurface Flows
- Computational Fluid Dynamics Applications on Advanced Architectures

This taxonomy also represents a technical crosscut through this theme of strategic importance to Los Alamos.

2.1 Connection to the Goals and Mission of the Laboratory

2.1.1 Discretizations and Closures for Climate Applications. Our efforts in developing algorithms for simulating the dynamics of atmosphere, ocean and land-ice flows is tightly tied to our Earth and Energy Systems Grand Challenge. This Grand Challenge is to "... develop the capability to measure, model, and predict, in a quantifiable manner, the impacts of energy choices on climate and their cascading effects on the environment and society." We expect that the rise of atmospheric carbon dioxide concentrations over the next century will lead to significant changes in the Earth's climate. One of the many prerequisites to an accurate simulation of future climate change is the availability of robust solvers for the motion of the atmosphere, ocean and land ice systems. This mission is closely aligned with the major sponsor of this work, the Climate and Environmental Science Divisions within DOE BER, whose goal is to develop "... a predictive, systems-level understanding of the fundamental science associated with climate change."

2.1.2 High-energy Multi-material Compressible Radiation Hydrodynamics. A primary responsibility of Los Alamos is to develop and apply science and technology to ensure the safety, security, and reliability of the US nuclear deterrent. The Advanced Simulation and Computing (ASC) Program supports the DOE National Nuclear Security Administration (NNSA) Defense Programs and its shift in emphasis from nuclear testing to computer simulation. Under ASC, computer simulation capabilities are developed to analyze and predict the performance, safety, and reliability of nuclear weapons and to certify their functionality. The Integrated Codes (IC) sub-program of ASC at Los Alamos constitutes Laboratory projects that develop and improve weapons simulation tools, physics, engineering, and specialized codes. The core of the ASC codes is high-energy, multi-material, compressible radiation hydrodynamics. Therefore, development of new methods and algorithms for such flows, along with their coupling to other physical processes, is absolutely critical for the stockpile stewardship Laboratory mission. It is also important to note that these same codes and methods are being used for a variety of other applications such as inertial confinement fusion research, astrophysics, and homeland security, which was alluded to in Figure 1 in Section 1.1.

2.1.3 Direct Numerical Simulations of Fluid Turbulence. Many of the problems of interest for the Laboratory involve fluid flows and mixing between different materials, occurring mostly in the presence of turbulence. Although routine calculations of such flows require coarse meshes for reasonably fast calculations, the present generation of DOE supercomputers has enabled accurate calculations for several flows of interest, albeit at very long simulation times. These types of calculations, commonly known as Direct Numerical Simulations (DNS), offers a wealth of information, inaccessible in physical experiments, and can be designed to isolate the importance of a specific physical phenomenon. Thus, DNS can be used to complement physical experiments to improve and device turbulence models, as well as verify and validate the DOE physics codes.

2.1.4 Computational Fluid Dynamics Applications in Astrophysics. Many applications for computational fluid dynamics exist in astrophysics research. Moreover, as additional physics is added to the fluid dynamic calculations, the scope of applications expands greatly. We review some of the astrophysics applications Los Alamos is working on, as follows.

- *Mixing in stars and s-process nucleosynthesis.* One of the outstanding problems in stellar evolution is explosive convection in the late stages of the life of intermediate mass stars. The mixing of fuel down to a burn region and the energetic feedback of this burning fuel is an ideal CFD problem. Calculations require a multi-material prescription with a simple nuclear burn network [Clayton et. al. 2007, Herwig et. al. 2008, Pignatari et. al. 2008, Hirschi et. al. 2008, Diehl et. al. 2008, Bennett et. al. 2010, Herwig et. al. 2010, Motl et. al. 2007].
- *Convection in the core-collapse supernova engine.* The convection in a core-collapse supernova and type Ia supernovae is critical to driving a supernova explosion [Fryer & Young 2007, Fryer et al 2007, Budge et al 2008, Raskin et al 2009, Livescu et al 2010]. This convection forms from the perturbations in the pre-collapse star. These perturbations grow in the collapse and bounce phase of the star. CFD calculations of this growth are crucial to understanding the onset of this convection. The addition of heating/cooling terms allows more extended calculations.
- *Mixing in supernova ejecta and supernova observations.* Mixing in supernovae brings radioactive nickel (that powers supernova light-curves) from its production site in the core into the outer layers of the star, altering shape and details of the emission observed from supernova. Multi-material CFD calculations, coupled with radiation transport, are required to accurately model this supernova emission [Fryer et al 2007, Fryer 2009, Young & Fryer 2008, Fryer 2008].

Many other CFD applications exist in models of planet formation and active galactic nuclei. There is a rich set of research at Los Alamos leveraging our CFD and multi-physics CFD assets and attracting new talented staff and postdocs to Los Alamos.

2.1.5 Subsurface Flows. A new era of computational power is emerging for modeling subsurface reactive flows derived from a new generation of massively parallel computing architectures. It is now possible to carry out simulations with billions of grid cells and a multitude of chemically reacting constituents that was heretofore impossible. As a consequence of this new capability (besides the ability to carry out simulations in three spatial dimensions at higher resolution), more realistic algorithms can be introduced to model the fate and transport of contaminants and other processes in multiphase systems. This new capability applies directly to Laboratory goals and mission related to energy security through applications involving remediation and monitoring of cold war legacy waste, carbon sequestration, geothermal energy and other energy-related applications, all of which relate to the broader issue of national security.

2.1.6 Computational Fluid Dynamic Applications on Advanced Architectures. This area is focused on developing programming models, coding abstractions, tools, and techniques to aid in making modern processing capabilities—including homogeneous and heterogeneous multicore, hybrid and accelerated computing architectures—accessible to CFD developers and domain scientists. The challenges associated with designing and developing simulation codes to run on these types of architectures are likely to dominate our efforts for at least the next decade. Our overarching goals are threefold, each addressing some aspect of integrating new technologies into our existing capabilities: 1) identify relevant hardware and software trends and begin to understand how they impact—or can be used to enhance—current development techniques, and how these can be abstracted to suit the specific needs of CFD research at the Laboratory; 2) experiment with using these tools and abstractions to implement pseudo-production level codes that incorporate substantially realistic physics capabilities, thereby further establishing what techniques and tools will ultimately be useful; and 3) integrating these "vetted" techniques into actual CFD production codes.

The goals of this effort span a spectrum that extends from bleeding-edge, high-risk investigations of new architectures and programming languages and tools, to moderately flexible projects that can absorb some risk and are designed to emulate the needs of production code projects, to the necessarily conservative, user-oriented, full production codes themselves. Our basic strategy is to establish a pipeline—focused on interaction and communication between representatives from each of the three goal-oriented thrusts listed above, through which, new ideas and programming models can be developed, validated and integrated into actual production codes using a staged approach. This co-design of new systems and codes is critical to the future of Los Alamos.

2.2 Research Breadth and Impact

2.2.1 Discretizations and Closures for Climate Applications. Modeling atmosphere and ocean dynamics over the duration of simulated centuries in a highly rotating system leads to the development of computational fluid dynamics algorithms that are distinct from their counterparts in other fields of science. Small secular drifts in the discretization of the governing PDEs can accumulate over the duration of the simulation and eventually corrupt the simulation. Of particular importance with the field of fluid solvers for climate applications is the requirement that the discrete solution mimic the continuous system with regard to invariants such as mass, potential vorticity, energy, and potential enstrophy.

Models of atmosphere and ocean dynamics are always (and will always be) under-resolved. We are thus continually confronted with the notion of sub-grid closures, i.e., empirical or theoretical models that predict the net impact of all unresolved motion on the simulated system. In addition, with significant energy existing at or near the grid scale, we are forced to pay special attention to the diffusion properties our numerical algorithms and, in particular, the transport algorithms. Given the highly nonlinear nature of the system, excessive diffusion at the grid scale propagates to much larger scales over the duration of century-long simulations.

To address these broad challenges in the development of algorithms for the robust simulation of climate dynamics, cutting edge algorithms are being developed at Los Alamos in the areas of spatial discretization, temporal discretization, transport, and closures.

In the area of spatial discretization, Los Alamos has developed the first multi-resolution finite-volume method applicable to simulation of ocean and atmosphere dynamics at time scales commensurate with climate change [Ringler et al. 2010, Thuburn et al. 2009]. Through the use of variable-resolution, centroidal Voronoi diagrams, resolution can be placed in specific areas of interest [Ringler et al. 2008]. This approach allows for the study of high-resolution, climate-relevant phenomena (i.e. ocean eddies or atmosphere clouds) in isolated regions within the framework of a global climate model. This approach is the basis for the next-generation global cloud-resolving model under development at the National Center for Atmospheric Research (NCAR). This approach also forms the basis of the next Los Alamos global ocean model.

In the area of temporal discretization, Los Alamos is at the forefront of the development of fully implicit time integration schemes for use in atmosphere and ocean models based on Jacobi-Free Newton Krylov Methods (JFNK) [Evans et al. 2009, Nadiga et al. 2006 and Reisner et al. 2003, Knoll, 2004]. JFNK allows highly nonlinear systems that exhibit a wide range of time and space scales to be integrated within a unified system without the need for dimensional or process splitting. JFNK methods can readily extended to high-order accuracy in time, thus providing the ability to adaptively control error accumulation over the course of the simulations. Since JFNK methods provide an approximation to the discrete system's Jacobian, sensitivity of the simulation results (such as the sensitivity of the ocean meridional overturning circulation to freshwater forcing), can be inferred [Dijkstra and Weijer, 2005]. Los Alamos has a long history in the development of transport algorithms and this effort has been leveraged into the climate modeling activities. The thrust of this work is to exploit the Lagrangian nature of transport while maintaining a computationally-viable mesh. One such transport scheme based on this approach, called incremental transport, has found application in Los Alamos's ocean, sea-ice and land-ice model [Dukowicz and Baumgardner, 2000; Lipscomb and Ringler, 2005; Lowrie, 2009]. The recent work by Lowrie (2010) has extended incremental remapping to arbitrary order-of-accuracy on arbitrary convex polygon meshes. This new advanced transport algorithm is a core component of the Los Alamos next-generation ocean model that is now under development.

The defining feature of the grand challenges in computational physics is that the available computational resources are not sufficient to resolve the full breadth of phenomena observed in the physical system being modeled. This is particularly true in climate modeling. For example, while ocean eddy activity is found throughout the entirety of the world's oceans, climate simulations on the time scale of centuries cannot simulate these ocean eddies directly due to lack of computational resources. As a result, a tremendous amount of effort is expended to develop sound, robust closures of the fluid system that model the net impact of the unresolved processes on the simulated system. Over the last decade Los Alamos has been at the forefront of developing a new class of closures that attempt to represent the sub-grid scale effects while respecting the important invariants of the underlying PDEs [Holm 1999]. Over the last several years, this new class of closures, called the Lagrangian-Averaged Navier Stokes (LANS-alpha) closures, has been incorporated into the Los Alamos ocean modeling activities [Hecht et al. 2008, Petersen et al. 2008]. The LANS-alpha closure in unique in its ability to incorporate ocean eddy activity at computational-tractable model resolutions.

The primary impact of the climate-related computational physics activities is through their integration into climate model components that are used to understand and quantify climate change. Los Alamos develops, distributes and supports comprehensive climate model components that utilize the methods described above for ocean, sea-ice and land-ice systems. These models are integrated into the NCAR Community Climate System Model (CCSM) that is used as a part of the Intergovernmental Panel on Climate Change (IPCC) assessment reports. The NCAR CCSM is also the only publicly available climate model in the US and is therefore widely used in the academic community.

2.2.2 High-energy Multi-material Compressible Radiation Hydrodynamics. The research in the development of methods and algorithms for modeling high-energy multi-material compressible flows is quite broad. It is critical that the methods and codes developed be applicable to the extreme regimes encountered in simulations of weapon performance. In particular this means that the hydrodynamic methods must support strong shocks, real materials, material strength, material mixing, reactive chemistry, large flow deformations, and turbulence; together with the coupling of these processes with radiation transport and other physical processes. A pragmatic measure of research success is the migration of the algorithms and methods developed here into working production codes. Furthermore, since these codes are intended to serve as tools for engineering design and assessment, they must provide adequate performance for simulation turnaround together with a rich set of tools for the analysis of the simulation output.

Two broad approaches are used in the design of hydrodynamic codes, a fixed spatial grid Eulerian approach (including dynamic mesh refinement) and a moving mesh Lagrangian approach. The two approaches are complimentary in that Lagrangian is best suited for moderate resolution sharp interface flows while Eulerian is well suited for high-resolution large deformation flows transitioning into turbulence. Both schemes have limitations, the addressing of which are major components of method development research. For Eulerian schemes, mixed cell treatments is major research issue, while mesh tangling or poor mesh quality in general is a central issue for Lagrangian schemes. Since a major technique for improving Lagrangian mesh quality is the Arbitrary Eulerian Lagrangian (ALE) approach, the issue of mixed cell treatments is an important component of Lagrangian codes too. Both approaches must address the properties of real materials, so high quality hydrodynamic equations of state (EOS) are a must. Research into high order thermodynamically consistent treatments of equations of state based on tabulated data is one component of the current research. This work includes EOS treatments for solids and materials in tension and the support of such flows for the hydrodynamic solvers.

Methodologies to handle mixed cells in the Eulerian approach include explicit interface tracking [Glimm, Grove et al. 2000; Glimm, Grove et al. 2002; Bo, Jin et al. 2008], volume of fluid interface reconstruction [Cummins, Francois et al. 2005; Francois, Lowrie et al. 2009; Schofield, Garimella et al. 2009; Francois and Swartz 2010], and dynamic models for non-equilibrium mixtures [Zhang, Ma et al. 2006; Grove 2010].

A major component of our work is directed at the coupling of material flow with radiation. Recent work includes Monte-Carlo methods for radiation transport [Densmore, Warsa et al.

2010], and verification via first-of-kind analytic solutions for radiative shocks [Lowrie and Rauenzahn 2007; Lowrie and Edwards 2008].

Conservative discretization of the flow equations on general polyhedral meshes [Caramana, Burton et al. 1998; Campbell and Shashkov 2001] has been a significant focus for Lagrangian hydrodynamics method development. It also includes development of closure models [Shashkov 2008] needed to capture sub-scale physics of mixed cells. Mesh rezoning including mesh improvement [Knupp, Margolin et al. 2002], mesh untangling [Vachal, Garimella et al. 2004] and mesh reconnection – [Loubère, Maire et al. 2010] is another focus area. Rezoning requires conservative interpolation, remap between Lagrangian and rezoned mesh, [Margolin and Shashkov 2003; Loubere and Shashkov 2005]. As in the Eulerian case, interface reconstruction is also an important research topic for Lagrangian codes [Ahn and Shashkov 2007; Dyadechko and Shashkov 2008].

This goal of all of this work is to provide a predictive capability for the ASC codes for high-energy complex flows.

2.2.3 Direct Numerical Simulations of Fluid Turbulence. The current petascale computers have enabled accurate simulations of complex turbulence flows, in non-standard configurations, away from the usual canonical flows extensively studied in the past. The current efforts at the Lab encompass a range of such flows: compressible and shocked turbulence [Petersen and Livescu 2010], compressible and incompressible buoyancy driven flows [Livescu and Ristorcelli 2007, 2008; Livescu et al 2010] and reacting turbulence with type Ia supernova microphysics [Livescu, Mohd-Yusof and Kelley 2010). These new simulations have revealed interesting new physics and are rapidly increasing the predictive capabilities of the large physics codes.

2.2.4 Computational Fluid Dynamics Applications in Astrophysics. Applied CFD problems span a broad set of programs and research entities: NNSA, DOE Office of Science, NASA, and NSF. These multi-physics problems tie strongly to many of the ASC and Campaign studies. Astrophysics problems provide additional verification tests for ASC codes and can be used for training and recruitment. They also tie Los Alamos code development to larger DOE interests such as nuclear physics and the facility for rare isotope beams. These projects tie extremely well into Los Alamos programs in nuclear, particle, astrophysics and cosmology (NPAC) and fit into the Astrophysics Initiative funded by ASC and Campaign projects.

2.2.5 Subsurface Flows. Research involves a number of different thrusts in geosciences including a SciDAC-2 groundwater project (Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows using Advanced Computing, Lichtner PI), Advanced Simulation Capability for Environmental Management (ASCEM, Dixon PM) project initiated by DOE-EM to develop a community-wide subsurface modeling code, and modeling coupled thermal-hydraulic-mechanical processes in fractured geological media (FEHM, Zyvoloski PI).

The SciDAC-2 project involves modeling multiphase, multi-component reactive flows in multidimensional fractured and porous media by leveraging massively parallel computation through development of the highly scalable reactive flow and transport code PFLOTRAN with application to energy and environment related projects. The code is currently being used to investigate cleanup options including natural attenuation of cold war legacy waste at Hanford, WA, carbon sequestration in deep geologic formations, and to help optimize geothermal energy recovery. Calculations carried out at the Hanford 300 Area bordering the Columbia River have helped resolve a long-standing issue of the slow release of uranium at the site. In the early 1990s it was predicted that uranium would be reduced to acceptable levels in ten years, but today the plume still persists exceeding EPA maximum concentration levels. The problem is complicated by the hourly fluctuations in the Columbia River stage of several meters causing flow of water to and from the river. Three-dimensional model calculations carried out with PFLOTRAN with 28 million degrees of freedom were able to predict the release of uranium into the Columbia River in close agreement with present-day field observations. It was discovered that the high frequency fluctuations in the Columbia River stage could be averaged out leading to a simple approximately linear behavior in the cumulative uranium flux with time. Contrary to expectations, the model calculations showed that sorption of uranium played only a secondary role in the uranium attenuation rate. The major factor controlling the release of uranium, not considered by previous investigators, appears to be the slow release of non-labile uranium located in a smear zone within the vadose zone that is periodically wetted by the rising and falling water table. Also unexpected was the lack of influence of meter-scale heterogeneity in the permeability field on the flux of uranium into the Columbia River. Multiple realization calculations, a novel feature of PFLOTRAN through its ability to run seamlessly multiple realizations with multiple processor cores per realization, found minimal effect from a heterogeneous permeability field on the flux of uranium into the river. Additional work is needed to investigate the role of site-scale heterogeneity on the flux.

2.2.6 Computational Fluid Dynamic Applications on Advanced Architectures. This topic primarily supports research efforts in two areas: 1) early-adopter experiments with the goals of understanding how modern architectural developments can be exploited in the short-term to adapt or enhance CFD methods and algorithms, and how these concepts can be abstracted into low or mid-level tools, programming models or techniques that will be useful and accessible to an applications developer within a 3-5 year time frame; and 2) longer-term efforts to define and develop high-level or domain-specific interfaces and languages that insulate methods developers and programmers from disruptive technological developments in the underlying computing architecture as an enduring solution to the volatility in this area. Research topics in this area include, but are not limited to, the following.

- Strategies for application-level fault tolerance with ties to systems developers to establish what role should be played by either side and what interfaces are needed to enable the development of resilient simulation codes.
- Development of portable programming models for multi-core/many-core and accelerated architectures.
- Development of algorithms and programming models that expose greater concurrency.
- Design of data structures for efficient CFD-specific requirements, e.g., efficient material data lookup or generation (EOS, opacity, nuclear data).
- Design of high-level algorithm descriptions for domain-specific language development.
- Algorithm co-design for simulation problems that do not map well onto commodity hardware.

Several of the above topics are also in direct preparation for the move to Exascale computing.

2.3 Comparison with Peers

2.3.1 Discretizations and Closures for Climate Applications. The climate modeling activity at Los Alamos is connected to the international community. Los Alamos scientists are key members of the NCAR CCSM activity by co-chairing working groups on ocean model development, sea-ice model development and land-ice model development. Within the DOE, Los Alamos scientists share joint efforts with ANL, LBNL, LLNL, ORNL, PNNL and SNL. This is a highly integrated, multi-partner, collaboration.

2.3.2 High-energy Multi-material Compressible Radiation Hydrodynamics. Our peers include DOE Labs (both NNSA and Science), other government supported laboratories (e.g. NASA and DoD), academic universities including the NNSA ASC alliance centers, foreign research laboratories (e.g. AWE (UK), CEA (France), and Russian Labs) and academic institutions. We have extensive knowledge of the numerical methods and codes used in these organizations because of their participation in conferences and meetings. We are confident that we are leaders in method development for high-energy multi-material compressible hydrodynamics and methods developed at Los Alamos have achieved a high penetration into codes developed around the world. This claim is supported by citation of Los Alamos papers.

2.3.3 Direct Numerical Simulations of Fluid Turbulence. Los Alamos researchers are at the forefront of large-scale turbulence simulations. This includes the first successful implementation, with excellent performance, of a large fluid dynamics code on the Cell architecture [Livescu, Mohd-Yusof and Kelley 2010; Mohd-Yusof, Livescu and Kelley 2009]. The recent simulations of the CCS-2 fluid dynamics team represent the state of the art for buoyancy driven and compressible turbulence and are the largest ever attempted in their configurations. Los Alamos researchers are also collaborating with other national laboratories and universities in order to examine very large simulations performed outside Los Alamos [Livescu et al 2009; Reckinger, Livescu and Vasilyev 2010].

2.3.4 Computational Fluid Dynamics Applications in Astrophysics. Los Alamos has produced a number of computational firsts in these arenas, from highest resolution mixing studies to the first detailed supernova spectra from radiation hydrodynamics calculations.

2.3.5 Subsurface Flows. Currently there appears to be no comparable computational subsurface codes that can meet the performance of PFLOTRAN. Other contenders such as STOMP developed at PNNL, TOUGH developed at LBNL, UTCHEM developed at the University of Texas, Austin, and others have not, to our knowledge, achieved petascale performance as measured by running on over 100k processor cores. Los Alamos's Finite Element Heat and Mass Transfer (FEHM) code remains a leader due to its unique capability for coupling mechanical stress and flow in porous media. Although it remains a serial code, it is a workhorse in uncertainty quantification studies with ensembles of single processor runs performed in parallel.

2.3.6 Computational Fluid Dynamic Applications on Advanced Architectures. Activities in modern architecture research at Los Alamos have been a pioneering effort in the HPC community, establishing many best practices tools and techniques for applications development on modern computing architectures. This effort has been so successful that it first led to the formation of the Emerging Applications and Architectures team and then subsequently to the formation of the Applied Computer Science Group (CCS-7). Members of this new group are extremely active in developing and guiding community efforts in this area. Some examples of Laboratory leadership under this theme are:

- Pat McCormick (programming models team lead) is the chair for the heterogeneous thrust area for the 2010 Supercomputing Conference;
- Ben Bergen (programming models team member) is the Los Alamos representative on the Khronos Group OpenCL consortium;
- Sriram Swaminarayan (CCS-7 Group Leader) is the chair for the applications development committee of the Hybrid Multicore Consortium (HMC, a partnership of LANL, ORNL, SNL, and LBNL); and
- Paul Henning (algorithm co-design team lead) is the chair for the programming models committee of the HMC.

Members of this group have community-recognized expertise and frequently receive invitations to present or to act as consultants to other laboratories and institutions. This group is also making significant contributions to programmatic code development and open science. An example of this that is gaining attention is the work done by Tim Kelley and Paul Henning for Implicit Monte-Carlo simulations of radiation transport, whose code is a staple on the Roadrunner supercomputer. Additional successes on Roadrunner include work done by Jamal Mohd-Yusof and Daniel Livescu for turbulent fluid modeling, work done by Swaminarayan and Tim Germann for molecular dynamics, and work done by Bergen for plasma physics simulations. Collaborative development efforts are underway to address the challenges of multiphysics on multicore and accelerated architectures under the MultiPhysics for MultiCore (MPMC) project headed by John Wohlbier and Rob Lowrie in CCS Division.

2.4 Status of the Capabilities

2.4.1 Discretizations and Closures for Climate Applications. The computational physics activities related to climate modeling are vibrant at Los Alamos. The work being done in spatial discretization, temporal discretization, transport and closure all have the potential to be defining features of the next-generation climate modeling system that will be constructed during this decade.

2.4.2 High-energy Multi-material Compressible Radiation Hydrodynamics. The Eulerian production codes have proven to be very receptive to the incorporation of methods and algorithms developed under this project. Capabilities include support for materials in tension in mixed and pure cells, interface reconstruction in one, two, and three spatial dimensions, Eulerian methods for materials with strength, radiation transport, non-equilibrium temperature models for mixtures, higher order Godunov treatments for adaptive mesh refinement. In all cases these tools and methods are incorporated into a code framework that is used for pure and applied research by a large set of individuals and groups.

Current research in Lagrangian hydrodynamics is focused on several issues. These include sub-scale modeling and void formations in mixed cells, reconnection-based methods, where connectivity of the mesh can change at rezone stage, and cell-centered discretizations as opposed to staggered discretizations, which are used in almost all current Lagrangian codes. We have developed solid mathematical foundation for high-speed multimaterial compressible computational hydrodynamics. It allows robust modeling of complex 3D multimaterial flows.

2.4.3 Direct Numerical Simulations of Fluid Turbulence. The main DNS code used by the CCS-2 fluid dynamics team is called CFDNS. The code has been developed within CCS-2 for the last 7 years and has been used up to 150,000 compute cores on BG/P Dawn at LLNL with very good performance. The Cell version of the code, CFDNS-rr, reaches speed-ups close to the theoretical peak: 30x compared to the serial version and 20x at scale. CFDNS consists of a suite of modules, for various turbulence problems: incompressible, compressible, or variable density multi-fluid turbulence. The flow can have periodic or non-reflecting BC and real materials with tabular material properties and EOS.

2.4.4 Computational Fluid Dynamics Applications in Astrophysics. Los Alamos science efforts in CFD using the latest computers and computing architectures are pushing the envelope in resolution studies. Los Alamos's Roadrunner is capable of modeling simulations with 64 billion zones, beyond the current high-resolution studies of convective processes. For applied astrophysics problems, such high-resolution studies are many orders of magnitude beyond the current state-of-the-art.

2.4.5 Subsurface Flows. Through the SciDAC-2 groundwater project, the massively parallel computational framework PFLOTRAN has been developed for modeling subsurface reactive flows in porous media. The code is DOE/Joule certified and has been run on 217 (131, 072) processor cores with 2 billion grid cells on ORNL's Jaguar XT5 computer achieving petascale performance. It is being applied to modeling uranium migration at the Hanford 300 Area and to carbon dioxide sequestration and geothermal energy recovery in deep geologic formations. A unique capability of PFLOTRAN is the ability to perform multiple realization simulations with multiple processors per realization limited only by the capability of the machine. Hanford simulations have typically employed 40k processor cores running 10 realizations with 4k cores per realization. This work is also supported by INCITE, for which the project has been awarded two three-year grants totaling roughly 30 million cpu-hours on ORNL's Cray XT4/5 (Jaguar), currently the number one computer in the Top 500 list. Presently, PFLOTRAN is being evaluated to serve as one of six codes to use to certify the next-generation Cray machine at the OLCF (ORNL Leadership Computing Facility) based on hybrid architectures. This machine is expected to be operational in 2012 and will serve as a first step towards exascale computing (and is related to the HMC discussed in section 2.3.6).

Advancements are being made in the ability to model coupled thermal-hydraulic-mechanical processes in fractured, porous geological media using the sequential code FEHM. Such modeling capabilities are of interest to a wide variety of projects across the EES Division related to energy (e.g. Oil & Gas, Geothermal), nuclear waste isolation, CO2 sequestration, and environmental management/restoration; as well as projects which study fundamental geophysical phenomenon. FEHM is currently able to handle multiphase, porous flow fully coupled with heat transfer; partial coupling with reactive flow; and partial coupling with linear elastic solid deformation. It is being extended to handle plastic behavior and to incorporate full coupling between the equations of solid deformation and fluid flow.

Recently, DOE-EM initiated the Advanced Simulation Capability for Environmental Management (ASCEM) project to develop a community-wide computer code for understanding and predicting contaminant fate and transport in natural and engineered systems. Central to ASCEM will be open-source modular toolsets that will be developed to facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for DOE-EM cleanup and closure activities. There are three thrust areas in the ASCEM project. First, is the Platform and Integrated Toolsets, which provides a flexible user interface for conceptual model development with advanced data management to support parameter estimation and uncertainty quantification for decision support and risk assessment. Los Alamos is leading critical tasks in this thrust, including conceptual model development and model setup (Carl Gable, EES-16), uncertainty quantification (David Higdon, CCS-6), and decision support (Velimir Vesselinov, EES-16).

The second thrust is the Multi-Process High Performance Computing (HPC) Simulator thrust providing a flexible and extensible computational engine to simulate coupled processes and flow scenarios relevant to legacy contaminated DOE sites. It will support a wide range of processes including hydrological, bio-geo-chemical, geo-mechanical, and thermal processes. In addition, it will treat complex source terms resulting from degradation of engineered barriers and waste forms. Los Alamos (David Moulton, T-5) is leading the design and development of this HPC simulator, with Los Alamos staff leading several key tasks. These include the design and development of the HPC Core Framework (Lori Pritchett-Sheats, CCS-2), the multi-process coordinator (Rob Lowrie, CCS-2), meshing infrastructure (Rao Garimella, T-5), spatial discretizations (Konstantin Lipnikov, T-5), geo-chemical and biological reactions (Peter Lichtner, EES-16), and nonlinear solvers (Niel Carlson, CCS-2). This strong leadership role in ASCEM for Los Alamos was made possible by the experience the team gained through research projects in the DOE ASCR Applied Mathematics program, the DOE ASCR/ERSP SciDAC program, as well as other programmatic projects under ASC.

The third thrust is Site Applications, which focuses on identifying potential EM waste sites for ASCEM to consider, developing the data sets from these sites, and making connections to new data collection and monitoring opportunities at the sites. In addition, Site Applications provides a connection to the user community through the User Steering Committee.

2.4.6 Computational Fluid Dynamic Applications on Advanced Architectures. Los Alamos has established extensive expertise in the identification and development of programming models and tools for hybrid computing architectures. Several staff members in this group have participated in tools development (aimed at making complex computing tasks and development models accessible to Laboratory domain scientists) and educational outreach. Some examples of the tools that have been developed that are in use in related research projects are: the SIMD Abstraction Layer (SAL), a vector intrinsics abstraction that allows cross-platform development of short-vector accelerated computational kernels; the PipelineManager interface, an abstract functional programming model for launching and controlling data and task-parallel processes across a variety of multicore architectures and the IBM Cell; and the Message Passing Relay (MPRelay), a communications framework that abstracts distributed-memory send/receive-style data movement to handle the hierarchical nature of modern hybrid supercomputers.

Our educational outreach program is designed to give domain scientists and applications developers the skills that they will need to meet the computing goals of the Laboratory mission. This group has sponsored introductory and advanced classes on programming models and techniques for developing on the Roadrunner supercomputing architecture, and has recently begun to offer seminars on using the Open Computing Language (OpenCL), an open standard for applications development on multicore/many-core and accelerated computing architectures.

2.5 Challenges and Issues

The challenges and issues related to this theme are common ones, related to the use of advanced computing architectures, staff retention, and so on. Such common issues are discussed in Section 8.

3.0 Theme 2: Partial Differential Equations

(Theme Leader: Dana Knoll, T Division)

The Partial Differential Equations (PDE) capability at Los Alamos is both broad and deep, and the theme has been divided into six sub-themes for the purpose of organization:

- Applied Math
- Deterministic Transport
- Solvers
- Computational Plasma Physics
- Computational Mechanics
- Meshing

We address these six sub-themes in that order. For some of these sub-themes the relevant Los Alamos community resides in one group while for others, the community is spread across divisional and directorate boundaries. This taxonomy also represents a technical crosscut through this theme of strategic importance to Los Alamos.

3.1 Connection to the Goals and Mission of the Laboratory

3.1.1 Applied Mathematics. In this subsection we focus on Los Alamos's capabilities in applied mathematics in partial differential equations and its evolution over the last ten years. Los Alamos's long history of world-class applied mathematics began in the 1940s with the Manhattan Project and its strong connection to the Courant Institute at New York University. At the present time, a strength that makes Los Alamos unique in the DOE complex is the Center for Nonlinear Studies (CNLS), an internationally recognized center of excellence in nonlinear, complex, and far-from equilibrium systems. This center acts as a gateway between Los Alamos and the academic world and is also a fertile recruiting mechanism for young scientists into the Laboratory. Applied mathematics underpins most of the DOE programs at Los Alamos and the capability is therefore spread out across divisions. Its main funding sources reach across the DOE and are principally DOE-NNSA and DOE-SC (ASCR, BER, BES, FES, HEP, NP) and Los Alamos Laboratory Directed Research and Development (LDRD).

3.1.2 Deterministic Transport. Deterministic transport methods research and the organizational thread it follows have a long history at Los Alamos. The goals of this research have remained relatively unchanged during the lifetime of the Laboratory. From its inception, this research has contributed to our mission by developing numerical methods to solve the transport equation deterministically. The capability to efficiently model the interactions of neutrons and photons is an important part of high energy density computational simulations. The complexity of the transport equation, together with the additional complexity associated with coupling neutron transport ("neutronics") and photon transport ("radiation") with multi-physics applications, means that efficient numerical solution methods must be developed. To keep pace with the growth in computational capacity and the increase in fidelity and complexity of multi-physics simulations, the need for more accurate and more efficient solution techniques for the transport equation has commensurately increased. The majority of this effort resides within CCS-2.

3.1.3 Solvers. There has been a long and successful research effort in the area of linear and nonlinear solvers research at Los Alamos. This has stemmed from the strong application potential in areas such as weapons simulation, climate simulation, environmental simulation and combustion (and others). Two of the primary equation systems driving much of the work have been deterministic transport (and diffusion), and various forms of semi-implicit and implicit CFD. Through much of the late 1990s until approximately 2006 there was a focused solvers project funded via the Los Alamos ASC program. This helped serve as a focusing collaboration for a number of methods researchers around the Laboratory. Currently growing desire for development and application of advanced solver methods in climate simulation and subsurface environmental management simulation may once again provide an all-important focusing application area for this Los Alamos community. This Los Alamos community can be found in T and CCS divisions.

3.1.4 Computational Plasma Physics. Computational plasma physics at Los Alamos has a very long history and mission support in NNSA, magnetic confinement fusion, inertial confinement fusion, other high energy density physics applications. Space plasma physics/space weather and astrophysics are also application areas with some level of support. Methodologies range.from collision-less kinetic modeling, collisional kinetic modeling, MHD/fluid models, and hybrid models. Many historic algorithm developments in computational plasma physics have roots at Los Alamos, such as implicit kinetic simulation, hybrid methods, semi-implicit and fully implicit methods for MHD, and particle methods for MHD.

Plasma theory and simulation groups and teams can be found in XCP, ISR, and T divisions. Traditional sources of programmatic funding have been DOE Office of Fusion Energy Sciences, DOE NNSA, NASA, and LDRD.

3.1.5 Computational Mechanics. As the nation's premier national security laboratory we are challenged with the responsibility of delivering to our nation solutions to problems associated with nuclear and conventional weapons systems and their effects. With current policy on maintaining a safe and reliable nuclear deterrent, we are faced with greater reliance on computational based certification and prediction of performance. This demands that we engage in these problems world-class researchers and deploy our nations best computational tools to enable numerically reliable prediction of highly complex material deformation histories. This includes not only advanced physics models but also advanced and robust computational tools and algorithms. Without the close and balanced coupling between these elements we will not be successful in achieving predictability for weapons performance. At present the work that is ongoing in solids computational mechanics occurs largely in T-3, T-1, XCP-5, XCP-4, CCS-2, and MST-8.

3.1.6 Meshing. Mesh generation is the subdivision of a geometric domain into many subdomains (elements, cells) of simpler geometry and topology. Mesh adaptation is the manipulation of meshes by point relocation or element subdivision to control element quality and size as desired. Mesh generation is a vital aspect of numerical solution methods for PDEs that require that the computational domain to be discretized adequately so that simplifying assumptions about the computational variables are valid over each element. Thus mesh generation pervades the entire range of applications critical to Los Alamos's mission from high-speed shock physics, to metal casting, to subsurface flow. High quality automatic mesh generation and adaptation tools are essential to the effectiveness of any analyst in efficiently conducting large scale computational simulations and even with the availability of such tools, analyses can spend as much as a third of their time in meshing and mesh adaptation of complex domains.

The focus of a majority of Los Alamos's simulations is in capturing complex multi-physics phenomena accurately rather than capturing complex features of the geometrical domain. Consequently, much of the meshing effort in Los Alamos concentrates on: a) generating carefully controlled meshes that accurately capture the physics and avoid spurious effects and b) adapting the meshes dynamically to solution features. Most of the meshing tools at Los Alamos are highly specialized tools tailored to the specific application. Typically, no off-the-shelf application exists to perform this task. This Los Alamos community can be found in T, EES and XCP divisions.

3.2 Research Breadth and Impact

3.2.1 Applied Mathematics. Rather than describe the complex organization across Los Alamos (and its even more complex relationship to DOE), we convey the unique capabilities and future directions through three sub-areas: 1) the example of applied mathematics in climate modeling, 2) the CNLS, and 3) the Los Alamos ASCR applied math program.

Applied Mathematics in Climate Modeling

POP-a: from theorem to ocean model simulation. This refers to the LANS-alpha model, which was discussed in some detail in Section 2.2.1. This is a major advance for the DOE thrust in climate modeling. Through this model, dynamical results are seen equivalent to a doubling of resolution (without actually doubling the resolution). This achievement means that at the coarse resolutions required for IPCC run scenarios, the Los Alamos ocean model can provide the most realistic circulation – crucial for understanding phenomenon like the shut down of the meridional overturning circulation and its relation to the onset of ice ages. No other ocean modeling team in the world has a model of this sophistication. This remarkable achievement was recently called out in the 2008 BER review of the COSIM project. This project was a long-term, low level-of-effort success supported by DOE-ASCR in fundamental development of PDEs, Los Alamos-LDRD in the development of the method to fundamental applications, and DOE-BER for the development of numerical methods for the alpha model into POP. It began as an effort supported by long-term research in ASCR and fostered by collaborations in the CNLS that created a new model of water waves [Camassa-Holm 1993], a paper that now has over 1000 citations. A Los Alamos LDRD-DR and several related LDRD-ERs expanded the work and had active participation through the CNLS by the international mathematics community. It appeared in the fundamental applied mathematics literature as theorems in [HMR 1998]. In 2000, the climate community started looking at key results related to fundamental ocean modeling [Holm and Nadiga, 2003; Wingate, 2004; Holm and Wingate, 2005]. Finally, in 2007, the first results of the full ocean model appeared in [HHPWa 2008, PHW 2008, HHPWb 2008 and HHMPW 2009]. The next two years will see investigations of POP-a in regional, global, and coupled configurations along with the incorporation of methods in statistical parameter estimation.

Multiscale-in-time: advancing beyond the hydrostatic approximation. As a consequence of the ASCR multiscale thrust a new applied mathematical result derives new slow equations that are non-hydrostatic [WHET 2010]. The new equations generalize the well-known Taylor-Proudman theorem to nonhydrostatic flows and predict columnar dynamics in the Arctic Ocean. Strong columnar vortices have been observed by [Woodgate 2001] and more recently by [Timmermans 2010]. These vortices can be as much as 4000 m deep and bring with them enormous kinetic energy making the abyssal Arctic Ocean more dynamically active than any other ocean in the world. This result is also having impacts on more fundamental mathematical results such as estimates of existence and uniqueness of the Boussinesq Equations. More importantly for DOE programs this result produces projection operators that take any vector and project it onto the null space of the fast operator. The consequence of this is a new generation of *asymptotically preserving* numerical methods that could efficiently lead the way past the hydrostatic balance that may not be accurate for the next generation of IPCC class ocean models. The numerical algorithm development will be supported by DOE-BER.

The Center for Nonlinear Studies (CNLS)
CNLS has had an exceptional history of contributions in nonlinear science with excellent postdoctoral fellows, many of whom have stayed as Laboratory staff, a varied and stimulating series of conferences and workshops, and interactions with top external academic, industrial, and national laboratory institutions. The Los Alamos Applied Math environment requires a multidisciplinary approach that is hard to find in new postdocs. We have been very successful in using extensive summer schools aimed at advanced graduate students to build a pipeline of young applied mathematicians interested in this approach to problems solving. For example, since 1995 more than 400 students went through the summer programs designed to create a path for the next generation of computational applied mathematicians to support the DOE mission through science-based simulations. These summer projects often became a seminal component in their PhD research. At the postdoc level, CNLS has played a key role in providing the right multi-disciplinary postdoc environment combined with access to a variety of computing platforms and compares well with some of the best postdoc programs in the nation. CNLS is funded by several overlapping LDRD grants. Each postdoc is supported at the 50% funding level in conjunction with a host from one of many groups around the Laboratory. This ensures that CNLS becomes involved in some programmatic effort right from the start. Historically, CNLS has been instrumental in providing high impact research in nonlinear analysis and PDEs, with applications in a wide variety of fields. This international impact can be measured by publications and by the large number of CNLS alumni playing important roles in Applied Math at Los Alamos, other laboratories, and academia.

The CNLS Annual Conference has often led to significant new developments in applied math. These multidisciplinary workshops have attracted as many as 300 international attendees and nucleated significant new collaborations and developments at Los Alamos and beyond. A powerful example is the 2003 CNLS Annual Networks conference. It led to several research efforts in various aspects of network science, nucleating several teams and led to the recruitment of many outstanding postdocs in this field. The origin of many important currently active research programs can be traced back to this conference, including: the analysis of multiscale, temporal networks with applications in cybersecurity, algorithm development and analysis of optimal design problems relevant to infrastructural grids, network methods and algorithms underlying several biological physics projects, networks applied to the interdiction of an adversary's activity, stochastic analysis applied to measures of robustness, and stability of sensor networks. The tools and algorithms in these projects are a blend of continuum and discrete approaches and provide important new connections between applied math, computer science, optimization, and also statistical physics and biology. In addition, the scale-free nature of the underlying networks provide exceptional challenges on new architectures. This is a great example of nucleating a new field before there was sufficient programmatic support and where scientific vision and strong strategic hires have led to exceptional multidisciplinary teams of applied and computational mathematicians. These network projects are funded from several sources, including SC, DTRA, DHS, NIH, and LDRD.

The Los Alamos ASCR Applied Mathematics Program
Office of Science funding in this field is traditionally provided by ASCR. Los Alamos has a long history of ASCR funded projects, originally mostly in PDEs and their numerical analysis. The total FY10 Los Alamos ASCR portfolio amounts to $5.2M (out of a Los Alamos total SC FY10 budget of $88.4M) and is divided into Applied Math ($2.4M), Computational Science ($1.2M), and Computer Science ($1.4M). Even in the computer science category, many projects have strong applied and computational mathematics components. In addition, there are many proposals (pending review) that involve a strong intersection between applied/computational mathematics and the goal of computing at the exascale. In this sense, the ASCR 2008 report on "*Applied Mathematics at the U.S. Department of Energy: Past, present and a view to the future*" [Brown et al., 2008] has had a strong influence on current research priorities at Los Alamos and also represents well some of the newer directions. The ASCR Applied Math program funds research in Mimetic Finite Difference Methods for PDEs, Predictability of Stochastic PDEs, Theory of Nonlinear Evolution Equations, Monte Carlo Methods for Problems with Large Deviations, and New Optimization Methods for Complex, Stochastic Networks. It also provides some additional funding for postdocs working in this area. Here we briefly highlight the first two of these projects, as they illustrate how fundamental research in applied and computational math can have significant impact on NNSA and DOE mission needs.

The *Mimetic Finite Difference Methods for PDEs* project provides a powerful example of how SC ASCR investment in numerical analysis research led to new algorithms or proven convergence and error estimates of existing codes and algorithms. This was then leveraged as several key contributions to the ASC program and world leadership for Los Alamos in (for example) multi-material ALE methods. (Refer to the Shashkov presentation on ALE methods and the Lipnikov poster presentation during the review). This project developed methods that mimic important properties of the underlying geometrical, mathematical and physical models. These can include: geometry (e.g. complicated dynamic material interfaces [Garimella-Lipnikov 2010, Ahn-Shashkov 2009, Dyadechko-Shashkov 2008]), conservation laws (e.g. in modeling flows with strong shocks [Shashkov 2007, Garimella-Lipnikov 2010, LMS-2008, LMS-2009, Lipnikov-Shashkov 2010]), symmetry preservation (as required in ICF [Lipnikov-Shashkov 2010]), positivity and monotonicity (e.g. of the density, pressure and concentration [Liska-Shashkov 2008, KSS-2009, LSV-2009, SVL-2010]), and the duality of important operators (as required by particular solvers. [BLSS-2007, LSY-2009, BBL-2009, BdVK-2010]). The successful development of a rigorous theoretical discrete calculus aimed at dealing with multi-scale, multi-physics problems on general polyhedral meshes, provided new algorithms and proofs of the convergence of some of the most advanced methods required for multi-material ALE techniques. It allowed provided order of magnitude improvement in the robustness and accuracy of codes required in the multi-physics, multi-scale simulations underlying stock-pile stewardship [Lipnikov-Shashkov 2006, BLSS-2007, Dyadechko-Shashkov 2008, Garimella-Lipnikov 2010]. At Los Alamos, these methods are playing an important role in complex, integrated hydro, radiation-hydro, and transport codes for application to Stockpile Stewardship, design and analysis of experiments, general purpose hydro and radiation-hydro problems, and analyzing radiation and particle transport problems for a variety of applications. In addition, codes based on these algorithms are utilized to simulate other dynamic events, including high-explosive, laser, and pulsed-power driven systems, sub-critical and AGEX experiments, inertial confinement fusion (ICF), and the response of energetic materials to thermal and mechanical insults. This project established very strong collaborations between T, CCS and XCP divisions, between Los Alamos and other national labs, as well as strong ties with academia in the US and Europe. It has attracted outstanding postdocs, some who were converted to staff. Outside Los Alamos, these mimetic methods in combination with results from the Los Alamos ASCR project on *Predictability with Stochastic PDEs (*PI David Moulton*)* are also having an important impact on our growing Energy Security portfolio. The above methods—combined together with new approaches to uncertainty quantification [VBCHR-2008, VBH-2009] and data assimilation [WT-2008]—will provide advanced algorithms for the simulation of groundwater and contaminant transport in porous media (modeled by hierarchical multilevel techniques [LMS-2008, LMS-2009]), as part of the new multi-lab, multi-million dollar ASCEM (Advanced Subsurface Capability for Environmental Management) project. This project will deliver the tools required to study the impact of massive future investments to manage groundwater resources and cleanup at all DOE facilities.

3.2.2 Deterministic Transport. The research necessary to provide the required capability has evolved through the years to keep pace with evolving needs that arise from changing Laboratory mission activities or out of scientific and technological concerns. It may be categorized into research areas as follows.

- *Parallel and Heterogeneous Computing Architectures*: parallel platforms have led to the development of new algorithms and techniques that can solve the integro-differential form of the transport equations. New insights and understanding of the problem have borrowed ideas from other areas of mathematics, including graph theory and linear algebra. New avenues of research have been created based on new or previously discarded algorithms that take advantage of new computer architectures.
- *Multi-physics Applications*: coupling with high energy density applications has led to new discretization methods, in both two and three spatial dimensions. The quest for greater fidelity in simulations introduces additional terms in the transport equation that increase complexity and thereby create an impetus to find more efficient solution methods. Research into finding the best algorithms, in terms of accuracy and efficiency, for solving the fully-coupled, non-linear overall system of equations is ongoing.
- *Theoretical Analysis*: techniques developed for numerical solutions need to have characteristics that make them suitable for use in the particular application areas. Such concerns require that theoretical analysis be conducted to determine the numerical properties of the discretization and algorithms employed. This can create new lines of research, leading to the modification of existing methods or to the development of new methods.

Recent research activities in these general areas have led to the following specific developments.

- Iterative solution methods tailored to implementation on the Roadrunner architecture [Rosa 2009].
- Parallel angular sweeps implemented on the Roadrunner architecture [Rosa 2010].
- Moving-material corrections for neutronics.
- Two-dimensional spatial discretization on unstructured polygon meshes [Warsa 2008].
- Efficient iterative solution methods for radiation [Morel 2007].
- Theoretical analysis for the numerical verification of SN transport discretizations in the thick-diffusion limit [Warsa 2010].

- Nonlinear algorithms for ensuring positivity of solutions [Fichtl 2010].Emphasizing the viewpoint that eigenvalue problems are essentially nonlinear, leading to new non-linear criticality and alpha eigenvalue solution techniques [Gill 2010].

3.2.3 Solvers. Over the history of solvers methods research at Los Alamos and number of diverse sub topical areas have been investigated. Multigrid methods have always had a strong focus at Los Alamos and over the years this direction of research has had a number of positive programmatic impacts. Here the noted software packages have been BoxMG [Dendy 1982,2010] and LAMG [Joubert 2006]. Another area of effective research has been in the development of advanced preconditioning strategies for Krylov and Newton-Krylov methods. For some period of time there was a focused effort on application of Jacobain-Free Newton-Krylov methods and the development of advanced preconditioners [Knoll 2004]. The primary goal of this effort was to provide more accurate options to multiphysics time integration as compared to standard operator splitting. This effort impacted computational plasma physics, atmospheric modeling, environmental modeling, mesh generation and some high energy density simulation efforts. There is currently a growing effort to utilize (and further develop) this technology within the computational mechanics and climate simulation communities at Los Alamos.

3.2.4 Computational Plasma Physics. VPIC [Bowers 2008a and 2008a] is an explicit kinetic plasma modeling capability. Ties to Los Alamos missions include ICF hohlraum energetics (presently the world's premier platform for modeling laser-plasma interaction in ICF hohlraums), ultraintense short-pulse laser-matter interaction, space, astrophysics, magnetic reconnection, magnetic fusion, thermonuclear burn modeling, radiography, and DARHT. Present research directions include r-z capability (presently only Cartesian); inclusion of radiation back-reaction for accurate particle orbits when laser intensity Iλ2>1022 (W/cm2)μm2; hybrid capability (fluid electrons, particle ions); electrostatic variant; more extensive use of heterogeneous computing hierarchy for soft/hard reboots and computationally extensive post-processing; Fermi GPU programming (Jaguar + upgrade); and acceleration over ignorable time/space scales (ala QuickPIC).

DREAM (Dynamic Radiation Environment Assimilation Model) is a growing ISR-based project that presently is a 1-D radial diffusion code that models the long-time evolution of the Earth's radiation belts due to natural changes in the magnetosphere caused by variations in the solar wind. This project is extending the present capability to 3-D and to include the injection of large fluxes of relativistic electrons from a high altitude nuclear explosion in space. This project significantly enhances the Laboratory's mission to analyze, access and mitigate threats to national security (and particularly space-based assets) from weapons of mass destruction.

Dense plasma modeling has also been an active area of research at Los Alamos. The ASC/PEM project (carried out jointly by T-5 and XCP-6 plasma physicists) supports the development and application of a specialized molecular dynamics code to model the transport in dense plasma that has both short-range screening and long range Coulomb interactions. The algorithm of choice is Hockney's Particle-Particle Particle-Mesh (PPPM) method, which calculates pair potential for short-range interaction but a Poission equation for the electrostatic potential in long range Coulomb interactions. An outstanding accomplishment from this tool is the resolution of the electron-ion temperature relaxation in dense plasma, which compares favorably with parallel effort nationally and internationally.

The Office of Fusion Energy Sciences supports a computational fusion plasma capability in the Plasma Physics Team of T Division's Applied Mathematics and Plasma Physics Group. The key capabilities are in four areas: 1) equilibrium and stability calculation of magnetically confined plasmas in toroidal (e.g. spherical tokamak, field reversed configuration, and spheromak) and linear (e.g. mirror) devices; 2) extended magnetohydrodynamics (MHD) modeling of toroidal plasmas; 3) neoclassical and gyrokinetic transport calculation using particle-in-cell methods; and 4) electrostatic kinetic simulation of nonneutral and quasineutral plasmas for plasma-materials interaction. These capabilities support the DOE's and Los Alamos's mission in energy security.

3.2.5 Computational Mechanics. Understanding material behavior under a given strain and strain rate, (i.e. constitutive relations or material model) is an important first step toward a simulation of material interactions. To successfully simulate material interactions, such as the interaction of an air shock with a porous material made of a linear elastic solid, requires a framework of model equations that can track the motions of the air and the solid material simultaneously. This material interaction is beyond traditional composite material theory, because this interaction cannot be described by a mean deformation field. One needs to track motions of both materials, air and solid, using two velocity fields. This is similar to modern two-phase flow theory, except most of two-phase flow theories are developed for disperse two-phases, where the solid phase is in a form of particles with a small characteristic length scale compared to the domain of the problem. To address this technology gap, a multi-material interaction theory was recently developed in T-3 [Zhang 2007].

The system of the model equations from the theory needs to be solved by an appropriate numerical method, especially in the cases of large deformation and breakup of the solid material. Currently available numerical methods are inadequate. The mesh based Lagrangian methods often encounter difficulties of mesh distortion and tangling; while particle based Lagrangian methods encounter difficulties related to accuracy of numerical differentiation. Eulerian based methods suffer numerical diffusion issues when advecting solid quantities. Many efforts have been devoted to improve Eulerian methods. Examples are volume of fluid, level set, and immersed boundary methods. These methods track material interfaces, but not the deformation in the interior of the solid material. Furthermore, there are cases such as the porous solid example where the length scale of the interfaces are below the grid resolution. To be able to solve this type of problem, we combine the multi-material interaction theory with the material point method. This method combines the advantage of Lagrangian and Eulerian methods while avoiding difficulties of both. This method has been built into a numerical code, CartaBlanca [Zhang 2008]. Recently, T-3 has also overcome several significant obstacles in the application of the method. The numerical code has been applied to simulate difficult problems essential to missions of the Laboratory such as safety of high explosive material, projectile-target interactions, and consequence of nuclear blast in an urban environment. This method and CartaBlanca code have also been applied to many problems to help our industrial partners.

3.2.6 Meshing. A large area of meshing research at Los Alamos is the adaptation of meshes in Arbitrary-Lagrangian-Eulerian (ALE) simulations of fluid flows. In pure Lagrangian methods, the mesh deforms according to material motion while in Eulerian methods the material moves through a fixed mesh. While Lagrangian methods track material interfaces and shocks accurately they suffer from the disadvantage that meshes can get tangled in the presence of large vorticity. ALE methods overcome this disadvantage by allowing the mesh points to be moved independent of the material motion in order to maintain the quality of the mesh.

The T-5 plasma physics team is also developing a method of mesh generation and adaptation based on Monge-Kantorovich optimization (MKO) [Finn 2008]. The MKO method for mesh adaptation is based on error equidistribution, minimizing the L_2 grid displacement from a previous grid. It has been shown it is closely related to minimization of mesh distortion. For this reason, grids generated by MKO are much less likely to fold than other grids while following solution features accurately.

A collaboration team from T and XCP divisions has developed a novel algorithm within the FLAG code to conformally subdivide a 3D unstructured polyhedral mesh along discontinuous reconstructed material interfaces. This subdivided mesh with pure material subcells is then used to compute solutions to the grey radiation equations with much higher accuracy than using averaged properties in the undivided multimaterial cells. This effort is more mature than a similar effort ongoing at AWE and has been published [Garimella 2008]. Future work involves making the procedure robust enough for production use. The main meshing challenge for the ASC setup team in the future will be the automated generation of general 3-D dendtritic meshes.

3.3 Comparison with Peers

3.3.1 Applied Mathematics. Our peer group is other national laboratories such as LLNL and SNL; each has strengths and weaknesses. Los Alamos's key strengths are as follows.

- A rich multidisciplinary environment, where applied math is immersed in a strong physics, materials science, chemistry, and computing community that, when combined, is larger than at any other laboratory. This multidisciplinary environment (CNLS is a good example) provides an incubator for new methods in applied mathematics. For example, in problems involving stochastic dynamics, fluctuations, and rare events, there is a very powerful local theoretical and computational expertise. When this is combined with new numerical approaches it can result in high impact research in several fields.
- Applied mathematics in climate modeling (POP-a), along with international collaborators.
- Mimetic differencing techniques and ALE algorithms.
- Applied mathematics for networks.

3.3.2 Deterministic Transport. The transport methods group (part of CCS-2) enjoys a global reputation for its quality research. The transport equation has a variety of application areas, including astrophysics, nuclear reactors, and radiation shielding. As a result, the deterministic (and Monte Carlo) method development published as a result of research areas that impact the Laboratory mission and capability has a far-reaching influence on the scientific community. Faculty visit on a frequent basis to conduct technical collaborations. Students regularly seek temporary and permanent positions within the transport group. One of the group's distinguishing characteristics is that research takes place hand-in-hand with code development and implementation, which means cutting-edge capabilities can be almost immediately leveraged for use in application simulations.

3.3.3 Solvers. As compared to peers at other DOE laboratories we have had varied relative impact. Los Alamos has not produced widely used solver software libraries such as PETSc, Trilinos, or Hypre. However, both BoxMG and LAMG are available under open-source libraries. In many applications here, non-Los Alamos packages provide the foundational solver needs in the particular Los Alamos simulation tool. However, in many applications, the generic preconditioners that reside within these standard packages are not optimal for any specific application. Here, Los Alamos solvers experts have been able to work with application users to develop unique preconditioners (often with significant physics insight) that provide significant performance improvements. Additionally, a number of Los Alamos solver concepts have found their way into other solver software libraries such as PETSc from ANL and Trilinos from SNL. These efforts have provided impact to the ASCI program and various Office of Science programs in fusion, climate, and environmental modeling. Los Alamos has had a leadership role in the application of modern nonlinear solvers to many multiphysics systems and in the development of physics-based preconditioners for such applications.

3.3.4 Computational Plasma Physics. In recent years, Los Alamos has defined how to map explicit, electromagnetic, plasma PIC codes to advanced parallel computing architectures. This is a definition that many others are now following. In a similar fashion, Los Alamos has defined how to apply Newton-Krylov solver technology to a number of important computational plasma physics problems.

3.3.5 Computational Mechanics. Activity at SNL and LLNL has been ongoing for many years. SNL is actively developing its Sierra framework collection of physics codes to address coupled physics problems. LLNL is developing its ALE3D code for use in complex weapons simulation problems. Increasingly these tools are being engaged in the DoD community for the simulation of conventional weapons problems.

3.3.6 Meshing. The research and development of meshing technologies at Los Alamos compares well with LLNL and SNL, although Los Alamos has not been as coordinated in developing well recognizable software packages for meshing. Our efforts are closest to those of LLNL due to the emphasis of both laboratories on capturing complex physics in high-speed shock simulations. LLNL's PMesh has capabilities that are somewhat similar to the capabilities of the Setup team at Los Alamos. Also, the ITAPS for developing mesh APIs is loosely related to the development of the MSTK mesh infrastructure (see section 3.1.6) at Los Alamos. LLNL does have a significantly more advanced effort in Structured Adaptive Mesh Refinement through a package called SAMRAI that is widely used. At SNL, the main meshing package is CUBIT, which is mainly focused on unstructured meshes for engineering type parts and not able to generate the kinds of meshes required by Los Alamos or LLNL (i.e. parallel meshes with some structure and symmetry, along with hanging nodes to reduce mesh density in narrow regions). The Sierra ToolKit is a similar effort as MSTK to develop mesh infrastructure to applications solving PDEs. Comparable work to Los Alamos has been done at SNL on the subject of mesh quality improvement and mesh untangling by node motion.

3.4 Status of the Capabilities

3.4.1 Applied Mathematics. Because the capability is spread throughout Los Alamos it is difficult to assess overall strength. The development of entirely new areas of applied mathematics, such as the new network capabilities, suggests overall health. However, two key issues discussed in more detail below prevail: first, loss of key applied math staff that participated strongly in CNLS, and second, not only do we need to replace those staff, but we also need to consider that new demands faced by DOE and our nation may require a new generation of applied mathematicians who are very different from what worked in the 80s and 90s. Our future depends on how we address those issues.

3.4.2 Deterministic Transport. The deterministic transport methods team currently supports two major code development projectxs PARTISN and Capsaicin, that are used in several application areas that support the laboratory mission for multiphysics simulations. A unique aspect of our code development effort is that research into new methods and algorithms largely takes place within the code projects. Therefore, any promising new techniques can be rapidly made available to the simulations. Ultimately, the capabilities of the two projects will be merged to provide a unified interface for neutral particle transport and radiative transfer calculations. PARTISN is the "neutronics" code that models the interactions of neutrons with materials. It has been undergoing development here for the last 40 years in an ongoing effort to extend capability, methods and algorithms to meet changing requirements that arise through continuing evolution of computer capacity and technical concerns involving multiphysics simulations. The code works on structured meshes with parallel decomposition in all phase space variables. Capsaicin is the "radiative transfer" that has been developed using modern software quality assurance and design principles during the past six years. The code framework includes the latest and most advanced solution methods and algorithms that have been primarily developed by CCS-2 during the past ten years. The code works on fully unstructured meshes with arbitrary topology, with spatial parallel decomposition. Much of the research that has been published on transport methods and algorithms has been tested and analyzed through implementation in Capsaicin, primarily to provide capability for parallel-decomposed unstructured mesh calculations. Neutronics capability through the NDI data package, unstructured 3D tetrahedral mesh capability, and JFNK eigenvalue calculations, in addition to the radiative transfer capability already in place for 1D and 2D meshes, are among the recent capabilities being implemented.

3.4.3 Solvers. A core of a solvers community still exists here, but due to ASC program priorities that community now resides within a variety of application codes as opposed to a unified, standalone effort.

3.4.4 Computational Plasma Physics. Algorithmically VPIC is an explicit particle-in-cell, electromagnetic, charge conserving code. It employs a 5th order Boris push, FDTD field solve, support for unary and binary collisions, nuclear and chemical reactions. VPIC uses a Trotter factorization, so possesses excellent numerical stability, accuracy. Single- and double-precision variants exist (but single-precision is most used). Native support for short-vector SIMD, including SSE, Altivec, and IBM Cell exists along with data alignment. Additionally, VPIC is accelerated for IBM PowerXCell8i processor (Roadrunner). The major DREAM capability is a numerical solution of a 3-D diffusion equation. The three dimensions are not physical space or velocity space, but instead are three canonical variables that involve very disparate spatial and temporal scales. The diffusion coefficients have widely differing magnitudes and the off-diagonal terms can be much larger than several of the diagonal terms, making the 3-D version of the code much more complicated than the 1-D version. In addition, the diffusion coefficients can vary widely in space and time and must be converted to canonical variable space. The diffusion coefficients are inferred from satellite data; data assimilation techniques must be employed to interpolate/extrapolate from a limited number of spatial positions (that are changing in time as the satellites orbit the Earth). The Los Alamos magnetic fusion energy effort uses Newton-Krylov method extensively as the core solver technology for both the nonlinear equilibrium solver and the initial value extended

MHD simulation. This is often combined with sophisticated spatial discretization such as spectral element and aggressive physics-based preconditioning. Our stability codes typically employs ARPACK as the underlying eigensolver and also, when applicable, innovative non-eigenvalue-based methods. The neoclassical and gyro-kinetic simulation capability, which is based on delta-f particle-in-cell methods, is a joint development with PPPL. Our emphasis has been on the algorithmic formulation and implementation of the collision operator, in addition to geometric flexibility such as allowing stochastic magnetic field lines. The adaptive-grid electrostatic simulation of kinetic equation is a more recent development at Los Alamos. It brings the power of a time-dependent grid adaptation strategy based n Monge-Kantorivich control to particle-in-cell simulation, which ensures high fidelity while retain full geometric flexibility.

3.4.5 Computational Mechanics. Los Alamos uses both EPIC (legacy code) and ABAQUS (commercial) for these same problems in computational mechanics. There has been some support for the development of new material point method (MPM)-base capability. More support will be required to mature this young capability.

3.4.6 Meshing. For the past few years the focus of the ASC setup team has been the efficient and automated generation of 2-D dendritic boundary-conforming meshes for high-speed shock physics simulations in Los Alamos codes FLAG and RAGE. These meshes are non-conforming (contain hanging nodes/terminating lines), have highly anisotropic geometry, and may contain multiple related meshes separated by slide lines. The team has also developed a 3-D CSG (Constructive Solid Geometry) modeler with massively parallel 3-D CSG model query, and automated input deck/problem specification. For the last 10+ years, T-5 at Los Alamos has been developing methods for optimizing the quality of unstructured 2D and 3D meshes in multi-material domains. This technology is being deployed in our production codes and being enhanced to optimize distributed grids during the course of ALE simulations [Vachal 2004]. Meshing for geological applications is another important area of research here and serves varied customers such as physics modelers of subsurface flow and transport (hydrology, waste repositories, C02, oil and gas, geothermal), shock physics (containment, hardened targets) and short-term tectonics (earthquake rupture, post-seismic deformation). Each application area has different requirements and data input types (geologic framework models) and EES-6 has developed a suite of tools and algorithms called LAGRIT (http://lagrit.lanl.gov) to meet some of those needs. For example, they have developed methods to mesh non-manifold geometries (fault surfaces embedded within a mesh) and methods for stratigraphy conforming Voronoi control volumes in 3D (hydrology, CO2 sequestration) and geometry adaptive mesh refinement methods using octree-based refinement. LAGRIT is a freely available to the geophysics community and offers a powerful alternative to purchasing multiple, expensive geological meshing software products. A meshing infrastructure, MSTK, [Garimella 2004] has been developed for simplifying the task of developing more advanced mesh based algorithms such as mesh generators, mesh optimizers and numerical solvers for PDEs (http://math.lanl.gov/~rao/Meshing-Projects/MSTK). MSTK allows application developers to store, query and manipulate multiple unstructured meshes in an object-oriented way without getting bogged down in details of mesh data structures. MSTK's interface to unstructured meshes is similar to that of SciDac's ITAPS (Interoperable Technologies for Advanced Petascale Simulations) effort and is among a handful of unstructured mesh frameworks available under an open-source license. Current efforts are focused on handling parallel, distributed meshes so that much larger simulations can be performed.

3.5 Challenges and Issues

Many issues in this theme are common to all themes in the CPAM capabilities and as a result appear in Section 8.0. Some specific challenges and issues for the PDE theme follow.

3.5.1 Applied Mathematics. Over the last decade, we have lost some of our most important applied mathematicians. The 2009 CNLS External Advisory Committee, comprised of internationally recognized scientists from academia, report prominently noted:

> "...Among the internal challenges noted ..., perhaps the most significant is the apparent diminution of the historically important role of the applied mathematicians—both individually and through the former T-7 group—in the recent work of the Center. Although this diminution may in part be comparative, given the increasing participation of biologists and physicists, the EAC noted a large number of individuals who have in prior years been strongly associated with the CNLS, who have either left Los Alamos or have become less involved in the Center. Among these are Mac Hyman, Darryl Holm, Charlie Doering, Pieter Swart, Aric Hageberg, Roberto Camassa, and Ildar Gabitov. Of course, since the CNLS does not have any permanent scientific staff positions (apart from the Director and Deputy Director), it cannot by itself guarantee the presence of applied mathematicians at the Lab. What the CNLS can do within its resources and structure is to seek out postdocs who may be paired with existing permanent staff to bring new applied mathematical techniques to the Lab. Specific examples might include a postdoc in stochastic equations (a hot area now in mathematics) or a postdoc in computer science, either of whom could be paired with one of the statistical physicists at the Lab. The EAC's concern is that, without sufficient nurturing, the role that the CNLS has played in bringing advances in the mathematical science to Los Alamos may diminish over time."

The concern was for CNLS but is true also for the Laboratory. One question we face is how to recruit the kind of applied mathematicians that are able to reach into academia and into the laboratories programs at the same time. DOE SC and NNSA are advancing the idea of achieving the exascale in computing. To meet this challenge applied mathematics will have to evolve into a much more collaborative process. Rather than the classical analysis of partial differential equations or numerical algorithms it will have to incorporate fundamental ideas from uncertainty quantification and the analysis of large data sets [Brown et al. 2008]. Mathematics will become more important and be part of the whole solution process. There are exciting new challenges and opportunities in applied math that require a closer connection between applied math and computer science than in the past. A good example is provided by the many new projects that Los Alamos applied mathematicians are attacking in the national security arena. We have projects at the intersection of network science with: 1) cyber security, 2) smartgrid dynamics, 3) cell-signaling, 4) interdiction of smuggling, and 5) detection of anomalous behavior and rare events via sampling. These projects demand new approaches that encourage combined backgrounds in both CS and applied math. Its success will rely on finding talented young people with an unusually broad background (including, for example, interest in optimization, discrete math, and large-scale computing on new architectures, to name but a few.) Our past efforts at helping such postdocs succeed by immersing them in an environment such as CNLS have not been overly successful, largely because a new computer science PhD has different goals, language and metrics for success compared to a postdoc in statistical physics, for example. It is not clear that a PhD is even required in many cases. The challenge is to design a program and environment that can attract young computational scientists who can effectively bridge between applied mathematics, computer science, and future exascale efforts.

3.5.2 Deterministic Transport. Current capabilities must continue to evolve with changing requirements and new computational platforms or paradigms. The importance of the connection between basic research and applications is clear and cannot be overstated. But capabilities need to be developed and expanded whenever new insight is realized. Because of the unique way in which research and implementation are connected, the viability of new methods can be determined quickly so there is little risk on the overall mission objective. Therefore, it is essential that funding for the basic research not always be tightly linked to applications. An open approach will provide freedom of research.

3.5.3 Solvers. There continues to be many challenges to a healthy solvers community here including fractured efforts and lack of support for direct research from large programs outside of specific programmatic application domains. Future direction will most likely focus on multiphysics applications, multiscale applications [Lipnikov 2008], and performance on advanced architectures (see Section 8.1).

3.5.4 Computational Plasma Physics. While the DREAM physical problem is somewhat straightforward, the numerical challenges are daunting. Algorithm development includes efficiency in three major areas: 1) solution of a very complicated and coupled three-dimensional diffusion equation in time, 2) canonical transformation between space-time variables (from satellite data) and canonical variables (needed for the diffusion coefficients in the diffusion equation), and 3) application of data-assimilation techniques to interpolate/extrapolate measurements of electromagnetic wave spectra from a few widely spaced satellites.

3.5.5 Computational Mechanics. We presently lack a single tool to successfully tackle nuclear and conventional weapons problems. As a result, new developments must address multiple codes. We need to develop a computational framework for solids problems that can be used for both nuclear and conventional weapons work, and dynamic material behavior research.

4.0 Theme 3: Monte Carlo

(Theme Leader: Francis J. Alexander, IS&T Center Leader)

The Monte Carlo (MC) method was invented here in the post-World War II era by Ulam and von Neumann to treat numerically the complexity associated with transport of radiation through fissile material. It was the numerical basis for the first large scale scientific computation performed on the world's first electronic computer. It was also the only method at the time capable of the task. In the 1950ss, Metropolis et al. invented the most widely used Monte Carlo method, the Metropolis algorithm (the original paper has over 12,000 citations), to study equations of states motivated by weapons research. The new algorithm was the only method at the time capable of the task. In between, Fermi, as a Laboratory consultant, offered that the Ulam-von-Neumann Monte Carlo Monte Carlo strategy could solve Schrödinger"s equation. It took the dawning of the age of supercomputer to realize Fermi's vision. These beginnings set the foundation not only for the legacy still benefiting important portions of today's research here, but also for today's world-wide use of the Monte Carlo method for classical and quantum problems.

The enduring power of the Monte Carlo method is its unique ability to "break the curse of dimensionality." Many deterministic methods scale exponentially with the complexity of the problem. Most Monte Carlo methods scale linearly. As the complexity of the mathematical, scientific, and engineering problems at the Laboratory keep increasing, Monte Carlo methods will remain the only simulation method capable of many tasks. Encouragingly, the still increasing power of computers keeps beckoning for more and more complex problems. Monte Carlo will thus remain in the Laboratory's future because it can do what other methods will be unable to do. Integrating Monte Carlo and exascale computing is likely to unveil a new dimension to this fundamentally powerful numerical method. The use and development of MC methods are ubiquitous at Los Alamos. In addition to the efforts described in detail that follows, MC is also being used and developed for modeling complex networks, social systems, classical kinetic theory, performance analysis, optimal estimation and more. This self-assessment will describe the larger efforts in the following eight areas.

- MC for Transport
- Kinetic MC
- Condensed Matter Physics and Materials Science
- Statistics
- Optimization
- MC for BioSecurity
- Phylogenetics
- QCD

4.1 Connection to the Goals and Mission of the Laboratory

4.1.1 MC for Transport. Modern Monte Carlo for radiation transport has its roots in the Manhattan Project at Los Alamos with renowned scientists such as Fermi, Ulam, von Neumann, and Metropolis. Monte Carlo research, methods development, and applications on the world's fastest and biggest computers and for the nation's most urgent needs remain a forte of Los Alamos, particularly in the mission areas of nuclear deterrence, global threats, and energy security.

For example, Los Alamos uses MCNP to design critical and subcritical assemblies using large quantities of special nuclear materials (bare and moderated/reflected). Some of the subcritical assemblies were built to support R&D associated with new detector designs and data analysis techniques with applications associated with nuclear material safeguards, homeland security, and nuclear emergency response. Some of the critical experiments were used to benchmark the computational ability of MCNP and the cross section sets used with MCNP to predict the critical masses of actinides where insufficient quantities of the materials exist to build a full critical experiment. Recent critical experiments of interest include the Neptunium critical mass experiment, one of the benchmark critical experiments performed on the Comet assembly machine, and the Planet HEU foil experiments. Recent subcritical experiments of interest include the BERP ball reflected by polyethylene, acrylic, and nickel. In addition, we have used MCNP to study neutron absorbing materials and spacing for criticality safety and to validate and optimize radiation detectors designs.

Detector Design. [Swinhoe 2009, Evans 2010, Fensin 2009a, 2009b, and 2009c, Peerani 2009, Lafleur 2008, Swinhoe 2007, Hendricks 2003, Langner2006]. MCNP6 is a simulation tool widely used for the design of detectors (neutron and gamma) for use in non-proliferation safeguards. Nearly all of the non-destructive assay (NDA) equipment used in nuclear fuel cycle facilities in Japan and elsewhere have been designed using MCNP6. In general the simulation results are within about 5% of the experimental measurements. In recent years we have added the capability for MCNP6 to perform neutron multiplicity detector simulation, which allows us to calculate coincidence counting rates in situations where our approximate theoretical models no longer hold. In N Division there is a major project to design instrumentation to measure the plutonium content of spent fuel. We use MCNP6 not only to model detector behavior, but also to calculate the composition of the spent fuel created during the reactor irradiation using the recent MCNP6/CINDER integration. Some other institutions carry out modeling work (European Union Joint Research Center, International Atomic Energy Agency, ORNL) but most use either MCNP6 itself or a modified version of MCNP. Los Alamos is acknowledged as one of the leaders (if not the leader) in this area (see ESARDA benchmark reference below).

Global Security. Part of our mission is to develop and apply science/technology to reduce the threat of weapons of mass destruction, proliferation, and terrorism. Los Alamos provides technical assistance and advice in accidents or incidents involving radiological or nuclear weapons. Monte Carlo simulations are well suited to predict the signatures from shielded radiation sources because of the three-dimensional and time-dependent nature of the problem. Specifically, the Monte Carlo methods, codes, and nuclear data developed and used here to provide assistance for these global problems are also used by dozens of other US federal agencies and foreign partners as the "gold standard" to design and optimize radiation detection systems for monitoring and performing radiological health and safety predictions. In some global security applications, radioactive threat objects are characterized by measuring a gamma-ray spectrum and analyzing the leakage of uncollided passive decay gamma-ray lines. In order to optimize the parameters of the threat object model so that forward calculations match the measurements, it is helpful to compute the sensitivity of the uncollided fluxes to the unknown parameters (system dimensions, material densities, etc.). We have developed the capability to compute these sensitivities in a general three-dimensional geometry using MCNP. The method also provides a much more efficient means of obtaining the uncollided pointwise flux than the standard point detector tally. Los Alamos is the leader in modeling and analyses based on uncollided fluxes; peers tend to use the entire gamma-ray spectrum. MCNP6 has the ability to model detailed delayed neutron and gamma emissions, which is particularly useful for Homeland Security applications where the primary detection method is active interrogation with delayed signatures.

Nuclear Fuel Behavior. MCNP/CINDER is used in T Division to study the detailed behavior of nuclear fuel elements, such as the formation and propagation of bubbles and cracks.

4.1.2 Kinetic MC. Kinetic Monte Carlo (KMC) is commonly used, and for reasons given in the overview is powerful and valuable, for simulations in various areas of materials science, physics, chemistry and biology, and in many cases the connection to the Los Alamos and DOE missions are clear. For example, KMC is often used to study the complex processes in radiation damage annealing, which is of course critical to understanding advanced nuclear waste storage, advanced nuclear fuels, and materials for fission and fusion reactors.

4.1.3 Condensed Matter Physics and Materials Science. The MC method is one of the main computational tools (along with Molecular Dynamics and Density functional theory) for modeling materials—a major thrust of the Laboratory. MC's continued support is required for advances in this area and for Los Alamos's signature facility, MaRIE.

4.1.4 Statistics. Monte Carlo is an essential part of statistical work as related to Lab projects in weapons (e.g., Gaussian process emulators for prediction and UQ), enhanced surveillance (system reliability estimates; sampling methods for complex populations), homeland security (design of, and performance assessment for, radiation detectors; transport of airborne particles; baselines for biosurveillance metrics), analysis of tomographic images, and environmental problems (climate modeling, underground migration of contaminants), to cite a few examples.

4.1.5 Optimization. The goal here is to find the best possible solution that minimizes a given cost function as efficiently as possible. Remarkably, almost any problem can be cast as an optimization one. Examples are the traveling salesman problem, find the shortest route that meets a number of cities, and the protein folding problem, find the configuration that minimizes the energy of a given protein. Optimization is naturally at the intersection of several scientific fields with tremendous impact in applied mathematics, computer science, network communications, physics, computational biology, and complex systems. There are several computational methods to attack optimization problems. Arguably, probabilistic methods based on classical and quantum Monte Carlo techniques (Markov chain Monte Carlo, MCMC) are the most efficient ones, allowing us to deal with large and complex problems. Some of these problems are of relevance in national security. For example, optimization provides more efficient ways to deal with large amounts of data, essential in scenarios where the data overtakes the amount of space for storage. High-performance computing is necessary to enhance the security of nuclear weapons. MCMC techniques for optimization are thus key to our mission. It is a strategic investment area of the LDRD program, addressed in the Science and Technology Grand Challenges.

4.1.6 MC for BioSecurity. Influenza kills an average of 40,000 people every year in the US during a normal seasonal epidemic. It is possible that millions can be killed during a pandemic, which occur for influenza every few decades (1889, 1918, 1957, 1968, 2009). We are developing spatiotemporal models to understand several epidemiological aspects of influenza, including the emergence of drug resistant strains under combination therapy and the sources of seasonality. Although the most basic mathematical models employ coupled ordinary differential equations, more accurate models employ stochastic methods that capture both the fact that populations are composed of individuals (and therefore represented by integers) and, more importantly, that most events can only be specified in terms of probabilities. Such a statistical description is necessary when populations are small, as with the emergence of a resistant strain, when the disease is invading a geographic region, or when new strains emerge to evade the immune system. To treat these processes, we are exploring kinetic Monte Carlo methods that are based on the Stochastic Simulation Method (SSA) introduced by Gillespie. As the SSA method is typically too slow for large populations (cities, states, countries), we are exploring faster methods, such as the approximate tau-leaping methods. We are exploring optimal adaptive time step tau-leaping methods that will allow us to construct large-scale kinetic Monte Carlo simulations that can simulate the global spread of the disease while including details of human movement.

4.1.7 Phylogenetics. [Bhattacharya 2007, Timm 2007, Gnanakaran 2007, Rousseau 2007 Brumme 2007, Rousseau 2008] The Laboratory has been on the forefront of developing theoretical biology as a field. A large number of applications (from systems biology to pathomics) and technologies (from attribution to intervention both against natural and against artificial agents) rely on a solid phylogenetics capability. Whereas a large part of this capability relies on point estimates derived by heuristic methods, the needs for robust estimates and quantification of the uncertainty involved in these calculations are rising. Monte Carlo methods for estimating the Bayesian posterior is the leading method of choice in this field. This nascent capacity is intimately tied to maintaining our lead in a variety of fields in theoretical biology. Coupled with this, the realization that phylogenetic methods may yield better classification tools in a wide variety of situations has increased the importance of this capability. In almost every field where the diversity of the objects being classified has a strong component due to descent with independent modifications, leading to lineages, phylogenetics is likely to provide better tools than other unsupervised classifiers. The Laboratory's interest in cybersecurity is an example of an extended application of phylogenetics. It can potentially be used to classify and rapidly intervene in the spread of malware, whether deliberately targeted or maliciously spreading.

4.1.8 QCD. The use of high performance computations to further the needs of Beyond the Standard Model Physics is an active area at the Laboratory. In particle physics, this translates to understanding the signals of new theories of physics in experiments carried out here and elsewhere. The problem with this approach is that one part of the currently known physics, Quantum ChromoDynamics, has no small parameter on which to base a perturbative expansion at some energies of interest. The only completely controlled calculations of these backgrounds come from Markov Chain Monte-Carlo evaluation of expectation values using "path integrals," which are infinite-dimensional integrals with number of dimensions scaling as the number of points on a discretized finite volume space time. We have a long history in carrying out these calculations and considered one of the leaders in this field. These QCD codes also form a standard part of the tests for newly emerging architectures. Because of their intensive floating point calculations and extremely regular grid communications, they exercise different capabilities of the machines than other codes.

4.2 Research Breadth and Impact

4.2.1 MC for Transport. Monte Carlo methods research, software development, and simulations of radiation transport are prevalent in many different application areas around the Laboratory.

- Neutron [Yesilyurt 2009, Solomon 2009] and gamma ray transport
  Codes: MCNP, MCATK
  Applications: MCNP, including criticality safety, radiography, nuclear oil well logging, fission and fusion nuclear reactor design, decontamination, decommissioning, waste transport and storage, and medical, radiology (detector design and image reconstruction)
- Thermal x-ray transport [Kelley 2010, Densmore 2010a, McClarren 2009, Densmore 2009a, Hykes 2009, Densmore 2009b, Urbatsch 2008, Densmore 2008, Densmore 2007a, Densmore 2007b]
  Codes: Jayenne IMC Project
  Applications: high energy density physics, astrophysics, inertial confinement fusion, and experiments at the Z-Pinch, NIF, and Omega facilities.
- Ion transport
  Codes: MCNP, Eulerian Application Project Package
  Application: medical including proton and heavy ion therapy, solar and cosmic ray shielding for astronauts, accelerator target design, active interrogation, plasma physics.
- Relativistic electron transport
  Codes: MCNP, Merlin
  Applications: Compton electron currents for EMP; solids, dielectrics, and plasmas for radiographic applications.

4.2.2 Kinetic MC. Our work has been in the early development of rate catalogs, the development of methods for accelerating KMC [e.g., Chatterjee 2010]. There have also been applications in radiation damage annealing and alloy segregation. Los Alamos also has a significant large-scale parallel KMC capability and expertise in kinetic theory aspects of the method.

4.2.3 Condensed Matter Physics and Materials Science. In condensed matter physics and materials science the breadth of the Laboratory's Monte Carlo applications samples the breadth of such applications worldwide. Examples include current activities such as:

- Condensed Matter Physics: electronic structure of Pu and metal-insulator transitions in solids, Novel ground states of strongly correlated electron materials,
- Quantum Information (Atomic, Condensed-Matter and Nuclear Physics): Cold Fermi atoms in optical lattices,
- Statistical Physics (Equilibrium): potential energy surfaces of explosives, Ionic potential energy surfaces for equations of state and high-pressure phase transitions, and
- Statistical Physics (Nonequilibrium): kinetics of colloids and granular materials.

The impact of this work varies with the application. Key components of the above are directed towards the theory, modeling, and simulation of explosives, and accordingly, directly link with major Laboratory programs. The cold Fermi atom work brings international respect for the Laboratory's science. Success with the electronic structure of plutonium work will impact both programs and scientific reputation.

4.2.4 Statistics. The Statistical Sciences Group (CCS-6) is a unique resource in the nation, and is responsible for the origination of Latin hypercube sampling for the design of computer experiments in the 1970s (the original paper has more than 1,200 citations). More recently, the group published the seminal proof of exponential convergence theory for adaptive biasing methods (also known as importance sampling), developed partial decoupling methods for auxiliary sampling, established the theoretical basis of ex post facto sampling for estimation of means from heavy-tailed distributions, and developed algorithms for so-called transition matrix Monte Carlo for condensed matter systems. CCS-6 has published numerous papers on the theoretical underpinnings of Monte Carlo algorithms in a variety of prominent journals, including the Journal of the American Statistical Association, Technometrics, Annals of Applied Probability, Statistical Science, Journal of Statistical Mechanics, Journal of Computational Physics, Mathematics and Computer Simulation, and the Journal of Computational and Graphical Statistics. Customized software for implementing Markov chain Monte Carlo has been written locally and used in Bayesian statistical analyses.

4.2.5 Optimization. Historically, Los Alamos has been a world leader in Monte Carlo simulations. Currently, a number of staff members at Los Alamos utilize and develop MCMC methods for problems in optimization such as finding the optimal configuration in quantum or classical spin glasses. Spin glasses are important because they provide simple models of many complex systems in nature. In fact, most combinatorial optimization problems can be related with spin glasses. It is well known that MCMC can be used to study a spin glass model by imitating a slow annealing process where the temperature is slowly changed in time. This is the basic idea behind methods like classical simulated annealing; a probabilistic heuristic method. By choosing a proper annealing schedule, it is possible to converge to the optimal configuration of a spin glass with large probability. While in the worst-case scenario the total annealing time is undesirably large, simulated annealing is still a very good linear-time heuristics for many related and important problems. In particular, classical simulated annealing implemented using MCMC could be very efficient when used to estimate the ground state energy of a spin glass (instead of obtaining its optimal configuration). [Krzakala 2009]

A more recent method, also based in heuristics, is quantum annealing. Here, the idea is to exploit quantum fluctuations to speed up a classical annealing process; the latter is driven by thermal fluctuations. While quantum annealing can naturally be implemented on a quantum computer (adiabatic quantum computation), it can also be imitated by means of (quantum) Monte Carlo methods. It was recently demonstrated numerically that MCMC for quantum annealing largely outperforms classical simulated annealing in a number of problems in optimization. A review of quantum annealing can be found in [Das 2005]. Apart from achieving unprecedented speed-ups, these Monte Carlo studies will likely be the foundation for future implementation of quantum annealing on quantum computers.

Batista and Somma, T-4, recently introduced a classical-to-quantum mapping that relates the classical simulated annealing method with a particular instance of the quantum annealing one [Somma 2007 & 2008]. This result implies that quantum annealing, if implemented on a quantum computer, is at least as powerful as classical simulated annealing. In fact, [Somma 2008] rigorously showed that some instances of quantum annealing always provide speed-ups with respect to the classical annealing method. The mapping in [Somma 2007] provides novel ways of using MCMC to simulate classical spin glasses by embedding them in effective spin glasses that live in larger space dimensions (Markov chain lifting).

4.2.6 MC for BioSecurity. The methods we are developing, spatial kinetic Monte Carlo with realistic human movement, can be applied to the spread of many diseases.

4.2.7 Phylogenetics. The use of Monte Carlo methods in phylogenetics is a nascent research area at the Laboratory. A large capability exists in the application of phylogenetics methods here, but the use of Bayesian methods necessitating Monte Carlo techniques is new. Phylogenetics has been used in biology for metagenomics, attribution, understanding pathogen evolution, and studying correlations relevant to vaccine development. The methods used have varied from distance-based approaches to heuristic search for the maximum likelihood answer. When the need arose for error bars, ad hoc methods have been used or standard Bayesian tools have been applied to small amounts of sequence data. The advent of large sequencing efforts using the newly emergent pyrosequencing techniques, and the development of that capability at the Laboratory has now spurred interest in developing Bayesian methods to deal with phylogenetics in this domain. Concurrently, the new generation of hierarchical parallel architectures has led to the need to adapt the methods developed on serial architectures to these efforts. The mapping of this Monte Carlo problem on to such architectures has just begun and algorithmic developments have started.

4.2.8 QCD. The collaboration centered at the Laboratory has been at the forefront of research in this area. The quantities that we have been traditionally focused on involve static properties of light hadrons and their interactions. This group has also been instrumental in showing how the discretization approximation [Bazavov 2009] can be systematically eliminated in a limit without resorting to perturbation theory at any stage. Recent work has focused on the properties of these theories at high temperatures relevant to the quark-gluon plasma transition being probed in various experiments around the world.

4.3 Comparison with Peers

4.3.1 MC for Transport. MCNP is a powerful, general-particle Monte Carlo transport code that is more than 32 years old and created directly from the algorithms derived from Ulam, von Neumann, and others. The MCNP team contains world-class leaders in the fields of variance reduction, parallel particle transport, high-energy transport physics, criticality, and electron transport. MCNP is widely distributed worldwide and is regarded as one of Los Alamos' most successful code development projects in its entire history. MCNP will soon be the first and only code with the capability to estimate sensitivities and reactivity changes using continuous-energy Monte Carlo. The current capability uses a differential operator to estimate the response to a perturbation, and this approach has been shown to have difficulties with neutron scattering and thus is not appropriate for eigenvalue sensitivity calculations. The closest peer and competitor is ORNL's SCALE code, which uses the usual inner product formulation, except only in multigroup, not continuous energy. SCALE also has the ability to propagate sensitivities and can compute adjoint-based sensitivities for reaction rates in criticality problems. MCNP's use of the fission probability interpretation of the adjoint flux to achieve continuous-energy sensitivities is a unique capability.

For Merlin, the peer capability is the Voss Scientific LSP code and its progeny. These codes are three-dimensional and have some internal capability for Monte Carlo photon transport and hydrodynamics. They also have certain additional physical models but are lacking others. Peers of the Jayenne Project are LLNL and the UK's AWE. One major difference is that the Jayenne Project operates mainly on AMR meshes and so it generally has many more cells than a Lagrangian or ALE mesh, which allows for more detailed studies of radiation-hydrodynamic behavior but also requires more particles to control statistical noise. Roadrunner has drastically reduced the incremental cost of particles and thus allowed Los Alamos to leapfrog its peers in computational efficiency while maintaining its more accurate course. AWE is very strong in general transport methods development, but the US appears to have more computing resources. LLNL has a competing hybrid method, but ours has more underlying mathematical research designed to maintain consistency and accuracy while speeding up the calculations. Another peer is Dan Casen (UCSC) who, as part of the Supernova Science Center SciDAC team, is beginning to couple his IMC transport with hydrodynamics in his supernova simulation capability and is looking to collaborate with Los Alamos.

4.3.2 Kinetic MC. Los Alamos is roughly at the state of the art in KMC. We do not have anyone developing parallel KMC methods as they do at LLNL or University of Toledo, but we import this technology. Los Alamos is known for some of the key development work in KMC; Voter has written a well-known introductory article in 2005.

4.3.3 Condensed Matter Physics and Materials Science. The Laboratory's Monte Carlo simulators are as good as any elsewhere, but the institution lacks recognition as a center of Monte Carlo oriented research in condensed matter physics. The Laboratory's efforts, while having clearly identifiable institutional justification, lack critical mass.

4.3.4 Statistics. Other researchers in statistical algorithms for Monte Carlo tend to be focused exclusively on its theoretical aspects (e.g., academia) or exclusively on applications and computational implementation (e.g., other national laboratories). In addition to its broad spectrum of MC applications, Los Alamos has a unique theory/practice that enables us to be productive in both arenas.

4.3.5 Optimization. Understanding and developing novel MCMC methods for optimization requires extensive studies and implementation of these methods for large instances of complex and computationally hard problems (e.g., spin glasses). Further, standardization of results requires averaging over large numbers of random instances of the problems. At the moment, Los Alamos is one of the best places in the world to carry on such a difficult project with our wide number of resources to implement large-scale computational methods. From smaller clusters in the research groups to Roadrunner, Los Alamos's researchers have access to execute their codes in high-performance computing centers. This unique environment at the Laboratory provides unconditional advantages with respect to other institutions. High-processing speeds and high memory capacities are especially important in Optimization where, for hard instances, the running time dependence of the MCMC method with the problem size is undesirably large.

4.3.6 MC for BioSecurity. Very few fully global models of disease spread have been developed and most use very simplified disease models with simplified kinetics (such as chain binomial methods).

4.3.7 Phylogenetics. Most Bayesian phylogenetics has been done so far using one of two big code suites: Mr. Bayes and BEAST. They, however, have followed standard Metropolis sampling techniques, which is an inherently serial technique that may be accelerated by parallel evaluation of the likelihood score using a co-processor model. This does not scale to the massively parallel architectures available today. There is limited amount of theoretical work that tries to understand the space of tree topologies and parallel tempering approaches applied to this problem, but no concrete implementation of these ideas capable of doing the required sequence analysis exists.

The work at the Laboratory is focused primarily at this niche of developing methods that can process large data sets using the computational power of the current generation of supercomputers. Since the use of supercomputers in these analyses is new, and the availability of deep sequencing leading to an increase in data set sizes by about three orders of magnitude has just started transforming the field, we are still in the forefront of this field.

4.3.8 QCD. These calculations are large and require huge collaborations. Los Alamos was lead of a small collaboration that was one of the leaders of the field, but recent movement has been towards bringing the world community together. In the domain of high-temperature QCD, we now work as a part of the US-wide effort, and our main competitors are similarly large collaborations in other countries. Recent work from this US collaboration on the equation of state was the first to demonstrate some control virtually all the systematic errors within the same calculation and is considered the state-of-the-art result.

4.4 Status of the Capabilities

4.4.1 MC for Transport. MCNP provides highly accurate results, using continuous-energy physics, ENDF/B-VII nuclear data, and explicit 3D constructive solid geometry. MCNP utilizes both domain replication with MPI and shared-memory OMP threading and has been shown to efficiently utilize both multiprocessor PCs and large, high-performance clusters. There are over 10,000 MCNP users worldwide. The MCNP Monte Carlo code is widely used in studies of advanced reactor concepts, either directly as a main-line design tool or indirectly as part of the verification/validation process. MCNP is routinely used to calculate k-effective and detailed distributions of power and reaction rates. MCNP has many special features for criticality calculations of reactors and has been coupled to burnup and thermal/hydraulic codes for multi-physics applications. MCNP6 contains the high-energy (10s to 100s of GeV) extensions for heavy charged particles, and includes the T-Division CINDER 2008 database of nuclear interactions and decays for 3100+ radioactive isotopes for production and depletion capabilities in nuclear reactor design.

Nonlinear collisional transport of energetic, relativistic electrons in condensed materials in the presence of external and self-consistent electric and magnetic fields is simulated with the Merlin electromagnetic particle code. A standard PIC technique for collision less field transport is coupled to a condensed-history Monte Carlo method for collisions against background materials. The models include atomic physics and Compton scattering of the propagating electrons. Because the method was initially directed toward moderate-energy electrons, an approximation was used for the nuclear Bremsstrahlung energy losses. The capability was originally developed for Compton electron generation and transport in dielectrics and in dielectric and vacuum Compton detectors. It has had numerous subsequent applications, including radiography using energetic electron beam Bremsstrahlung converters and compact rod-pinch x-ray diodes. Because self-consistent fields and beam neutralization are usually not important inside metallic targets, a link to the MCNP electron/photon code was provided to model photon generation inside the target and subsequent transport and radiographic imaging. Special-purpose links were employed to model energy deposition and disassembly of targets.

The Monte Carlo Application Toolkit (MCATK) provides a suite of components from which a client may compose targeted applications that meet their requirements. It is currently focused on delivering eigenvalue estimates using continuous energy cross section data running on serial, parallel shared memory and parallel partitioned memory architectures. In addition to stand-alone applications built entirely from toolkit components, the teams also provide components to aid existing applications by allowing new features and/or replacing capabilities that are difficult or expensive to maintain by the application code team. The Jayenne Project is for simulating thermal radiative transfer in the x-ray regime for high energy density physics applications such as supernova explosions, inertial confinement fusion, and radiation flow experiments at facilities such as Sandia's Z-Pinch, Omega Facility, and the National Ignition Facility. The Jayenne Project uses the Fleck and Cummings Implicit Monte Carlo (IMC) method, its software is powerful, robust, and massively parallel; it is multi-dimensional, runs on AMR meshes, and has different parallel schemes. These underlying components are used in the radiation-only code Milagro, which is also used as a testbed for advanced numerical methods research. The underlying components are also used in Wedgehog, which is a high-level IMC component that hooks into multi-physics application codes and provides the transport capability for radiation-hydrodynamics simulations. The Jayenne Project codes have run for countless millions of CPU-hours on the DOEs supercomputers. One application of radiation-hydrodynamics simulations using the Jayenne IMC Project software is the modeling of emission from supernova. This simulation capability allows observational astronomers to constrain, to a degree not possible before, aspects of the supernova explosion mechanism using the diagnostics of their observations. The Jayenne Project devoted substantial effort to adapting its code to the heterogeneous architecture of Roadrunner. This effort has realized overall speedups ranging from 3 to 15 for users. Ongoing methods research includes hybrid methods, Compton scattering time step control, and software design for heterogeneous architectures. Finally, the transport of ~MeV light ions in a thermonuclear plasma is an important physical mechanism for ICF applications and diagnostics. In the Eulerian Project's plasma codes, this process is modeled by continuous-slowing-down energy loss to the thermal plasma, combined with a Monte Carlo treatment of the large-angle binary collisions and in-flight reactions. The upscattered plasma ions and energetic reaction products serve additional sources for the charged-particle cascade. All suprathermal particles Z=1-4 and their principal reactions are tracked in the code.

4.4.2 Kinetic MC. The Kinetic MC capability has grown recently due to a new hire in the area. The capability is located primarily in T and MST divisions and is in a steady state at the present time.

4.4.3 Condensed Matter Physics and Materials Science. The Monte Carlo method is more of an approach to numerical problem solving than one technique. It is in fact a vast range of techniques. Overall, it is an extremely flexible method. In many cases, this flexibility permits the approach to adapt optimally to specific applications. In general, the approaches being used at the Laboratory range from standard to state-of-the-art.

4.4.4 Statistics. The ever-increasing reliance on computing that we see in major programs such as weapons, surveillance, and other computational applications, should continue to sustain and advance existing capabilities.

4.4.5 Optimization. Los Alamos is hosting a number of staff members with experience in Monte Carlo methods that simulate classical or quantum annealing processes for optimization. Some of these staff were connected with the development of field of quantum annealing from its very early stage and contributed substantially to its understanding. One of them (Arnab Das) implemented the first quantum Monte Carlo method for annealing of small samples of computationally hard spin glasses. Outside Los Alamos, several groups use MCMC methods to study related problems. A well-established group that uses MCMC for quantum annealing is Nishimori's research group in the Tokyo Institute of Technology. Another group is Tosatti's group in SISSA, Italy. Some of Los Alamos's recent contributions have put the Laboratory at the forefront of this field and generated new external collaborations with these groups. Particularly, a recent article by Tosatti and Santoro in Nature Physics (2007) describes the impact and contributions of our work in Optimization. Understanding and developing novel MCMC methods for optimization requires extensive studies and implementation of these methods for large instances of complex and computationally hard problems (e.g., spin glasses). Further, standardization of results requires averaging over large numbers of random instances of the problems. At the moment, Los Alamos is one of the best places in the world to carry on such a project as it offers a wide number of resources to implement large-scale computational methods. This unique environment provides unconditional advantages with respect to other institutions. High-processing speeds and high memory capacities are especially important in Optimization where the running time dependence of the MCMC method with the problem size is undesirably large.

4.4.6 MC for BioSecurity. We currently have several small tests codes for ODEs, SSA, and tau-leaping. We also have two small spatial codes using the coupling and metapopulation methods. Once we have quantified the kinetic Monte Carlo methods we wish to use it will be incorporated into a metapopulation model for the most important global airports with realistic travel. This should be in place by late summer. We hope to work closely with the NM State Epidemiology Office as part of this ongoing LDRD-ER project.

4.4.7 Phylogenetics. The capability is still in the development stage and has not yet been deployed. Keen interest in this arena is evident in the biology community: early results using small-scale non-monte carlo importance sampling has already been accepted for oral presentations. The development efforts are currently funded by Exploratory Research LDRD funding, but the NIH funded CHAVI initiative is willing to fund development once the capability has been demonstrated.

4.4.8 QCD. The capability ranges from both the theoretical to the computational end of this subject. Our code to do these calculations is written in Fortran with parallelization implemented either using Fortran 90 or the Message Passing Interface, but the core computational routines are hand tuned for each architecture. Through collaborations we also use codes from other scientists and implement scripts to control the continual running, some times over months, reliably.

4.5 Challenges and Issues

Issues for the MC theme that are common to all themes appear in Section 8.0.

4.5.1 MC for Transport. One issue for the Eulerian application project package is that there are several deficiencies in the existing light ion Ace cross section data now being worked on. Some modifications to the cross section capabilities will be required.

4.5.2 Kinetic MC. No issues except as presented in Section 8.0.

4.5.3 Condensed Matter Physics and Materials Science. The main generic problems that Monte Carlo faces are the cost of precision and the possibility of broken ergodicity. The precision (error) of the simulation is proportional to the reciprocal of the square root of the number of independent samples. When this is a problem, the cure is not just asking for faster and more processors but rather asking for new algorithms that reduce the error scaling's proportionality constant and/or increase the rate at which independent samples are generated (faster processors addresses the latter in a brute force way). Broken ergodicity refers to the sampling being too infrequent for some (rare) events that can and must occur. It renders the simulation invalid. These problems underscore the need to continually develop new algorithms. With the Laboratory's commitment to MARIE arises both the need and opportunity for new Monte Carlo initiatives. MARIE will permit novel and penetrating explorations of dynamics and quantum phenomena. While dynamics seems unnatural for Monte Carlo, in fact the method is commonly used to simulate non-equilibrium systems. "Kinetic Monte Carlo" is the rubric for one type of such approach. Sampling rare events is the challenge for this particular important form of Monte Carlo. Except for simple problems, numerical solutions of the partial differential equations of quantum mechanics are impractical. Quantum Monte Carlo techniques developed at the Laboratory can extract useful dynamical information. The inherent probabilistic nature of quantum mechanics suggests broader dynamical information should be accessible by Monte Carlo methods. Support is needed to develop them. Part of the institutional commitment to MARIE should be a commitment to computational physics as an essential supporting tool. Monte Carlo methods should be allowed to play a prominent role in this. They will often be the only method capable of the task.

4.5.4 Statistics. No issues that are not common ones, addressed in Section 8.0.

4.5.5 Optimization. While MCMC methods for optimization were proven successful a number of times, some challenges remain to be addressed. One challenge regards the design and implementation of novel MCMC methods for optimization to simulate alternative annealing processes that could combine both, the classical and the quantum annealing ones. Another important issue is the lack of interdivisional collaborations that could be improved with new, collaborative, projects between staff members with interdisciplinary backgrounds including physicists, computer scientists, and software developers.

4.5.6 MC for BioSecurity. The challenges are: 1) having a very fast kinetic Monte Carlo method, 2) having an accurate and fast spatial model, and 3) knowing human movement patterns across various spatial scales. For influenza in particular we are developing new disease progression models and exploring environmental impacts on that progression, such as humidity effects that lead to seasonality.

4.5.7 Phylogenetics. No issues that are not common ones, addressed in Section 8.0.

4.5.8 QCD. No issues except those addressed in Section 8.0.

5.0 Theme 4: Molecular Dynamics

(Theme Leader: Tim Germann, T Division)

Like its predecessor, the Monte Carlo method, Molecular Dynamics (MD) simulations were first developed to study equations-of-state for the post-WWII Atomic Energy Commission. Alder and Wainwright's pioneering 1950s calculations at Livermore of the equation of state for a system of a few hundred hard spheres, and importantly the demonstration that their MD results and Metropolis MC calculations of the same system by Wood, Parker, and Jacobson at Los Alamos were in quantitative agreement, helped to establish the MD technique for computing equilibrium properties. This initial work was followed up in the 1960s for atoms interacting via continuous potentials such as the Lennard-Jones pair potential by other early MD pioneers such as Aneesur Rahman at Argonne National Laboratory, and Loup Verlet in France. At the same time, MD simulations were being used to model nonequilibrium processes. George Vineyard and colleagues at Brookhaven National Laboratory published the first study of radiation-induced damage in crystalline solids in 1960. In these simulations a primary knock-on event is modeled by giving one atom a sudden velocity impulse, and following the resulting collision cascade and residual defects, primarily interstitial atoms and vacancies. At Livermore in the early 1970s, Bill Hoover and graduate student, Bill Ashurst, began developing nonequilibrium MD (NEMD) techniques to compute transport properties such as thermal conductivity and viscosity, particularly in extreme conditions not amenable to experimental measurement. In order to model such driven systems, both an energy *source*, such as boundary reservoir regions with a constrained velocity and/or temperature, as well as an energy *sink* to account for heat which would be lost to a system's surroundings, such as a thermostat, are required. Despite this early development and adoption of MD simulations at national laboratories, it was not until the late 1970s that Los Alamos seriously entered this field. Brad Holian, in collaboration with Hoover, studied the strongly nonequilibrium, and nonlinear, process by which a steady shock wave develops. They showed that the structure of weak shocks in dense fluids is reasonably well described by continuum Navier-Stokes equations and how Navier-Stokes begins to become less accurate for stronger shocks. MD work at Los Alamos grew throughout the 1980s with work on surface science and an emerging leadership position in interatomic potential development for metals in the 1990s, primarily embedded atom method (EAM) potentials such as Voter-Chen, and into the 2000s with modified EAM (MEAM) potentials for elemental plutonium [Baskes 2000], alloys, and helium gas bubbles [Valone 2006] as well as continued investigation of new interatomic potential forms for complex metals [Baskes 2007; Taylor 2009].

At present, MD simulations play an important role in a variety of Laboratory programs, including energy storage, environmental remediation, etc. Here we focus on five particularly active fields of research, four broad application areas, and one method development:

- Nuclear Energy, particularly thermomechanical properties of nuclear fuels;
- Material Dynamics, including shock and other high strain-rate conditions;
- Energetic Materials;
- Biomolecular Modeling, in particular biofuels and protein folding; and
- Advanced Algorithm Development, specifically AMD.

Accelerated Molecular Dynamics (AMD) refers to a class of methods developed in the late 1990s at Los Alamos that are designed to achieve time scales beyond the reach of standard MD methods, which require a timestep of order 1 fs = 10-15 s in order to numerically resolve atomic vibrations, and are consequently limited to roughly one microsecond of total simulation time. These AMD methods are applicable to infrequent-event systems, in which transitions from one state to another happen at intervals that are infrequent relative to the time scale of vibrational motion in the system. These are typically systems involving activated processes, such as the diffusion of a defect in a solid material or on a surface, although the overall class is much broader than this. A key concept is that a molecular dynamics trajectory, if it can be integrated for a long enough time, will escape from the current state of the system in an appropriate way – i.e., it will "pick" an escape pathway with a probability that is proportional to the rate constant for that pathway, despite the fact that it has no prior knowledge of what pathways exist. The unifying theme in the AMD methods is that they exploit this property of a trajectory, but they coax the trajectory into making the escape-path choice sooner, thus accelerating the dynamics. This philosophy is in contrast to methods such as kinetic Monte Carlo, in which the user must pre-specify all possible escape pathways. Although AMD is substantially more computationally expensive than kinetic Monte Carlo, the payoff comes from the fact that the escape pathways in the system often exhibit a complexity that exceeds what is possible to guess in advance to capture with kinetic Monte Carlo. There are currently three AMD methods: hyperdynamics [Voter 1997], in which a bias potential meeting certain requirements is added to the potential energy surface; parallel replica dynamics [Voter 1998], in which trajectories run simultaneously on many processors provide the effect of parallelizing time; and temperature accelerated dynamics [Sorensen 2000], in which rapid escape events at high temperature are filtered to find the first escape event at the lower, desired temperature. Parallel-replica dynamics gives exact state-to-state dynamics when implemented carefully and represents a good match to the increasingly parallel nature of computers. The other two methods rely on the transition state theory approximation, but offer speedup on a single processor. All three of these methods are most powerful when the events are very infrequent, i.e., when the barriers are high relative to the temperature of the system. They have been employed on a variety of processes such as surface growth, bulk diffusion, grain boundary sliding, nanoscale friction and plasticity, and radiation damage annealing mechanisms, achieving time scales from microseconds to milliseconds and in some cases, seconds.

An approach related to AMD is one generally known as adaptive kinetic Monte Carlo (AKMC). In AKMC, repeated searches are performed to find saddle points for escape paths from the current state of the system. After many saddles have been found, one assumes that the list of escape paths is complete enough that one can be chosen in a fashion analogous to a standard KMC move to take the system to a new state. The AKMC approach can be attributed primarily to Barkema and Mousseau (late 1990s), Munro and Wales (1999), and Henkelman and Jonsson (2001). The AKMC approach is somewhat more approximate than the AMD methods, in part because it is hard to guarantee that all relevant saddle points have been found, but is very efficient and powerful when saddle point-based dynamics are appropriate. An introduction to both the AMD methods and the AKMC methods can be found in [Voter 2002].

5.1 Connection to the Goals and Mission of the Laboratory

5.1.1 Nuclear Energy. Predictive materials science requires understanding of defects and how they interact with the lattice to determine materials properties. Defects both limit and enable all materials. The ability to identify and subsequently control multidimensional defects (where 0-D = point defects, 1-D = dislocations, 2-D = surfaces, grain boundaries and interfaces, 3-D = voids, bubbles and second phases) is the next frontier of materials research and will lead to materials of superior performance and an overall implementation of the "materials-by-design" paradigm. For nuclear fuels, which is an important component of addressing the energy security issues currently facing the nation, these relations are exemplified by binding between point defects such uranium vacancies and fission gases such as xenon, which subsequently interact with dislocations and grain boundaries acting as sinks to form a second phase in the form of gas bubbles. Gas bubbles eventually form inter-linked structures leading burst release and degraded fuel properties. Fuel performance is critically governed by fission gas release, thermal conductivity and geometry changes (swelling), properties that are all directly linked to multi-dimensional defects, e.g., via fission gas and void evolution. The two primary reasons to pursue atomistic modeling for nuclear fuel performance are the ability to investigate fuels of variable composition (i.e. other than for which irradiation data already exists, e.g. UO_2 and U10-Zr), and the ability to explicitly consider microstructural features (such as dislocation, grain boundaries, interfaces and voids/bubbles). Both of these reasons critically enable engineering scale fuel performance codes to be predictive and in the process decrease the reliance on empirical data from integrated experiments. Indeed, without such atomic scale insight, engineering scale models will continue to rely upon empirical data. The step from atomistic simulations to engineering applications would naturally involve further simulations within a multi-scale framework. In summary atomistic simulations are essential for innovation and technology improvements in the nuclear energy field and thus support missions related to energy security and threat reduction. Atomistic approaches also allow us to gain insight into the non-equilibrium materials properties that emerge in extreme environments such as high-burnup and fast reactor concepts.

5.1.2 Material Dynamics. The missions of the Laboratory in nuclear security and stockpile stewardship without nuclear testing require accurate, validated models of dynamic materials phenomena over a wide range of densities, temperatures and rates of deformation. The goal of the Laboratory as a world leader in materials science underpins such model validation. The detailed microphysics of dynamic deformation, in situ, is a long-term goal for facilities such as MaRIE. One of the signal characteristics of NonEquilibrium Molecular Dynamics (NEMD) simulations, pioneered at Los Alamos, is the ability to simulate the microphysics on weapons relevant time scales, giving detailed information for the development of dynamic materials models. Such simulations provide both microscopic parameters, for theories at larger length scales and longer time scales, and detailed spatial and temporal information about the relevance of competing mechanisms thereby constraining the set of physical model parameters.

5.1.3 Energetic Materials. The inherent metastability and rapid reactions of high explosive (HE) formulations makes it difficult to characterize them completely. Molecular dynamics is used to supplement and expand the experimental information. The Equation of State (EOS) of the product mixture (N_2, H_2O, CO_2, CO, solid C, and a wide variety of minor products) is the furthest advanced of these. Classical potentials are formulated on the basis experimental data for pure materials, simple mixtures and actual formulations, and quantum chemical calculations, and these are used in Monte Carlo simulations to determine the equilibrium composition as a function of pressure (density) and temperature (entropy) to establish the EOS, which is then reduced to analytic or tabular (Sesame) form (e.g., see [Coe, 2009]). Probable dynamic issues dealing with the slow solid product formation (solid carbon or metal oxides) can be inferred from these studies and treated analytically. Non-reactive potentials for the components of the formulations (HE crystals, polymeric binders) have been determined in collaboration with academic groups, in particular Smith at Utah and Thompson at Missouri. These have been used to calculate a wide variety of physical properties (elastic constants, thermal conductivity, strength and fracture properties) that are used in mesoscale studies of the response of the composite materials [Menikoff 2002], particularly for accidental initiation scenarios. Current studies are performing detailed analysis of the temperature profiles formed during void collapse, shear banding and general deformation processes [Cawkwell 2008]. The results are compared with studies performed on well-prepared single crystal samples synthesized at Los Alamos in group DE-9. Reactive molecular dynamics for realistic materials are performed with the Reax Force Field to formulate reactive models as a function of pressure and temperature. To first order, these models reproduce the simple one-step Arrhenius models used to interpret the basic kinetics of HE decomposition, which span the range from rapid cook-off [Zhang 2009] to the inferred kinetics required for detonation. Current studies are extending this analysis to a multi-step model that could be compared to the empirical cook-off models (such as those formulated by Henson and Tarver) developed for accidental initiation scenarios and provide a physical basis for greater extrapolation and prediction. Reactive molecular dynamics simulations for idealized materials (energetic AB dimer) are performed with REBO-type potentials that are formulated to reproduce realistic material properties [Heim 2008]. These studies have demonstrated a well-resolved reaction zone with the expected properties of the von Neumann spike, reaction zone profile and the Chapman-Jouget propagation conditions, with a system that was demonstrated to be following rational Arrhenius kinetics. Current studies are formulating more complete analyses of the initiation kinetics associated with void collapse initiation. These studies establish a path to connect the more realistic Reax studies with continuum level treatments (see Tarver, JTF, DSD).

The primary customer for this is the NW ASC program, with a strong emphasis on PBX9501 (Conventional High Explosive: HMX and Estane) and PBX9502 (Insensitive High Explosive: TATB and Kel-F), their associated detonator chains, and the interactions with neighboring materials. Phenomena associated with aging, performance at the limits of operating ranges, changes in the manufacturing conditions, accident scenarios and geometric perturbations would benefit from more complete physical models for these systems. Secondarily, the DoD has interests in developing safer and greener munitions, and in reducing their development time and costs for new formulations, which require an enhanced fundamental understanding of these materials. DHS and DoD must deal with a wide-range of unusual HE formulations (Improvised Explosive Devices, IEDs) whose properties are not well understood. Improved means for assessing the performance characteristics, sensitivity and disposal issues, and methods for detection would benefit from more accurate physical models where molecular dynamics can supply important pieces of information.

5.1.4 Biomolecular Modeling. Our use of MD simulations to characterize molecular recognition of virulence factors from bacteria and surface proteins from viruses is closely tied to the goal of developing therapeutics to fight pathogens, the mission of Los Alamos' biosecurity center. Our MD simulation based approaches to characterize biomass and its degradation for biofuels is closely tied to the Laboratory's mission on energy security.

5.1.5 Accelerated Algorithms. The three AMD methods compliment MD methods by offering a powerful approach for accurately simulating complex activated processes in materials that occur on time scales beyond nanoseconds. Such processes are ubiquitous in problems relevant to the Laboratory mission. Examples include radiation damage annealing [Bai 2010], material deformation and failure, surface growth [Shim 2007], and surface catalysis.

5.2 Research Breadth and Impact

5.2.1 Nuclear Energy. The work on atomistically informed meso-scale simulation models for applications in nuclear fuel performance codes and for development of new advanced fuels is an important part of LANL's current civilian nuclear energy programs. It will continue to be so as the importance of nuclear energy is anticipated to remain significant for the nation's energy portfolio. Nuclear energy represents one particular application of the concept of interactions between multi-dimensional defects. The tools and knowledge thus developed will find application in other areas such as advanced ceramics applied in batteries, fuels cells and electronics. Development of experimental techniques to resolve materials behavior down to the atomic level under static as well as dynamic *in situ* conditions will eventually enable validation of simulation predictions and will assist interpretation of these experiments.

5.2.2 Material Dynamics. The areas of importance for dynamic materials modeling that have particular relevance to science campaigns and the ASC and DPE programs are the: 1) physics of plastic flow and melting in shocked materials [Holian 1998], 2) physics and kinetics of phase transformations in metals [Kadau 2002 & 2007a], 3) physics of correlations and phase transformations in strongly coupled plasmas, 4) physics of damage nucleation and growth in metals [Germann 2005], 5) physics of interfacial friction [Hammerberg 2004], 6) physics of Richtmyer-Meshkov and Rayleigh-Taylor [Kadau 2007b & 2010] instabilities, 7) physics of particulate ejection at shocked interfaces [Swaminarayan 2008], and 8) physics and chemistry of detonation in energetic materials, including homogeneous and inhomogeneous detonation, carbon clustering effects, and reactant/product equations of state [Cawkwell 2008, Heim 2008, Menikoff 2002, Zhang 2009].

All these areas of non-energetic and energetic materials have been addressed in the past three decades at Los Alamos by T and X Division staff in concert with developing computational platform advances and programmatic needs. The earliest NEMD simulations in fluids, solids, and shock-wave physics were carried out here as well as the first massively parallel Connection Machine simulations of shock-wave and interfacial phenomena, which were recognized with two ACM/IEEE Gordon Bell Prizes (for Performance in 1993 on the CM-5, and Price/Performance in 1998 on an Alpha/Linux cluster). High-rate materials deformation simulations using the LANL-developed SPaSM (Scalable Parallel Short-range Molecular dynamics) code, in support of the ASC Physics and Engineering Models (PEM) program, have been among the initial scientific applications run on both the LLNL BlueGene/L [Germann 2005; Kadau 2006; Germann 2008; de Supinski 2008] and LANL Roadrunner [Swaminarayan 2008; Germann 2009] platforms, becoming a finalist for the ACM/IEEE Gordon Bell Prize in both cases [Germann 2005; Swaminarayan 2008]. Areas where Laboratory advances in NEMD have had particular influence have been in the characterization of the development of substructure in shock loading and release in metals, kinetics of phase transformations, characterization of dislocation motion in metals [Zhou 1998] and the general methods for NEMD using Embedded Atom Method (EAM) and Modified EAM (MEAM) potentials for dynamic phenomena and multiphase equations of state. These have led to regular sessions and invited talks at American Physical Society meetings such as the Conference of the American Physical Society Topical Group on the Shock Compression of Condensed Matter (SCCM). LANL's leadership in this field is indisputable; Holian was elected President of the SCCM Topical Group, a position normally held by experimental shock physicists, and Germann is the scientific advisor for the May 2010 biennial international conference on New Models and Hydrocodes for Shock Wave Processes in Condensed Matter.

5.2.3 Energetic Materials. Our current performance and safety models are largely empirically based and heavily calibrated to experimental tests. Although HEs are very heterogeneous composite materials they are typically treated as homogeneous materials in continuum codes with homogenous temperature and stress distributions. Because initiation and safety phenomena are controlled by localized fluctuations, these models are not directly tied to our limited fundamental understanding and cannot be relied upon outside of their calibration regime. For safety considerations, there are a large number of accidental initiation scenarios that must be considered (manufacturing and processing, damage from dropping or insult, nearby flame or explosion, electrostatic discharge) such that we cannot confidently bound these readily by experiment where we have limited understanding of the inherent fluctuations in these scenarios. Development of improved models has been a major challenge for the current NNSA ASC program and has attracted growing interest from DoD as well. This is being addressed at the mesoscale level where the heterogeneous nature of the materials is explicitly represented. These typically include the crystalline explosive base (~100 micron crystals, typically quite brittle), a polymeric binder (may be present in submicron thicknesses, with highly temperature dependent viscoelastic properties), and voids of various sizes (both internal to the crystals and between the crystals and binder). Analytic evaluations indicate that voids are critical focusing agents that instigate ignition and that resulting "hot spots" of dimension ~0.1 micron are required for self-sustaining reaction. The experimental characterization of these materials over this range of length scales is just now becoming accessible. Characterization of the dynamic damage evolution processes is a current grand challenge. Many damage evolution models are based on the concept of fracture of the crystals by an initial wave, followed by frictional heating by sliding between those surfaces. Accurate modeling of the fracture, frictional heat generation, thermal conductivity, phase transitions (melting), chemical reaction and gas generation should be incorporated within a realistic geometry. This would require very large scale three-dimensional simulations with an accurate description of phenomena at interfaces. Current work is associated with two-dimensional simulations on model geometries as a means to prioritize the various aspects for further study. Accurate material properties over a broad range of temperature and pressures are also required, where we have limited data because of the inherent instability of materials.

Atomistic simulations can provide an explicit representation of these various phenomena and link them to chemical reactivity. However, these cannot reach realistic length scales required to characterize the microstructure and dynamic response. For example, electronic structure calculations on ensembles of hundreds of atoms are currently used to characterize the EOS of both the reactants and primary products. However, clusters of solid products (soot, metal oxides) are likely much larger and cannot be included in the analysis. Reactive molecular dynamics simulations can now be performed on many millions of atoms, which gives us a base understanding of the chemical reactions but is not sufficient to understand propagation or coupling to gradients in stress or composition. Non-reactive molecular dynamics on 100 million atoms (~1 micron^3) are being used to understand deformation processes and model the collapse of a single void, but are insufficient to understand in the interactions between multiple voids.

5.2.4 Biomolecular Modeling. Our implementation of embarrassingly-parallel molecular dynamics algorithms for enhanced sampling, and the development of more accurate force fields, have allowed the all-atom simulations of peptide and protein folding and aggregation from physical principles [Sanbonmatsu 2005 & 2007]. We have also shown how these simulations can be carried out under volume and pressure conditions consistent with the water-vapor coexistence curve. Currently we are expanding MD based approaches to systems beyond proteins (such as membranes, carbohydrates and aromatic polymers).

5.2.5 Accelerated Algorithms. Currently, the effort to develop and apply the AMD methods consists of a small, highly active group of two in T-1 and one from MST-8 funded from DOE Office of Science and LDRD sources. Impact has been substantial as can be seen in the large number of invited talks, teaching courses at international venues, and collaborations on outside proposals and in general. The AMD methods are also now starting to show up in standard molecular dynamics simulation packages, such as LAMMPS and DL_POLY. Impact on Los Alamos programs is growing especially for problems involving radiation damage annealing (e.g., [Bai 2010]) and evolution of post-shock plasticity. Neither process can be easily treated with molecular dynamics nor existing kinetic modeling methods.

5.3 Comparison with Peers

5.3.1 Nuclear Energy. Our present effort has a unique focus on studying length and time scale bridging issues pertinent to micro-structural features in nuclear fuels. Most peers address either atomic or mesoscale problems in a separated fashion.

5.3.2 Dynamic Materials. We have been the clear leader in this area, in part because high-rate materials deformation is primarily of relevance to nuclear and non-nuclear weapons issues, and because of the NNSA leadership position in high-performance computing platforms. For instance, MD modeling of shock compression was mainly a curiosity, with at most a handful of talks at the biennial APS SCCM conferences (Section 5.2.2) until a publication from Los Alamos appeared in *Science* [Holian 1998] and SCCM invited plenary talks were given by Holian in 1999 and 2001. Since then, national laboratories throughout the US (e.g. Bringa, Rudd, and Streitz at LLNL, Lane and Thompson at SNL), UK (Park at AWE), France (Maillet, Mazevet, and Soulard at CEA), and Russia (Dremov at VNIITF) have launched or greatly expanded similar efforts and awarded early and large amounts of cycles on flagship supercomputer platforms for MD shock and high-rate deformation simulations. In addition, ASC university partnerships such as the Predictive Science Academic Alliance Program (PSAAP) and its predecessor, the Academic Strategic Alliance Program (ASAP), have spawned related efforts at CalTech and Purdue. As a result, SCCM conferences have regularly had multiple invited talks, and a separate sorting category, for MD simulations to accommodate the large number of recent participants in this community.

5.3.3 Energetic Materials. Our primary competition is the LLNL effort, which is primarily funded through their ASC and DoD (JMP-MOU) program. Their work often highly complements our program. For EOS studies, they use similar atomistic Monte Carlo methods to formulate results, which they distribute to a large number of customers through the program Cheetah (and derivatives). However, they have a preference to reduce this data to a particular mathematical form (JWL EOS), which can obscure information concerning phase changes. They also have a program to calculate the EOS with atomic potentials on-the-fly embedded in their continuum codes. While likely accurate, it is time-consuming and precludes uncovering simple reduction rules (phase changes). LLNL does not emphasize large-scale classical MD for HE applications, but focuses more on the *ab initio* prediction of EOS and chemical reactions. This restricts the size of their simulations, but is more in line with understanding the EOS at higher pressures (ionizations, excited states) which HEs would not normally generate, but are important for NIF applications. SNL has a program similar to ours, but much smaller as their strategic emphasis is not on bulk HE properties.

The Army Research Laboratory is developing a large program similar to Los Alamos in terms of emphasis on large-scale quantum chemical and molecular dynamics simulations to service the DoD needs for munitions development. However, they do not have a coherent mesoscale effort, so there is a lack of focus on delivery of significant properties. Several other DoD laboratories also have small modeling programs at this length scale for particular materials of interest to them (e.g. White, NRL), but do not address the subject in a general way. There are several universities with expertise in HE MD (Goddard at CalTech, Sewell and Thompson at Missouri), with funding sources primarily based in the DoD. These programs normally do not have access to large-scale computing unless there is a collaboration with either Los Alamos or SNL.

5.3.4 Biomoleuclar Modeling. We are one of the world's leading groups on implementing all-atom molecular dynamics to study immunological and biofuel related problems. With respect to immunological problems, we are integrating MD simulations with sequence-based analysis for HIV vaccine design. With respect to biofuels, we are at the forefront on characterizing material properties of biomass that is predominantly carbohydrates. Recently we published a first replica exchange MD study on cellulose [Shen 2009].

5.3.5 Accelerated Algorithms. The AMD concept and methods were invented here and Los Alamos remains the undisputed world leader in AMD development and application. The most substantial AMD development efforts outside of Los Alamos are those of Fichthorn at Penn State, who develops hyperdynamics methodologies, and McCammon at UCSD, who develops an adaptation of hyperdynamics for biomolecular systems. The closely related AKMC approach discussed above is most strongly represented in the groups of Henkelman at University of Texas and Mousseau at University of Montreal.

5.4 Status of the Capabilities

5.4.1 Nuclear Energy. See section 5.2.1.

5.4.2 Dynamic Materials. See section 5.2.2.

5.4.3 Energetic Materials. See section 5.2.3.

5.4.4. Biomolecular Modeling. Our current challenges and accomplishments are directed at two fronts. First, how one extends some MD based methodologies that have successfully applied to proteins to other systems such as carbohydrates, aromatic polymers, membranes and nanomaterials. Here, we faced challenges with respect to force fields and conformational sampling, but have made significant advancements in carbohydrates. The second concerns how to characterize the interactions (molecular recognition) involving these different heterogeneous systems (eg. Membrane-carbohydrate, nanomaterial-protein interactions).

5.4.5 Accelerated Algorithms. The AMD methods have been demonstrated for a range of infrequent-event problems in materials science, chemistry and physics (see [Perez 2009]). Time scales of microseconds are now routine and time scales beyond seconds are possible in favorable cases. Two main technical challenges have been the size scaling problem (AMD has typically worked best for systems on the order of 1000 atoms or smaller) and the low-barrier problem. The low-barrier problem is more serious, and a general solution is being sought as discussed in Subsection 5.5.5. In some cases, an understanding of the characteristics of the system allows the low barriers to be ignored without compromising the accuracy. For example, this approach has been used in the parallel-replica dynamics study of hydrocarbon pyrolysis (in which the conformational transitions were ignored but bond-breaking transitions were respected) [Kum 2004], and in a demonstration of accelerated metallic surface dynamics at a solid-liquid interface (in which the ultra-fast transitions in the liquid were ignored) [Perez 2009]. Advances on the size-scale problem have included the development of a spatially parallelized version of the temperature accelerated dynamics method [Shim 2007] and the very recent development of a reformulated local hyperdynamics that can be used on arbitrarily large systems. This local hyperdynamics has been incorporated into the SPaSM spatially parallel MD code as part of the LDRD-DR project "Spatio-temporal frontiers of atomistic simulations in the petaflop computational world" (Germann, PI). All three AMD methods will continue to improve in range and power as they are developed further and more experience is gained. The parallel-replica dynamics method is especially well suited to the massively parallel future of computing. Recently, a version of the parallel-replica code ported to Roadrunner was used to study deformation of metallic nanowires on the millisecond time scale. For small systems (e.g., 1000 atoms) in which the state-to-state transitions are less frequent than roughly once per 10 nanoseconds this code is capable of achieving more than a microsecond of simulation time per minute of wall-clock time.

5.5 Challenges and Issues

Challenges and issues common to all themes are covered in Section 8.0.

5.5.1 Nuclear Energy. Although atomistic simulation is poised to make significant contributions to the multiscale, multiphysics approach of materials performance predictions, technical challenges still exist, e.g, pair potentials for relevant many relevant materials do not exist or are limited in their predictive power. Although it is possible to consider bulk phenomena for several metal fuel compositions via DFT there is a limitation in the number of atoms that can be simulated thus preventing the consideration of relevant microstructural features via DFT. There is also room for improvement in the DFT treatment for many of the actinide materials relevant for nuclear fuel applications. Charge transfer potentials that can capture valence variability of many systems (and will also permit the consideration of metal/oxide interfaces) are also under development. Additionally, new approaches to bridging time and length scales are always being developed. A particular technical challenge that might be addressed by improved simulation techniques going forward will be the improved description of radiation effects in fuels modeling. We foresee that radiation effects will be included at the mesoscale predominantly via the concentration of multidimensional defects (including points defects from radiation damage, fission products in solution, secondary fission product phases, dislocations, evolved microstructure and bubbles) and the role of these defects on thermal and mass transport.

5.5.2 Material Dynamics. The future of NEMD simulations and their impact on the fundamental understanding of dynamic phenomena in fluids and solids can be grossly characterized under the rubrics of *bigger, faster, smarter.* The current limitations in size and time scales are micron sizes for ns time scales now standard algorithmic implementations of NEMD. Over the next ten years one can reasonably expect an order of magnitude increase in both due to platform enhancement. However, scales of interest for truly predictive model development are 10-100 micron length scales and microsecond time scales to understand phenomena such as plastic deformation, strain localization, shock phenomena in heterogeneous explosives, kinetics of phase transformation, and the evolution of interfacial phenomena. This is the multiscale or mesoscale barrier that must be surmounted for true prediction in dynamic materials theory. In the context of NEMD, our research is addressing the final rubric via development of accelerated methods of NEMD with the potential of increasing the temporal range by three to six orders of magnitude. Such methods, already showing promise in damage nucleation and localization, will be frontier areas in NEMD research and dynamic materials modeling in the future. A key challenge has been retaining a critical mass in this area, a problem exacerbated by retirements (Holian, Lomdahl) and departures or extended leaves of early and mid-career staff (Kadau, Strachan, Sewell) that were active in this area and related energetic materials MD simulation-based studies. Support from LDRD and BES programs, including an Energy Frontier Research Center on "Materials at Irradiation and Mechanical Extremes" has ameliorated this issue, enabling the conversion of postdocs to staff such as Cawkwell, Liu, Perez, Taylor, and Wang, and recruitment of several new postdocs.

5.5.3 Energetic Materials. The core technical challenge here is to couple extensive chemical reactions and hydrodynamics in an inhomogeneous system. The length scales of these phenomena overlap so they cannot be decoupled but must be treated as an integrated whole. Further, this happens in a condensed phase system at high temperatures and pressures where we have limited capability to probe the system or maintain steady-state conditions. Consequently, we must rely extensively on calculations to supply the information that cannot be obtained from experiment, which requires well-validated models that can be linked across length and timescales. Atomistic simulations can provide strong guidance, and are certainly the only way to obtain an explicit representation of chemical reactivity, but cannot yet reach realistic length scales required to characterize the microstructure. The accurate coupling between chemistry and microstructure of these materials is critical for the development of predictive models. Current reactive molecular dynamics simulations are limited to nanosecond timescales for millions of atoms using classical interatomic potentials. The reaction zones for high-order detonation processes (the faster possible reaction rates) are estimated to be 10-100 microns in linear extent and 1-10 nanoseconds in temporal evolution. It is to be emphasized that there are strong pressure and temperature gradients in the profiles as well, so analysis of a static box supplies insufficient information. It is the location of the sonic plane in this dynamic structure that controls detonation propagation characteristics known to depend on confinement and initial temperature. Additionally, the interaction of this wave with chemical fluctuations, interfaces and voids are unknown, but suspected to play significant roles in refined models. Such simulations would require ~10 micron^3 of material or ~10^{12} atoms observed for time periods in excess of 10 nanoseconds. Initiation and deflagration processes extend out several orders of magnitude larger in both length and time scales. Non-reactive molecular dynamics can extend these scales out an order of magnitude or two in both space (>100 micron^3) and time (>1 microsec). Those simulations can resolve the mechanical effects for multiple voids, stress waves propagating across binder layers, and crack propagation at moderate strain-rates. This information will resolve many issues that are inadequately addressed in current mesoscale models because of limited ability to characterize interfacial phenomena. These results will be needed to provide stronger closure relationships for those models.

There has been significant progress in the last several years in the scale of calculations accessible. In particular, SPaSM and LAMMPS have been adapted to many high performance platforms, and the Reax Force Field has been implemented into LAMMPS. Simulations on millions of atoms are now commonplace, simulations on billions of atoms are not unusual, and simulations on trillion atom systems will likely soon be feasible as we approach exascale computing. Billion atom systems correspond to roughly a cubic micron of material so that a realistic representation of macroscopic phenomena (void collapse, shear bands, grain boundaries) is achievable. This has been the major focus of our program. Future emphasis should be placed on improving accuracy (and complexity) of non-reactive atomic potential functions (adding polarization functions, allowing adjustable charges), understanding sensitivity of the results to input potential functions and geometries, and quantifying the uncertainties of the results of the models and comparison to experiment. The reactive potential functions present a much more complex fitting/optimization challenge, where there will be some obvious limitations in representing spin interactions (singlet-triplet separations) within a classical ensemble. Semi-quantum approaches (tight-binding) may become competitive if higher levels of accuracy are required. Because of the high frequency vibrational modes in these light element systems, purely classical mechanics incurs a significant error (especially with respect to temperature for $T < 1500K$), and semi-classical approaches for correcting this need to be further developed and included [Kendrick, Wyatt]. Finally, the scale of the simulations here (>billions of atoms) requires more sophisticated techniques for the extraction of data from the simulations. Storage of all of the data from such simulations is neither feasible nor desirable, so learning methods that identify, classify and reduce the significant features during the simulations need to be developed. This is particularly critical for the accurate evaluation of the dynamics and thermodynamic properties of the physical processes. Comparisons of multiple simulations for sensitivity analysis and uncertainty quantification will require a similar format of metrics to be established that can be identified and counted during the complete dynamics run.

5.5.4 Biomolecular Modeling. In the past, we utilized all-atom MD simulations to provide microscopic details of the folding and to map-out the free energy landscape that governs folding of small proteins and individual secondary structural motifs such as short helices, β-hairpins and β-turns. One major challenge is the extension of all-atom MD based to larger, medically and biologically relevant biomolecular systems. Currently we are facing size and time scale limitations on these systems.

5.5.5 Accelerated Algorithms. The main challenge here is the so-called "low-barrier" problem. In many realistic systems, there is a mix of low barriers and high barriers. Reaching the time scale of the high barriers may be important for the problem under study, but frequent transitions over the low barriers limit the computational speedup that can be achieved. In fact, this is a very general problem in kinetic simulations, plaguing adaptive kinetic Monte Carlo and regular kinetic Monte Carlo as well. Thus, a substantial part of the AMD development effort here is currently directed at making progress on this problem. Various attacks are being pursued, but one main theme is development of methods for on-the-fly recognition of sets of states that can be grouped into Markovian superstates.

6.0 Theme 5: Discrete Event Simulation

(Theme Leader: Stephen Eidenbenz, CCS Division)

Discrete event simulation (DES) is a simulation technique that uses discrete events as a main driving force to simulate the evolution of a complex system. The notion of DES and most of the theoretical underpinnings were established in the 1970s and 80s. DES is used predominantly for engineered systems that follow a set of prescribed rules, such as the Internet and communication networks, vehicular transportation networks with discrete traffic light logic, epidemic modeling, or war games simulation. Any other process with discrete events can and has been modeled using DES, most notably biological and chemical processes. Discrete event simulations also play a role in composite systems where physical systems interact with social systems, such as modeling global warming. The physical processes of greenhouse gas generation, atmospheric mixing, oceanic interactions, and terrestrial uptake are relatively well understood. However, social processes such as agriculture, land use, electric power generation, transportation systems, and economic choices at multiple social levels affect the production of greenhouse gases but are much less well understood than physical processes. Agents attempt to approximate the perceptions and decisions of humans despite the acknowledged difficulty in predicting human behavior.

Distributed discrete event simulation (DDES) simulates processes on a complex system on multiple processors through separate threads, called logical process (or LP); DDES presents the designer with a set of challenging problems, in particular synchronization and load balancing. While the theoretical underpinnings are largely established (despite a few very recent attempts to awaken this dormant field), many real-life engineering challenges remain to fully exploit the potential of DDES in many application areas. We focus mainly on concrete application codes in this section; for a general introduction to discrete event simulation, refer to [Banks et al, 2004]. Perhaps the best-known early example of a discrete event simulation project at Los Alamos is the TRANSIMS project, which simulated vehicular traffic using a discrete automata model starting in the mid 1990s. A large number of DDES codes have since been developed here and can be grouped into 1) Technical Domain Applications, 2) Agent-based applications, and 3) Simulation and Design Frameworks. Following, we present a few example codes for each.

Technical domains. The FastTrans project, which simulates vehicular traffic on a nationwide level, grew out of the legacy of the TRANSIMS transportation simulation code. The telecommunications simulation code MIITS (Multi-scale Integrated Information and Telecommunications System) has been used to simulate the nation's communication fabric. BotSim is a specialized tool designed to understand the cyber threat of botnets (i.e., rogue networks of compromised computers that can start cyber attacks). A final example is CyberSim, which simulates the spread of malware through technical and online social networks.

Agent-based applications. These codes focus on simulating the actions and thought processes of agents such as humans. EpiSims code simulates the spread of an epidemic, such as H1N1 through a population of millions of human agents who go about their daily activities. AFS (Agent Framework for Simulation) simulates the complex processes of an intelligent agent, such as a dam operator. ActivitySim generates activities for a population of millions of humans (which can be used by EpiSims) based on optimizing an objective function.

Simulation and design frameworks. Any discrete event simulation code relies on a simulation engine that it either implements as part of the code or calls as subroutines. A few such codes exist; SimCore is the simulation framework in use at Los Alamos.

6.1 Connection to the Goals and Mission of the Laboratory

DES is a key component in the predictive science objective of Los Alamos' IS&T thrust. A Laboratory goal is to leverage our science and technology advantage to anticipate, counter, and defeat global threats and meet national priorities; the range of applications is broad.

6.1.1 FastTrans. Large-scale simulations are an important tool in the emerging field of infrastructure modeling, where simulating the behavior of millions of entities and their interactions with various interdependent infrastructure networks (like transportation, communication, electric power) demand significant computational resources. Here, FastTrans is one of the key modules in a suite of simulators that have been used to provide detailed analysis to the DHS for quick turn-around "what-if" scenario simulations.

6.1.2 MIITS: Multi-scale Integrated Information and Telecommunications System. MIITS is a SimCore-based DES application that aims to simulate the world's communication fabric to packet-level detail if necessary. MIITS is a scalable, end-to-end simulation environment for representing and analyzing extremely large, complex communication networks of any type, including cellular networks, public switched telephone networks (PSTNs), the Internet, and ad hoc mesh networks. MIITS offers network representation in several resolutions, ranging from packet-level simulation to flow-based approaches.

6.1.3 BotSim. Cybersecurity is of both immediate and long-term concern to the nation and Los Alamos. One of our goals is to develop modeling and simulation tools to quantify the effects of large-scale cyber-security incidents. Botnets have emerged as one of the most severe cyber-threats in recent years. To evade detection and improve resistance against countermeasures, botnets have evolved from the first generation that relies on IRC chat channels to deliver commands to the current generation that uses highly resilient P2P (Peer-to-Peer) protocols to spread their C&C (Command and Control) information. We developed a high-fidelity simulation tool called BotSim to understand behaviors of P2P-based botnets.

6.1.4 CyberSim: Malware Propagation on Online Social Networks. The wide spread acceptance of the Internet by the masses has made the international community ever more interconnected and dependent; we are now more than ever a knowledge-based society. Along with this, there has been a growing realization in the knowledge and information security sciences communities of the important challenges posed by cyber-infractions into a country's strategic security envelope. Los Alamos is in an unique position of technical capability and responsibility in providing and maintaining a set of tools for analyzing the impact of cyber-security loopholes and vulnerabilities as soon as they are recognized. CyberSim has been developed in response to the IS&T grand challenge at the Laboratory and provides the capability to model malware propagation in online social networks.

6.1.5 EpiSims. Protecting the nation against emerging and re-emerging infectious diseases directly supports the Laboratory's Global Security mission, the Information Science & Technology pillar, and the Bio-Security initiative.

6.1.6 The Agent Framework for Simulation (AFS). Many Los Alamos missions require the investigation not only of physical systems, but the embedded interaction of human individuals with various components of the physical system. Many examples exist that demonstrate that human choices have a strong, if not determining, effect on the behavior of the joint human-physical system. Global climate is believed by most scientists to be influenced by human behavior over the last century. People make choices based on their values, perception of the environment, internal goals, and desires. AFS provides mechanisms to model these elements and investigate the properties of mixed human and physical systems.

6.1.7 ActivitySim. The DHS aims to model, simulate and analyze critical infrastructure and their interdependencies across multiple sectors such as electric power, telecommunications, water distribution, transportation, etc. Most infrastructure sectors rely on an underlying network that gets used by individual people and business entities. Alternatively speaking, there is a demand for service the network supplies. This demand is largely generated by people's daily activities, driving to work, using energy to cook or heat, using water and sewage systems, making phone calls, etc. Thus, an accurate model for daily activities of individuals is a pre-requisite for a simulation of demand. An agent-based approach is the only modeling paradigm that allows us to generate demand shocks as an emergent property of the simulation. Demand can vary from a normal day to emergency scenarios. ActivitySim is part of the NISAC portfolio of large-scale detailed infrastructure models. This work contributes to the Global Security mission for the impact of natural events on regions and societies and is part of the IS&T capability.

6.1.8 Simulation Framework, SimCore. SimCore is a scalable simulation engine coupled with a modeling philosophy expressed in base classes of entities, services, and information. It is an enabling technology for most of the DDES codes mentioned above.

6.2 Research Breadth and Impact

6.2.1 FastTrans. FastTrans is a scalable, parallel microsimulator for transportation networks that can simulate and route tens of millions of vehicles on real-world road networks in a fraction of real time. FastTrans uses parallel discrete-event simulation techniques and distributed-memory algorithms to scale simulations to over one thousand compute nodes. Vehicular trips are generated using agent-based simulations that provide realistic, daily activity schedules for a synthetic population of millions of intelligent agents. Utilizing a queue-based approach to road network modeling, which been shown to be significantly faster than traditional approaches based on cellular automata models, FastTrans can execute simulations of large cities up to 20 times faster than real time, while at the same time capturing road link and intersection dynamics with high fidelity. The routing algorithm, which is the most computationally intensive part of FastTrans is a heuristic search variant of the classic Dijkstra shortest-path algorithm (A*). FastTrans uses a highly optimized version of A* that uses the structural properties of the road network and

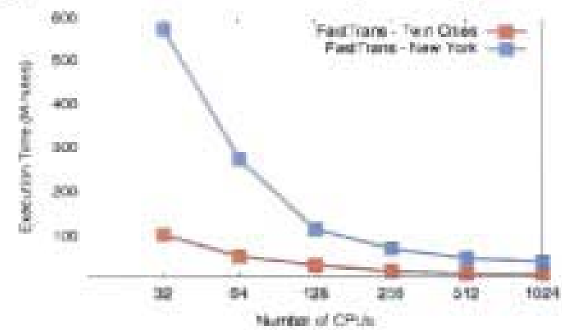
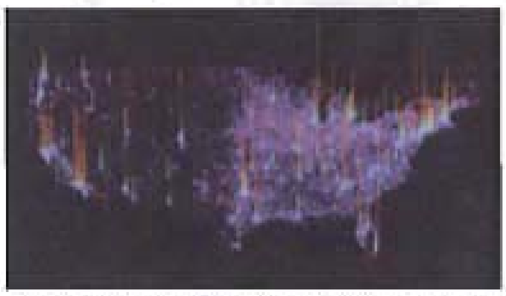


Figure 2. Performance scaling with increasing cluster sizes has been encouraging

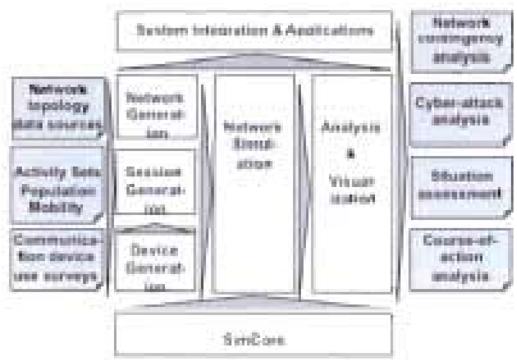
performs a goal directed search to find the best path toward the destination. Experimental results have shown up to 30-fold improvements in routing performance compared to naive implementations of shortest path algorithms.

FastTrans is also able to achieve near-perfect load-balancing on distributed clusters, through an optimal assignment of simulation entities to processors through a technique called explicit spatial scattering [Thulasidasan 2010]. With optimized routing and partitioning, FastTrans is able to simulate a full 24-hour work-day in New York – involving over one million road links and approximately 25 million vehicular trips – in less than one hour of wall-clock time on a 512-node cluster. The quick turn-around capability of FastTrans has been employed in numerous NISAC transportation studies that simulated and analyzed infrastructure disruption studies in New York and Southern California. FastTrans is also currently being used for detailed road asset ranking at a national scale.

6.2.2 MIITS. At one end of the spectrum, MIITS constructs detailed representations of network loads based on individual device usage and real survey data. At the other end, MIITS employs multiple abstraction levels for network protocol stack simulations paired with powerful distributed discrete-event simulation technology to achieve scalability. MIITS has been developed to fill the technology gap that exists in methods for design, analysis, and development of current and future large-scale communication networks and infrastructure-interdependency-aware simulation and analysis tools for wireless and wire-line networks.



In this plot of the aggregate call volumes at each of the roughly 25 000 public switched telephone network wire centers in CONUS, each wire center is represented by a vertical bar whose height denotes the call volume. The top 100 wire centers are shown in orange, the remaining wire centers in purple.



MIITS' modular architecture (white boxes) allows for efficient extensions by other network types. MIITS takes detailed population data as key input, supplemented by various network topology and communication device use surveys (left grey boxes). MIITS' output is a set of analyses (right grey boxes).

Figure 3. MIITS has a modular structure that is shown in the right panel of the figure above (taken from [Waupotitsch 2006]). The left panel shows an example simulation result for a Public Switched Telephone Network (PSTN) model (CONUS is CONtinental United States).

The MIITS sub-module Network Generation creates a realistic model of network infrastructures such as PSTN switches or Internet routers. MIITS receives demographic, mobility, and device ownership information for individuals in a synthetic population as input data. The Device Generation sub-module creates end-devices (e.g., desktop computers, phones) for the population. The Session Generation sub-module creates sessions (e.g. calls, e-mails) between individuals of the population. Synthesizing the outputs from those sub-modules, the Network Simulation sub-module simulates the time-dependent load in the network with a user-defined abstraction level. Individual MIITS sub-modules are implemented as a SimCore applications, which guarantees scalability through use of state-of-the art distributed discrete event simulation technology. SimCore provides the distributed discrete-event simulation engine that the other sub-modules rely upon and the System Integration & Applications sub-module prepares the output analyses with the help of the Analysis & Visualization sub-module. MIITS's modular design provides the following advantages.

- Directly interoperable with other infrastructure simulations built on SimCore technology (such as ActivitySim, FastTrans, DemandSim) as well as through Hydra web services with other NISAC tools (IEISS, TransOpt, AFS), permitting interdependency-analysis studies, such as the effects of a power outage on communication networks.
- Designed to scale to 1 billion nodes in the long term. It is also designed for technological scaling.
- Accommodates new types of networks, such as novel wireless ad hoc mesh networks, sensor networks, or Wi-Fi hotspots accurately and efficiently.
- Can be used to evaluate federal policies on the use and operation of communication network infrastructures, especially regarding the potential effects of the policies on national security.
- Designed to discover and respond to communication network vulnerabilities through its contingency analysis and its cyber-attack analysis features.

6.2.3 BotSim. BotSim, a distributed event-driven botnet simulator, can be used to explore the strategy space of both the attacker and the defender for P2P-based botnets. Using large-scale simulation to understand the behaviors of botnets has a few advantages. First, due to the destructive nature of such botnets, implementing them in the real world may lead to ethical or legal issues. A simulation testbed eliminates such a concern. On the other hand, a large-scale botnet often has hundreds of thousands of compromised machines, or even millions of them, which renders it costly to study them on a real testbed.

6.2.4 CyberSim. The CyberSim suite consists of a high performance distributed discrete event simulation engine built on top of the proven scalable SimCore framework and along with a small set of pre- and post-processing code. Malware spreads through a computer network by simultaneously exploiting software vulnerabilities on individual machines and utilizing some social network's small diameter community structures.

Figure 4. An example of the geographic spread of a malware propagated through online social networks after a few days.

The CyberSim suite is capable of generating realistic social networks from of a database of networked geo-coordinated physical devices such that they conform to widely adopted power-law behaviors and demonstrate geographical sub-community clusters. These social networks are used to closely model real life social networks arising out of personal and business email contact lists and online communities such as Twitter, Facebook, and LinkedIn. Each physical device on the network can be thought of as a computer that is further endowed with a list of installed operating systems (Windows, Mac, Linux etc), application software (Microsoft Office, OpenOffice.org etc), email clients and web browsers. The suite is further capable of online parsing and retrieving software vulnerabilities that are routinely published by reliable sources such as the National Vulnerability Database (http://nvd.nist.gov/) maintained by the National Institute of Standards and Technology (NIST) for the DHS National Cyber Security Division. The user can chose an initial set of source devices in the network where the exploit for a particular software vulnerability originates. The DES engine then simulates the spread over the social network of the malware, which exploits that specific vulnerability. Network packet delays and user online behavior are modeled using either a simple probabilistic Poisson process model or more complicated specific behavior. The tool is furthermore loosely integrated with a post processing code producing a Google Earth based visualization that shows the time evolution of the malware spread, its severity, the businesses likely to be affected the most, etc., to the analyst. The tool is flexible enough to allow the analyst to tweak various social network parameters such as the probability of location based clustering and scale free nature of the interconnections arising as a consequence of the power-law nature of the network's node degree distribution. It also allows the modeling of inter- and intra-organizational interactions within various business sectors and categories based on their market share statistics. Using the CyberSim tool-set, we have been able to analyze the geographical spreading patterns, time evolution patterns as well as severity of impact on various business sectors for several commonly deployed vulnerable software such as email clients, browsers and office documentation software. The preliminary results of this research has been encouraging and we have been invited to present results in the Telecom, Web, Networks Track of the WinterSim 2010 Conference [Santhi 2010].

6.2.5 EpiSims. The highly structured Epidemic Simulation System (EpiSimS) is an agent-based discrete event simulation engine that explicitly represents every person in a city or region and every place therein where people interact [Eubank 2004; Barret 2005; Stroud 2007; DelValle 2007; Mniszewski 2008a; Mniszewski 2008b]. The synthetic population consisting of 265,796,301 individuals residing in households in the contiguous US are simulated. The nationwide population can be divided into parts (e.g., states or regions) to make the simulation manageable. Each individual in the simulation is instantiated according to actual demographic distribution drawn from the 2000 census data. The business directory database, Dunn & Bradstreet[1], provides business addresses, industry classification, and number of employees, so that businesses can be assigned to locations. EpiSimS models each business as a separate location. Each individual in the simulation is assigned a schedule of activities to undertake throughout the day. Each individual's schedule specifies the starting and ending time, type, and location of each assigned activity. There are seven types of activity: home, work, shopping, visiting, social recreation, school, and college; plus a activity designated other. Information about the time, duration, and location of activities is obtained from the National Household Transportation Survey[2]. From these three components, EpiSimS computes which individuals are together at the same location at the same time and can therefore simulate disease spread through a population. EpiSimS can simulate disease spread, school closures, and workforce absenteeism at a sufficient fidelity to capture geospatially varying demographic characteristics, travel patterns of individuals, and transmission opportunities through household, work, school, social, and casual contacts. EpiSimS has been used to analyze the impact of disease spread for different diseases

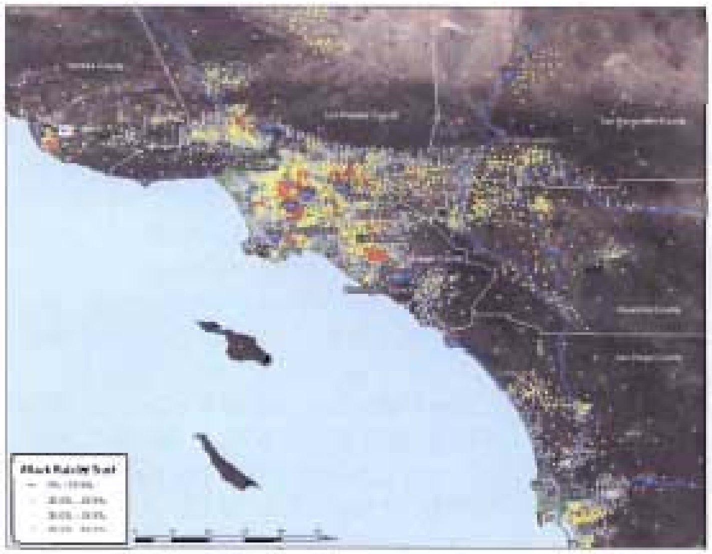
[1] http://www.dnb.com/us

[2] U.S. Department of Transportation, Bureau of of Transportation Statistics, NHTS 2001 Highlights Report BTS03-05, Washington, DC (2003).

including smallpox and influenza and to analyze the social network that emerges from the synthetic population.

Smallpox. EpiSimS has been used to model the potential impact of the spread of smallpox and mitigation strategies such as mass versus targeted vaccination [Eubank 2004; Barret 2005]. The results showed that the speed with which people withdrew to their homes or were isolated by health officials was the strongest determinant of the outbreak's extent. The second most influential factor was the length of delay in officials' response.

Influenza A (H5N1). In response to limited outbreaks of influenza A (H5N1) and its potential to generate a pandemic of catastrophic proportions, EpiSimS was used to assess the magnitude of impacts of pandemic on the US population [Stroud 2007, Mniszewski 2008]. Results demonstrate that the attack rate (percentage of population infected) is strongly correlated with the average household size. In addition, temporary behavioral changes have the potential to generate waves of infection if they are relaxed before the pandemic dies out. Results from this study were used by the national Strategy for Pandemic Influenza Implementation Plan. An example visualization is shown in Figure 5.

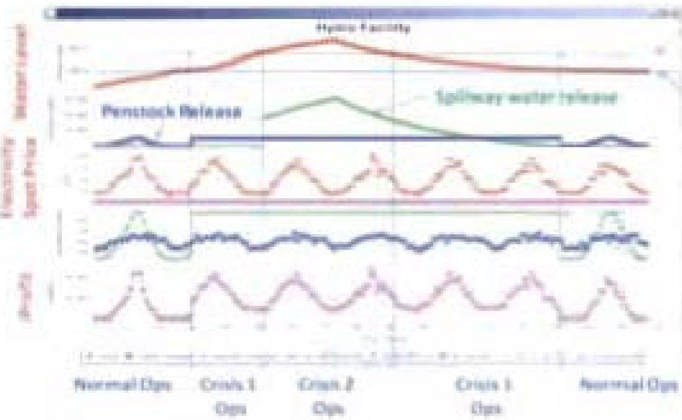


2009 Influenza A (H1N1). Most recently, in response to the appearance of a newly mutated 2009 influenza A (H1N1) virus in Mexico, EpiSimS was used to study the potential impacts that H1N1 and co-circulating strains would have on the US population [DelValle 2009 & 2010]. EpiSimS projected low workforce absenteeism due to disease characteristics. Although EpiSimS assume uniform infectivity across all ages, the simulation showed that school-age children were more likely to become infected and spread H1N1. Results from this study were briefed to high-level officials and were used for planning purposes.

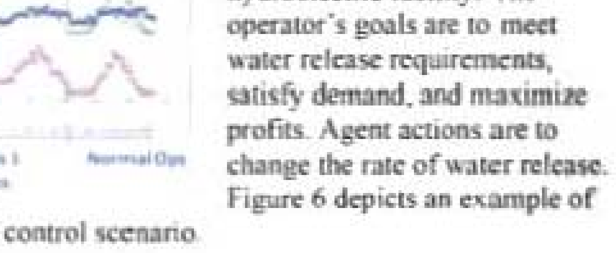
6.2.6 AFS. AFS is a Java software framework that promotes the development of agent-based simulations using components. Agents are software entities that can operate autonomously, perceive the environment, and map perceptions into actions. The framework includes a discrete event engine and a set of standard components to reduce development time and improve software reliability. There are many different types of agents as well as many applications in which they are used. The AFS supports the building of agent-based simulations for almost any agent type. This provides a uniform development platform that can support a wide variety of applications. In AFS, a simulation is a component that contains a scheduler to sort and execute events and an optional virtual environment. Simulation objects and agents are components normally found in the virtual environment. Simulation entities are elements in the simulation that interact. SimObject is a class that can post simulation events. Agents are SimObjects that can reason on their perceptions of the virtual environment. Agents reason by using Cognitors, a class of components that allows the application developer to specify agent behavior. Cognitors can be based on a variety of approaches, from simple rule sets to arbitrarily complex algorithms. Cognitors can implement existing architectures such as InterRap (integrated reaction and planning [Muller 1996]). This architecture has three layers of increasingly complex cognitive capabilities.

- Behavior-based Layer: agents recognize and respond to situations using programmed behavior patterns. This reactive mechanism provides substantial capability for an agent.
- Local Planning Level: enables simple means-ends planning when the reactive mechanism fails to match goals to actions.
- Strategic Planning Level: the agent attempts to account for the actions of other agents in creating plans to achieve its own goals.

An Agent Communication Language (ACL) can enable agents to exchange information by using a special information class, Performative. A performative is a literal that maps to specific agent actions, much like a command. An agent receiving a performative will normally execute the associated action. A rich ACL allows more general exchange of information among agents, potentially including goals, plans, and motivational state, enabling sophisticated agent behavior.



AFS is used to model decision-making entities in a variety of environments. One example is the Hydro Operator, which models the decisions of a dam operator in charge of a hydroelectric facility. The operator's goals are to meet water release requirements, satisfy demand, and maximize profits. Agent actions are to change the rate of water release. Figure 6 depicts an example of the Hydro Operator responding to a flood control scenario.



In the Global Pandemic application, AFS agents represent public health decision makers for a nation. Their role is to develop a pandemic response strategy and implement it if a pandemic is detected. The strategy is constrained by available national resources and influenced by the relative costs and availability of mitigation measures. Agent actions include creating a pandemic strategy, developing a pre-pandemic stockpile, and implementing the strategy when a pandemic is detected. Figure 7 depicts the modeled spread of pandemic influenza. The radius of the circle is representative of the number of people with influenza in the host nation. This application represents a global framework, enabling the representation of assets in 220 nations. Multiple agents can be created for a nation, where each agent is responsible for a specific function; in this case the function is public health. Another application under development with AFS is a simulation of the US healthcare system, HCSim, for the DHS.

6.2.7 ActivitySim. ActivitySim is a parallel discrete event hybrid agent-based model of activity generation. Supporting functionality for choosing activity locations and activity execution operates concurrently. As a simulation, daily activity schedules for individual agents are generated based on their demographics and the utilities, priorities, and time constraints of a chosen set of activities. Traditional agent-based technology and numerical methods are combined. It has been developed as part of a larger effort to understand the interdependencies among national infrastructure networks and their demand profiles that emerge in baseline and emergency scenarios. It operates both as a standalone model for population analysis and can be coupled with other infrastructure models.

ActivitySim is an object-oriented scalable simulation tool that relies on a synthetic, but statistically accurate population of the US that was obtained using disaggregation methods applied to US census data. ActivitySim is a member of a family of simulation applications that follow the SimCore modeling paradigm. SimCore is a library for building large-scale distributed-memory, DES using the open-source discrete event engine from the Parallel Real-time Immersive Modeling Environment (PRIME) for passing events, event queue maintenance, and synchronization. It is composed of Entities (an object or component in the system that we want to model), Services (functionality or behavior of an Entity), and Infos (an event exchanged between Entities or Services). ActivitySim's architecture includes the "reactive agent" extension to SimCore called AgentCore with additional Entity capabilities to perceive, think and act and process patterns of behavior or production rules. Persons, Locations, Households, and Zones comprise the entity types used to represent a model of a geographical area. A Person is also an agent that reasons about daily activity schedules. State (current activity and location), demographics, activity location choices, and a current schedule are all part of a Person. A Location tracks Persons as they participate in its activities. A Household is associated with a Location, has aggregated income, and members. A Zone is an aggregation of Locations used when selecting where a given activity will take place. Each Person-Agent is assigned an activity set composed of a subset of activities available within a model based on demographic attributes (age, gender). Each activity has an associated utility function (sigmoid) that gives a certain amount of utility depending on how long the activity is being executed. An activity also has a priority function (sigmoid), where the priority of an activity increases with the time that has passed since the activity was last executed. Activities have constraints that guide when they can be scheduled and their duration. An activity can be tuned through its utility and priority function parameters and a weekend factor to suggest regularity (attending work/school on weekdays, shopping once a week). An activity set can be very specific (e.g., sleep, personal care, lunch, dinner, leisure) or more general (e.g., home, work, school, shopping, social recreation, daycare). A Person's schedule consists of a sequence of these activities with start time, activity, location, and duration. Each Person reevaluates and modifies their activity schedule as required and plans new activities in advance. This is accomplished by pre-calculated schedules, randomly generated activities, or a more sophisticated utility-based approach using a meta-heuristic and optimization. The utility-driven approach to planning and re-planning scheduled activities consists of an optimization loop composed of the following: 1) a meta-heuristic (local improvement, gradient method) that assembles and modifies scheduled activities based on priorities and constraints; 2) an objective function (a weighted sum of utility, priority, and travel contributions) used to evaluate a suggested schedule for replacement; and 3) an exit condition (number of iterations, when an improved schedule is found). An agent chooses "favorite locations" for their activities relative to base locations such as home and work/school. This involves assembling a distributed network of Zones or aggregated sets of Locations with attractors per activity (number of employees). The base Zone or a close Zone is first chosen based on sampling from the distribution of aggregated attractors for that activity. Then a location choice is made based on the Zone's Location attractors. ActivitySim has been used to simulate the daily activities of a Twin Cities, MN, synthetic population composed of 2.6 million individuals, with about 1 million households and more that 480 thousand different locations. The simulation was executed on Los Alamos' Coyote cluster and was run for ten simulated days. ActivitySim has been coupled with other models via activity execution events. For example, agents select their activity schedules in ActivitySim and travel between locations using the FastTrans transportation simulator or contribute to demand per service area or infrastructure through the coarse multi-infrastructure demand model, DemandSim.

6.2.8 SimCore. SimCore is a generic DES framework that provides an entity-service level interface on which specific simulation systems can be built. Its first application was an end-to-end packet routing simulation system, NetSim. However, in the meantime its versatility has been recognized and it is being considered in applications that are not Internet related. As of now, tools like ActivitySim, DemandSim, FastTrans, SessionSim and MIITS are all built on top of SimCore. SimCore isolates the implementation of simulation systems from the simulation engine details or logical processes (LPs). Simulations are implemented in terms of entities that receive packets, handle or service those packets, and send packets to other entities, where they are handled in a similar fashion. The details of the actual location of the receiving entity (on which LP, and on which CPU) are hidden from the implementation. This is facilitated by an API level specification of the interface based on a generic programming paradigm, and a generic data input mechanism that can be used for any combination of entities and services. The usage goals of SimCore are the following.

- Simulation of nationwide socio-technical infrastructure.
- Hundreds of millions of simulated elements (people, computers, etc.).
- Requires as-of-yet unknown approximation techniques of the elements and processes.
- Obtaining results that are meaningful and provide useful information.
- Limits approximation mentioned in previous bullet.
- Ease of combining simulations that were developed independently.
- Simulation of people generating phone calls, and simulation of phone infrastructure (combining the two allows feedback to session generation in case of overloaded network, for example.)

SimCore's goal is to provide basis for creating simulations of various socio-technical aspects, altering their functionality as the used models develop and combining the simulations into more complex ones. From the usage goals, we have identified several important design requirements for the SimCore library, listed here roughly in order of importance.

- Extensibility: adding new functionality is easy and does not require changing much of the existing code (changes are localized). For example, adding a new protocol to MIITS does not require changing the already existing code, which also means that removing an unused protocol is seamless.
- Expressive power: the library does not restrict the user to only certain constructs, the full power of C++ language and any library is available. This is important so that any

computation and simulated element interaction technique can be implemented if needed, even if it does not fit well into the SimCore design. Unknown approximation techniques may require unforeseen implementation steps.

- Conceptual simplicity: the places where the different components interact (like different MIITS protocols) should be well defined. This is important so that as it grows, it doesn't become an impenetrable jungle.
- Scalability: the library does not result in significantly higher memory usage or lower running speed, compared to when the simulation code is tailored to a particular application. In particular, it runs efficiently on parallel architectures.

There are relatively many DES tools and libraries already available but none that fulfills all four design requirements at the same time. SimCore is responsible for providing the user (an end simulation, such as MIITS) with concepts and tools for fulfilling the extensibility and conceptual simplicity design goals. The expressive power goal comes for free by SimCore being a library in C++ (as opposed to being a simulation definition language, which could be limiting in allowed constructs). It is not a DES engine, e.g. it is not directly responsible for passing events between computing nodes, event queue maintenance and synchronization. For this, SimCore uses an external software package. Currently, PRIME is used but any parallel distributed memory simulation engine would work. The scalability design goal is largely determined by the simulation engine used. SimCore simply tries to impose as little performance overhead as possible. The "library stack" is hierarchical, from top to bottom: End Simulation (e.g. MIITS), SimCore, Simulation Engine (e.g. Dassf), and Message Passing layer (MPI). Note that the end simulation is not supposed to interact with the simulation engine directly (let alone message passing layer), which makes them easily portable.

6.3 Comparison with Peers

6.3.1 FastTrans. Traditionally, traffic microsimulations of transportation networks have employed a time-stepped cellular-automata approach. A prominent example of this is TRANSIMS [Smith 1995], developed at Los Alamos, where vehicular dynamics are modeled at a high level of spatial granularity. This allows one to capture phenomena such as lane changing and vehicular emissions, but comes at a high computational cost. Other simulators using the microscopic simulation paradigm include CORSIM [Prevedouros 1999], VISSIM [Concepts 2001] and PARAMICS [Cameron 1996]. An alternative approach to traffic simulation, where road links are modeled as queues, was described in [Eissfeldt 2006]. A time-stepped, parallel implementation of this approach is described in [Cetin 2002]. [Charypar 2006] first proposed a discrete-event queue-based model for a sequential, single-processor environment. A parallel discrete-event approach to microsimulations was described in [Perumalla 2006], though the modeling paradigm employed here is conceptually closer to the cellular-automata approach. Experimental results presented here on a 1000-node grid network indicate speed-ups of up to 1000 over real-time. The FastTrans approach is to combine the discrete-event queue model with scalable parallelization. This allows us to simulate large-scale, real-world networks and realistic traffic scenarios involving tens of millions of vehicles in a fraction of real time. Also, since FastTrans simulates the behavior of each vehicle or traveler at the individual entity level, it retains some of the advantages of microsimulations. In addition, the congestion feature implemented in FastTrans, which updates the state of the routing graph on all simulation processes, allows one to observe the macroscopic behavior of the network.

6.3.2 MIITS. The multi-scale and integrated nature of MIITS is a unique property. MIITS has competitors in the commercial and the academic field. The tool of choice for most computer science and electrical engineering departments at the world's universities is the ns-2 simulator, which does not have a distributed feature and in turn leads to very limited scalability. The follow-on ns-3 simulator has limited distributed features, improved scalability, but as of today does not yet see a very large following. SFFNet is a fully scalable network simulator built at Dartmouth and later UIUC; it focuses on Internet traffic; the software philosophy of SSFNet is somewhat different from SimCore and it also does not cover the entire end-to-end range of traffic generation. In the commercial domain, the QualNet simulator (by Scalable Solutions, a UCLA spin-off) has a small but loyal following. QualNet scales better than ns-2, though not as well as SSFNet of MIITS and is a stand-alone tool that does not integrate well with other simulator tools. OPNET is a successful tool used by industry to assess their small- to mid-size networks and is by far the most user-friendly of all tools (albeit it still does not offer real-time visualization). Scaling is limited to about 200 nodes for any realistic traffic volumes. Various smaller efforts exist that tend to address one of the classic shortcomings of network simulators, including GTNetS (good scalability), SwIM (good wireless channel models), pdns (parallel computing), and OMNet++ (good shared-memory scalability).

6.3.3 BotSim. We have not yet seen other work that attempts to model and simulate P2P botnets at such a high resolution as BotSim. Our work has been published at the IEEE/IFIP International Conference on Dependable Systems and Networks; another paper is currently under review.

6.3.4 CyberSim. Malware and vulnerabilities analysis is a relatively nascent subject; related concepts and technology are actively undergoing reviews and standardization efforts in the international peer community. In an attempt to standardize the naming conventions and to maintain an authoritative database of currently known exploits and fixes, the NIST is maintaining a public database of Common Vulnerabilities and Exposures (CVE). NIST also provides a somewhat limited online analysis tool. A rather comprehensive list of CVE analysis software and complementing exploit databases is maintained online by MITRE (http://www.cve.mitre.org/compatible/compatible.html). While these tools and databases are extremely valuable, the massively distributed discrete event design of CyberSim makes it extremely flexible while at the same time providing comprehensive and realistic analysis capabilities. For example, using CyberSim, we can statistically analyze the business sector impact and temporal swiftness of spread of an internet worm. We may analyze the dependence of the spread on the initial geographical distribution of the malware. We can also analyze the dependence of the spread on the inter-connectivity of personal and work related social networks. To our knowledge, CyberSim is unique in providing this kind of capability.

6.3.5 EpiSims. There are several research teams including [German 2006], [Ferguson 2005], [Longini 2004], [Lee 2008]. However, most teams use community-based simulation systems and/or individual-based simulations with small populations. We have the only model in the world that includes high fidelity, second-by-second activities, and simulates large regions.

6.3.6 AFS. There are roughly 25 commercial and 40 academic agent development frameworks ranging in capability from simple to highly specialized. Some notable packages include Star Logo, MASON, Swarm, and Repast. AFS is comparable in functionality to all of these, although it could use additional development in ontology support, planning, and learning. The existing AFS functionality is sufficient for all but the most demanding applications. Further, AFS can be used in high performance computing environments. AgentCore is a C++ port of AFS that executes under the SimCore high performance simulation library.

6.3.7 ActivitySim. A model of dynamic demand that generates realistic data is an open research area. TranSims activity generation creates static ground-hog day household schedules based on the National Household Transportation Survey and US Census data [Barrett 2004]. ActivitySim builds and extends the utility-driven approach to activity scheduling by [Joh 2001] with the addition of a priority function, objective function, and compound operators. Charypar and Nagel use a genetic algorithm approach to create and modify all-day activity plans and utility/priority functions and a fitness function (similar to ActivitySim's objective function) for evaluation [Charypar 2005]. Bhat et. al. (University of Texas) employs econometric models for activity patterns of adults only at the household and individual level in CEMDAP [Baht 2004]. Feil et. al. (Swiss Federal Institute of Technology) generates activity schedules in PlanotmatX using Tabu search, utility and fitness functions (similar to ActivitySim), with the addition of recycling schedules [Feil 2009]. ActivitySim additionally schedules activity-by-activity drawn from a set based on an agent's demographics, whereas the previous three work with sequences of activities as tours or patterns. Multi-day activity scheduling and re-scheduling is a compute-intensive process for those models that are capable.

6.3.8 SimCore. In terms of simulation engines, a few alternatives exist. The venerable DaSSF and its successor PrimeSSF implementations of the scalable simulation framework still can be used as the basis of SimCore, though we have replaced their functionality by a series of direct MPI calls for some of the clusters at Los Alamos. SimCore is more than just a simulation engine, though as it includes a modeling philosophy expressed through the base classes of entities, services, and info. Frameworks with such philosophies exist mostly in the very specific agent-based design world (for a listing of such frameworks refer to the AFS Section 6.3.6).

6.4 Status of the Capabilities

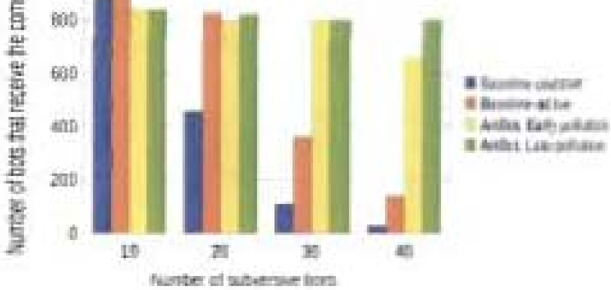
6.4.1 FastTrans. Currently FastTrans is capable of simulating regional transportation networks including mass-transit networks involving multiple states in the US faster than real-time. Future capability augmentations include hierarchical routing for whole-nation studies, and multi-scale simulations on hybrid architectures. We have published modeling and scaling results for FastTrans at various venues [Thulasidasan 2009a, 2009b, & 2010].

6.4.2 MIITS. MIITS has been used in the Tier asset ranking studies as part of the NISAC program since 2005 for PSTN assets and since 2008 for Internet assets. MIITS is routinely used in the FastResponse cycle to respond to all major threats including hurricanes, wild fires, and earthquakes. Open literature versions of MIITS results include a description and overview results of the PSTN ranking methodology [Ramaswamy 2007] and the Internet ranking methodology [Yan 2009]. MIITS contains a large number of scripts that make it usable for an intermediate user, albeit it is still a command-line tool.

6.4.3 BotSim. To understand the behaviors of P2P-based Botnets, we developed a distributed high-fidelity P2P botnet simulator that uses the actual implementation code of aMule, a popular P2P client. aMule implements the KAD protocol, which is a variant of the original

Kademlia protocol. Kademlia is a DHT-based P2P routing protocol, in which each data object or peer is identified with a 160-bit ID. The distinguishing feature of Kademlia is its XOR metric that measures the distance between any two 160-bit identifiers. KAD differs slightly from Kademlia as it uses 128 bits for its node and data object IDs and supports more diverse messages. Our choice of aMule is based on the observation that the first version of the Storm botnet used the Overnet P2P routing protocol, which is also based on Kademlia. Despite the great realism obtained by using the actual implementation code of a popular P2P client, simulating a large P2P botnet with high fidelity demands intensive computation. To improve simulation scalability, we develop our simulator on a distributed computing platform. The simulator is a component of MIITS, a local distributed simulation framework for simulating large-scale communication networks. MIITS is built on PRIME SSF, a distributed simulation engine using conservative synchronization. When porting the aMule code into MIITS, we intercept all time-related system calls (e.g., gettimeofday) and replace them with simulated time function calls. Similarly, we substitute socket API calls in the original code for network functions developed in MIITS.

In a case study, we use BotSim to study the resilience of P2P-based botnets against pollution mitigation. In some earlier work, it has been shown that polluting the command keys used by bots to search C&C information is an effective approach to disrupt operations of P2P-based botnets. In the simulation study, we demonstrate that a hypothetic P2P-botnet called AntBot can make pollution mitigation less effective. AntBot uses a tree-like structure to propagate botnet commands in P2P networks. The key idea of AntBot is that there are far more low-level bots that are closer to the bottom of the tree than high-level bots so that if a bot is seized by the adversary, it is highly likely that it is a low-level bot and polluting the keys that this bot uses to search or publish the command affects only a small number of bots at lower levels. The effectiveness of AntBot against different pollution mitigation schemes is illustrated in Figure 8.



6.4.4 CyberSim. The CyberSim tool set is functional at present, however, it is maintained as a loosely connected collection of scripts and a distributed object oriented code. It is desirable to further integrate the code and make it more interactive. Currently the CVE database from NIST has to be retrieved and manually updated prior to using the CyberSim tool. It is desirable to automate this process of retrieval and simulation, given that on an average there are currently 20 or so exploits discovered every day. The post-simulation visualization is currently provided using Google Earth, which has limited interactive ability, and it is desirable to seek alternate visualization techniques. Additional, continued funding is required to maintain and enhance our cyber analysis capabilities.

6.4.5 EpiSims. EpiSimS assigns static activities to their agents, thus, the next logical step would be to include dynamic activities and allow agents to modify their behavior based on surrounding environment (e.g., disease). We have been trying to extend EpiSimS for awhile but due to lack of funding we have not be able to do so.

6.4.6 AFS. As a framework, AFS is judged by its usability and completeness in supporting agent-based development for discrete event simulations. User reviews have been mixed; consensus is that AFS provides a broad capability without being tied to a specific agent structure or cognitive architecture. Most developers rapidly become productive with the tool. As an ongoing development, AFS is incomplete. Currently its strongest capability is reactive agents. Additional capabilities are under construction to provide local and strategic planning functions.

6.4.7 ActivitySim. ActivitySim is one of the newest large-scale DES infrastructure models. The initial version included a framework of the relevant objects, schedule processing (pre-calculated, randomly-generated, an early utility-based approach), and activity execution [Galli 2009]. The utility-based schedule processing proved to produce too many gaps in scheduling. A newly redesigned version has been developed with constraints and priorities to eliminate gaps in scheduling; compound-style operators for meta-heuristics; a modular optimization loop; reformulated utility, priority, and objective functions; demographics-based activity sets, distributed location choice, weekend handling, and is easily extendable to include new utility functions, priority functions, meta-heuristics, objective functions, and optimization loop exit conditions. Next steps include the additions of household coordination, social contacts per activity for communication, activity set changes due to a natural disaster/emergency, a mixing model per location activity, and scaling to larger regions up to the entire US.

6.4.8 SimCore. The library is a relatively mature code, with half a dozen simulators running on top of it. Nevertheless, there are various improvements we are working or planning. One is a support for blocking message exchange between simulated entities, when a question can be sent to another entity, and answer received, in one function call. Future extensions include check-pointing and on-the-fly debugging capabilities.

6.5 Challenges and Issues

DES is a key technology component in the predictive science objective of Los Alamos' IS&T thrust. A Laboratory goal is to leverage our science and technology advantage to anticipate, counter, and defeat global threats and meet national priorities. While some threats are natural in origin, for example, near-space collisions, earthquakes, severe weather, other threats arise from social systems, such as terrorism, nuclear proliferation, and civil violence. These threats often interact with complex engineered systems: terrorists attack the electric grid through the Internet, a hurricane disables a 911 emergency call center, or an earthquake destroys a transportation hub. In all cases, an engineered system enables the natural or human attackers to amplify damage. DES can be applied in the context of providing information to decision-makers for real-world situation awareness or in terms of representing the process of situation awareness in the agent-based model. When used to inform decision-makers about expected outcomes of decision choices, models and model outputs can provide a reduction in uncertainty over a suite of potential actions with respect to defined metrics. As we have seen, the breadth of research at Los Alamos for DES is quite broad, encompassing cognitive science, statistical methods, risk analysis, decision theory, game theory, sociology, anthropology, machine learning and classification methods, complex systems. While there are some basic theoretical underpinnings, the quick availability of a DES modeling approach is a great advantage. The Los Alamos developed SimCore framework provides an easily accessible and intuitive modeling philosophy that has already resulted in a number of interoperable tools. DDES simulation tools typically face some technical problems in terms of achieving sufficient scalability, but the set of solution approaches is well known. Tool performance optimization can easily turn into a never-ending software engineering nightmare.

A second, perhaps more fruitful focus area is that of actual modeling issues. The challenge of modeling human behavior on a large scale continues to be a fundamental challenge having many intriguing facets. Not the least of these is the problem of verification and validation (V&V). A thorough discussion of the V&V issue is beyond the scope of this report. Many other challenges are associated with the overall scale and complexity that agent modeling demands. Computing power alone cannot resolve the problem; rather it is an issue that brings together core issues of model representation, software design and high-performance computing. To expand on just a small portion of this challenge, consider that agents representing human behavior must be capable of mimicking complex reasoning, including the use of cooperative or competitive strategies, as well as routine behavior and simple reactive responses. They must do this in response to a changing simulation environment that includes the agents themselves as an essential element. All of this must be done in an authentic way and as efficiently as possible. Fundamental social science also needs to be advanced; we still do not have good fundamental models or constructs of how people make decisions, form groups, etc.

The third area for DDES focus is the seemingly obvious one of actually using DDES tools in operations and in scientific discovery. At Los Alamos, we unfortunately have a tradition of building large software DDES tools that then see relatively little use due to lack of funding. DDES tools need to be used more regularly in the scientific discovery process. The MIITS team has in fact discovered structural properties of the Internet topography that would have been hard to identify without DDES. EpiSims has probably seen the most use of all Los Alamos DDES tools, but even so remains underutilized.

Scientifically supported national preparedness, especially in the realm of Homeland Security, is driven by the whims of public opinion. Although this is exactly the sort of forward-looking, multi-disciplinary science in which Los Alamos ought to excel, this capability has two or three funding sources at any given time, with differing technical emphasis points and agendas, making it difficult to cultivate a sustainable, top-notch program. The current portfolio of DDES projects at Los Alamos is dominated by the NISAC project, which is subject to painful oscillations in funding, as is any single project. More diversification is necessary. There needs to be an ongoing institutional commitment to developing and expanding Los Alamos's DDES capability, resulting in a long-term investment in this important capability. Funding is often from WFO sources resulting in spotty funding. Future solutions to complex issues like mitigating global warming will rely on modeling and simulation–a key element of which will be agent-based models of the response of social systems to the warming and mitigation processes.

6.5.1 FastTrans. Issues covered in Section 8.0.

6.5.2 MIITS. The main technical challenge for MIITS is efficient code maintenance as it has been developed by a multitude of programmers. New application protocols (such as Twitter) often gain popularity within a matter of a few months. MIITS' objective of always having all relevant Internet traffic modeled on an application level is sometimes put into question as we are not always able to secure funding for implementing a model for the newest technology in short enough time frames. MIITS has had some success in diversifying its sponsor base, which now includes internal LDRD and DOE National SCADA Testbed (NSTB) in addition to the NISAC program, but guaranteeing a steady funding stream remains a challenge.

6.5.3 BotSim. One challenge is to integrate it into a more comprehensive network simulator, which models not just the nodes in P2P networks but also routers and domain name servers. Another important part is to model the activities and geographic distribution of both normal peers and bot machines in a realistic manner. We will continue to improve BotSim along these two lines.

6.5.4 CyberSim. The CVE database format is currently evolving and lack of proper standards makes it harder to maintain automatic parsing code. There is also a lack of reliable data on the currently installed software on user's computers. It is also difficult to associate physical computers with individual users: for example a given user may use a friend's computer to access a social networking website, which infects the friend's computer. While it is possible to statistically model such complex social interactions, this remains a work to be done. Another future research area is the manner in which work related and personal social networks interconnect and interact. We also plan to study in detail how the spread on malware depends on the geographical distribution of initial corrupted nodes.

6.5.5 EpiSims. The greatest non-technical challenges is funding; some technical challenges include computer resources to run our simulation (e.g., limited time on institutional HPC clusters) and representing accurate human behavior (e.g., fear).

6.5.6 AFS. Issues covered in Section 8.0.

6.5.7 ActivitySim. Detailed large-scale DES infrastructure models such as ActivitySim are time-consuming in their design, development, tuning, testing, and validation. This is required to ensure defensible study results. This needs to be recognized and addressed to ensure the future of these models. Due to lack of adequate funding for quality talent, the future of this work is at risk.

6.5.8 SimCore. No issues except those covered in Section 8.0.

7.0 Theme 6: Integrated Codes

(Theme Leader: Stephen Lee, CCS Division)

For the purposes of this review, an "integrated code" is defined as a software application that makes use of multiple methodologies, models, data, and/or algorithms working in unison to solve problems. Los Alamos has an impressive collection of such integrated codes, *which represent the integration of our scientific and engineering experience*, experimental data, and (of course) CPAM capabilities. In fact, there are too many individual integrated codes at Los Alamos, built for specific purposes, to accurately count. However, Los Alamos has assessed its integrated code assets and determined which assets are *strategically important*: solving multiple problems with significant visibility to sponsors and have longevity (and for which development is planned for the foreseeable future). This analysis produced a table with over 100 individual entries, which is summarized below.

Approximate Code Category	Approximate Number of Codes
CFD	25
PDE	15
MC	10
MD	8
DES	11
Other (do not fit in above categories or fit in too many)	45

In addition, total numbers of source lines of code (SLOC) were also estimated as part of this survey. SLOC is a useful software metric that can be defined in multiple ways, but here it is simply a count of the number of lines in source code files. The SLOC metric is typically used to predict software development efforts, estimate programming productivity, and indicate software complexity. In this case, it is used as a simple metric indicative of the pervasiveness of strategic integrated codes at Los Alamos, their complexity, and to compare the size of such efforts to other well-known software projects and products from an "order of magnitude" perspective. From the survey conducted, Los Alamos has approximately 10 million lines of code in over 100 strategic integrated applications. This number is significant, which becomes obvious in Figure 9.

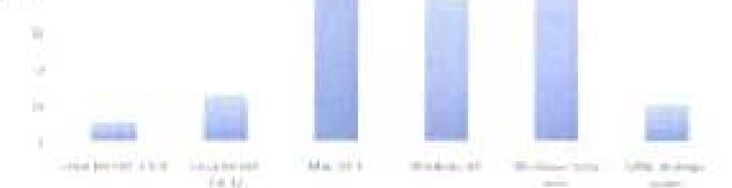


Figure 9. SLOC at Los Alamos versus other well-known software projects. Note the growth in SLOC between Linux versions, which is common

In Figure 10, we see the SLOC measures for other commonly known software products (in this case, operating systems) as compared to the Los Alamos strategic codes enterprise. This is an interesting comparison, as the Los Alamos strategic codes within the scope of this review are *all computational physics and applied mathematics oriented*. Clearly, our strategic code effort is deep, broad, and important to Los Alamos.

Relative LANL Organizational Contribution to SLOC Total

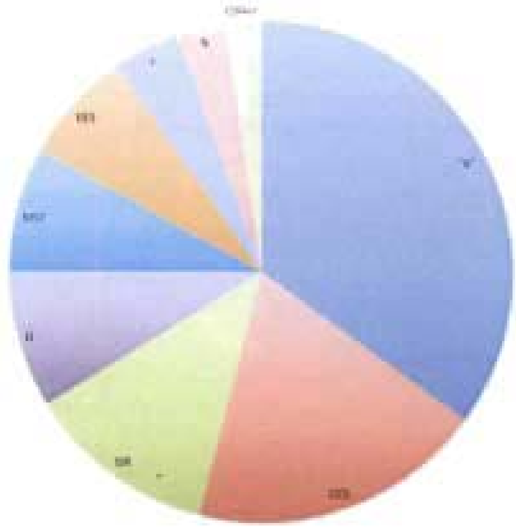


Figure 10. Relative SLOC comparisons by Los Alamos technical division ("X" refers to a combination of the recently bifurcated X Division: XCP, Computational Physics, and XTD, Theoretical Design).

Finally, a metric to understand the strategic value of such applications to Los Alamos and the nation is through licenses and technology transfer activities. The Technology Transfer (TT) Division assessed software codes that have been disclosed to TT and that fit into the theme areas for this review. From FY05 through present, TT received 432 software disclosures. This means that, while not all such software have licenses associated with them, there was an intent to share these codes outside of Los Alamos with peers, collaborators, and so on. The codes included in this particular assessment were *only those for which Los Alamos has asserted copyright* (meaning TT requested permission for DOE to take title to them in the Laboratory's name). The reason only these codes were included is due to the simple fact that the copyright assertion processes exposes more information about these codes than other avenues. Therefore, there are a large number of codes that have been disclosed and licensed through other mechanisms (noncommercial or government licenses) that were not assessed here. With this caveat, the following summarizes the TT analysis.

- CFD:
  - ⇒ Six integrated codes with both commercial and non-commercial licenses from CCS, T, and XCP divisions. The codes have multiple users, from 10s to 1000s.
  - ⇒ Nine integrated codes licensed for open source distribution (GPL, LGPL, and/or BSD licenses) from CCS, EES, HPC, MST, and T divisions.
- MC:
  - ⇒ Three integrated codes from AOT, ISR, D, T, and XCP divisions with tens of thousands of users worldwide and include some of our most successful code efforts to date (e.g. MCNP).
  - ⇒ Five separate codes licensed for open source distribution from EES, ISR, P, T, and XCP divisions.

- PDE:
  - ⇒ No separate identifiable commercially or non-commercially licensed codes, which is not surprising given that at Los Alamos PDE solution techniques are imbedded in applications as previously described.
  - ⇒ Five separate codes/solver packages licensed for open source distribution that fit the TT assessment criteria, from CCS, ISR, T, and W divisions.
- Other integrated codes that do not fit well within any one of the previous three themes (or fit in too many simultaneously):
  - ⇒ Six integrated codes from B, D, EES, and ISR divisions. Some under evaluation for commercialization, others have has many as 500 commercial and non-commercial licenses.
  - ⇒ One code, from CCS division, is licensed in this category for open source distribution.

Since FY05, Los Alamos has asserted copyright on 129 separate software codes. The copyrights were asserted for commercial or open source distribution (depending on the software in question). In addition, licensed codes have generated $1.6M in revenue for Los Alamos in FY07. This information is a clear indicator of our reputation and strength in this area. During this review, two classes of integrated codes were assessed: 1) Climate, Ocean, and Sea Ice Applications and 2) Nuclear Weapons Applications. As with the other theme areas, each of these will be briefly discussed below along the lines of the review assessment criteria with the note that much of what has been discussed in the other theme areas has already addressed the review assessment criteria and is not repeated here.

Finally, while not a separate theme in CPAM, Uncertainty Quantification (UQ) is a core strategic strength at Los Alamos and a key integrator of capabilities in applied mathematics and computational physics. UQ is the process of carrying out scientific inference (prediction uncertainties, parameter estimates, sensitivities, etc.) and typically combines physical observations, computational models and high performance computing to make these inferences. In this regard, UQ has played a key role in multiple programs. Our competitive advantage in this area stems from its broad range of experts from multiple fields and our environment that fosters significant and deep collaboration. As a result, we are leaders in the broader UQ community.

7.1 Connection to the Goals and Mission of the Laboratory

7.1.1 Climate, Ocean, and Sea Ice Applications. Climate modeling has been a traditional strength at Los Alamos, born out of an effort studying nuclear winter many decades ago and has grown into a world-leading and stable program of critical importance to the nation. Los Alamos, as the premier national security laboratory, includes energy security in its primary mission and goals. Energy security has a strong tie to our climate modeling efforts.

7.2.1 Nuclear Weapons Applications. The connections of this capability to Los Alamos are obvious. Los Alamos is one of two nuclear weapons laboratories and, as such, responsible for the technical certification of the physics packages under its responsibility. The nuclear weapons applications are central to this responsibility.

7.2 Research Breadth and Impact

7.2.1 Climate, Ocean, and Sea Ice Applications. Climate models have many uses, from technical to political. Climate modeling integrates knowledge of the climate system, is used to understand and quantify feedbacks in the system, attributing tracers in the system, and projecting future climate changes. Few other technical activities have an equivalent reach and impact worldwide. Los Alamos contributions to this area have been described in previous sections of the document.

7.2.2 Nuclear Weapons Applications. The transition from underground testing to a certification program based entirely on simulation and small-scale experiments represented an unprecedented shift for such a complex non-linear system and large-scale scientific and engineering enterprise. This shift is now complete, and the impact of this shift will be measured for decades to come. There are already several examples of similar shifts ongoing in multiple other areas (nuclear energy, environmental remediation, carbon sequestration, and so on). Furthermore, specific technical achievements for the weapons program manifest themselves in other areas the scope of which cannot be discussed in this document.

7.3 Comparison with Peers

7.3.1 Climate, Ocean, and Sea Ice Applications. The principal peer institutions are also partners in this endeavor, with different institutions playing different technical roles. This is a well-integrated and aligned national project.

7.3.2 Nuclear Weapons Applications. The only peers in this area are LLNL, AWE, and CEA. A detailed discussion and comparison of the capabilities of these institutions cannot be made in this document.

7.4 Status of the Capabilities

7.4.1 Climate, Ocean, and Sea Ice Applications. Los Alamos develops the advanced ocean and ice models for climate science, and focuses on high latitude climate change impacts throughout the globe. This includes ice sheets and sea level rise, rapid ice retreat, ocean circulation stability, eddy-resolving ocean modeling, and high latitude biogeochemistry and clathrates.

7.4.2 Nuclear Weapons Applications. As was illustrated during the classified presentation at the review, nuclear weapons applications are making seminal contributions to a multitude of national security interests.

7.5 Challenges and Issues

Most of the challenges and issues in this theme are common to all themes and therefore covered in Section 8.0. However, both nuclear weapons codes and climate modeling are closely tied to national policy and, as a result, funding support tends to ebb and flow with the political climate and interest in climate, nuclear weapons stewardship and technology, and proliferation. Particularly in the nuclear weapons program, this can make hiring and retaining staff a challenging issue.

8.0 Challenges and Issues for the CPAM Capability

In this section, challenges and issues common to the CPAM capability (often common to all scientific capabilities at Los Alamos) are briefly described.

8.1 Advanced Computing Architectures: Our Co-Design Future

The primary challenge to computational physics and applied mathematics over the next decade will be the sea change in computing technology. The first instantiation of this was the Roadrunner supercomputer, the first system in the world to achieve a petaFLOP/s of sustained performance. This system has a variety of architectural features that underscore where computing is heading, including accelerators of a different technology design than the base system (heterogeneity), different and complicated memory hierarchies, multiple networks, multiple compilers, and other complexities that required a complete re-design of application codes and algorithms for the architecture. Our current codes and algorithms often rely on high resolution schemes that depend on a rich set of data for discrete solution, thereby requiring large dependency stencils and frequent evaluation of constitutive properties – this translates into significant memory requirements (speed of access and availability) which can be limited on accelerated architectures. Furthermore, the lack of common programming tools for various architectures has become a significant barrier to the development of advanced applications to take advantage of newer architectures.

In addition to these challenges, as the nation drives toward exascale, computing resiliency and fault tolerance will also become issues that applications must face, demanding new strategies that go beyond the current checkpoint and restart methods employed today. In future Exascale systems, applications will have to tolerate node-level failures that occur at a frequency measured in minutes, and will require scalable recovery solutions that do not rely on globally accessible checkpoint data. This will drive significant changes in the programming models that will run on these systems, but will also require hardware and software capabilities that do not currently exist.

It is obvious that in order to exploit emerging architectures, computer scientists and computational physicists will be required to work even more closely together and develop long-standing collaborations in order to effectively map new computational physics algorithms onto new computer architectures. We have embarked on a serious and well-funded co-design philosophy in which methods developers, computer scientists, and computational physicists work together with industrial partners designing and creating new computing technologies to *co-design* the technologies and the applications that will run on them. This is not a new approach, as space-based computational assets have been designed in this manner for some time. However, the scale of effort, technical scope, and approach are different. Los Alamos has created a new group as an institutional resource within CCS Division (the Applied Computer Science Group, CCS-7) for this purpose. The group has multiple teams, projects, and activities intended to move strategic applications along the right trajectory and at the right pace to be ready for the future. This includes the development of new programming models, the training of staff in other organizations, and working directly with computing technology vendors and project staff on specific co-design activities. We are further extending this successful approach to co-design of experiments, theory, models, algorithms, computational infrastructure, and applications.

8.2 The Exascale Wave: High-end Computing for Everyone
Somewhat related to advanced architectures that are challenging to exploit, there is a wave of new programs that have heretofore not relied heavily on high-end modeling and simulation in the pursuit of their goals. Many of these are energy-related programs (nuclear energy, combustion, carbon capture, and so on) while others involve environmental remediation (e.g., ASCEM). Programs that have not made use of high-end computational science often initiate extremely ambitious projects with high expectations and seem to be under the impression that to make serious use of computational science requires nothing more than a checkbook to buy a big computer and a few people to string together existing tools into a large "plug and play framework." Nothing could be further from the truth and it is up to national assets such as national laboratories to help guide the development of these programs based on our collective experiences in this area. This is an excellent opportunity for Los Alamos to set the national agenda for computational science that will positively impact a host of issues of importance to the nation.

8.3 Open Computing Resources
One of our challenges is that our largest computing assets are behind the security perimeter and not accessible for unclassified work. The Laboratory has continued to invest in institutional computing resources, but we lag other national laboratories in unclassified computing assets. Los Alamos will continue to make open computing investments, and we will continue to partner with other organizations (such at ORNL) on joint projects (climate modeling is a good example), thus advancing the science and making use of larger open computing systems outside of Los Alamos. While this can lead to recruiting challenges, it is the only viable model for the future as exascale systems will be large, unique, and expensive – and therefore be few and far between.

8.4 Retention of Existing Staff and Attraction of New Staff
Los Alamos must continue to compete for people in the open market, both to retain critical staff we have now and to attract new talent. While Los Alamos cannot match the perks offered by some of our competitors, we can offer interesting work and the Laboratory should be prepared to compete on salaries, both for people we currently have and the talent we are trying to attract. In recent years, we have lost critical computer science and computational science staff at an alarming rate to non-NNSA laboratories and universities. Where we can, we should endeavor to ensure solid support for CPAM capabilities (e.g., in the LDRD component) before we drop below critical mass in some key areas. Having a multi-disciplinary environment and challenging problems to solve are no longer sufficient to compete for technical staff. Retention and hiring are also strongly affected by the issue discussed in the next section.

8.5 The Compliance Effect
Over the past several years, Los Alamos has come under increasingly restrictive measures meant to enhance compliance to a variety of regulations. Increased security requirements, particularly in computing, are significantly damaging the stature of Los Alamos in the scientific community and making it difficult to compete for staff and projects. In addition, compliance measures are driving our costs up making competition difficult on that basis alone. Few sponsors are receptive to the argument that working with an NNSA laboratory requires paying a share of the high security profile or the footprint of large experimental facilities, particularly when they are not making use of those facilities. CPAM in particular relies on computing and computing infrastructure to accomplish its science. Los Alamos has

become increasingly restrictive on what types of computers scientists are allowed to use and deploy, what software may be used on them, and how and where they can be used. While there is an exception policy in place, the restrictions are so severe as to require essentially every CPAM scientist to go through the exception process to acquire a computer (everything from allowed display sizes, to disk drive size, to memory sizes are specified as "default" systems; any variations from this default triggers an exception). While the exception policy work, it is unique to our environment and a significant barrier to attracting new 21st century minded scientists who are used to a host of tools at their disposal to solve problems and can see no compelling reason to select Los Alamos over another institution with fewer restrictions. For CPAM scientists, the computer is a very personal device, intimately coupled to the science they are pursuing. The industries, national laboratories, and universities that recognize this (as many do) are the ones that will successfully compete for new staff and programs in the real world. Striking a better balance between security compliance and scientific accomplishment is something Los Alamos needs to continue to address as an institution.

In addition to these issues, two specific issues are sufficiently acute to require further elaboration.

8.5.1 Working with Foreign Nationals. Our ability to stay at the forefront in computational physics and applied mathematics depends on our ability to work with external and foreign collaborators since the US education system is not graduating sufficient citizens with the requisite skills. A barrier to collaborations, including constraints on foreign collaboration and the hiring of foreign nationals, is a major problem. Increasing security requirements, particularly in computing, significantly affect both classified and unclassified work. New requirements need to be evaluated carefully in terms of their benefit, their impact to technical work, and true costs. Recent changes in procedures for foreign visitors, clearances, and computer access are making it increasingly difficult to host external collaborators. The loss of DOE Q-cleared affiliates will severely impact technical interaction and peer review for classified projects and will affect the ability to recruit and train students over summers, which represents a significant talent pipeline for the Laboratory.

8.5.2 UCNI. External collaborations are significantly hampered due to simulation codes developed at Los Alamos being designated Unclassified Controlled Nuclear Information (UCNI), while a code with the identical capability developed at a university is not designated as such – *even if written by DOE-funded, Q-cleared faculty*. This classification practice limits collaborations with universities, harms recruitment, and is a significant frustration for our scientists who need to participate and be competitive in the scientific community. We also encounter export control issues with our unclassified codes, particularly in astrophysical collaborations. While there is a process for removing an export control designation, it is tedious and has not been exercised for many important codes. There is no process to remove the UCNI designation, which would not exist if the exact same code were developed at a university.

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Invited Talks and Presentations

The distinction between invited talks and other presentations is often difficult to ascertain. At some meetings, the distinction is clear and relevant, while not so in others. Because such efforts would be subject to considerable error, we do not track this distinction in our databases. The following list of 76 invited talks and presentations reflects the major international involvement of the CPAM Capability Area staff.

Aluie, H., Compressible Magnetohydrodynamic Turbulence, Center for Magnetic Self-Organization bi-annual meeting 2010 (CMSO10), Swarthmore, PA, June 9-11, 2010.
Carrington, D.B, KIVA and Combustion Modeling at LANL, Engineering Graduate Seminar Series, University of Nevada, Las Vegas Mechanical Engineering, Las Vegas, NV, February 18, 2010, (from LA-UR-10-00727 and DUSA. Fossil).
Carrington, D.B, T-3 Combustion Modeling KIVA-4mpi and KIVA-hpFE Development, University of New Mexico Mechanical Engineering Seminar, University of New Mexico, Alburquerque, NM, March 5, 2010 (from LA-UR-10-00727 and DUSA: Fossil).
Chartrand, R., A Simple Algorithm for Solving the Monge-Kantorovich Problem, Monge-Kantorovich Optimal Transport, Theory and Applications, Santa Fe, NM, October 19-21, 2009.
Chartrand, R., Fast Algorithms for Nonconvex Compressive Sensing, Physics of Algorithms Conference, Santa Fe, NM, August 31-September 4, 2009.
Chartrand, R., Fast Algorithms for Nonconvex Compressive Sensing, International Symposium on Mathematical Programming, Chicago, IL, August 23-28, 2009.
Chartrand, R., Fast algorithms for nonconvex compressive sensing, Compressive Sensing Workshop, Duke University, Durham, NC, February 25-26, 2009.
Chartrand, R., Nonconvex Compressive Sensing and Dvoretzky's Theorem for Quasi-normed Spaces, 13th International Conference on Approximation Theory, San Antonio, TX, March 7-10, 2010.
Chartrand, R., Nonconvex Compressive Sensing, Institute for Pure and Applied Mathematics Workshop, Numerical Methods for Continuous Optimization, Los Angeles, CA, October 11-15, 2010.
Chartrand, R., Nonconvex Compressive Sensing: Getting the Most from Very Little Information, Joint Mathematics Meetings, San Francisco, CA, January 13-16, 2010.
Chartrand, R., Nonconvex Compressive Sensing: Getting the Most from Very Little Information, University of British Columbia Institute for Applied Mathematics, Vancouver, BC, Canada, November 1, 2009.
Finn, J.M., Line-tied Reconnection? U. S. -Japan Workshop on Magnetic Reconnection, Madison, WI, Oct. 2009.
Finn, J.M., Reconnection in Line-tied Systems, Center forMagnetic Self-Organization (CMSO) general meeting, Santa Fe, NM, April 2009.
Francois, M.M., A Balanced-Force Algorithm for Modeling Interface Dynamics with Surface Tension, Sandia National Laboratories, January 25, 2010.
Francois, M.M., Progress and Challenges in Modeling Interfacial Flows, Oak Ridge National Laboratory, Computer Science and Mathematics Division, April 24, 2009.
Francois, M.M., Progress and Challenges in Modeling Interfacial Flows, Idaho National Laboratory, Nuclear Energy Directorate, January 20, 2009.
Gintautas, V., Identification of Functional Information Subgraphs in Complex Neuronal Networks, University of Rostock, Rostock, Germany, 2009.

Gintautas, V., The Physics of Interreality Systems, Katholieke Universiteit Leuven, Belgium, 2009.
Gnanakaran, S., Assembly and Disassembly of Biopolymers: From Alzheimer's to Biofuels, University of Arizona, Tucson, AZ, January 2010.
Gnanakaran, S., Conformational Variability of Cellodextrins, Anselme Symposium, American Chemical Society Meeting, San Francisco, CA, March 2010.
Gnanakaran, S., Deconstructing Nature's Biomaterial for Biofuels, IMMS Soft-matter Seminar Series, Los Alamos, NM, February 2010.
Gnanakaran, S., Deconstructing Nature's Biomaterial for Biofuels, Department of Chemistry, University of California Santa Barbara, CA, April 2010.
Gnanakaran, S., Deconstructing Nature's Biomaterial for Biofuels, Biotechnology Center, Rensselaer Polytechnic Institute, Troy, NY, April 2010.
Gnanakaran, S., Multiscale Modeling of Biomass and its Degradation for Biofuels, Neutrons in Biology, Santa Fe, NM, November 2009.
Gnanakaran, S., Proteins Behaving Badly: Link Between Misfolding and Alzheimer's Disease, Invitation by the Q-bio Public Seminar Series, Santa Fe Science Complex, Santa Fe, NM, February 2009.
Grove, J.,Non-equilibrium Temperature Modeling in Eulerian Hydrodynamics, SIAM Conference on Computational Science and Engineering, Miami, FL,2009.
Gutfraind, A., Understanding Terrorist Organizations with a Dynamic Model, 5th Conference on Mathematical Methods in Counterterrorism, March 2009.
Habib, S., Cosmological Simulations at the Petascale, Institute for Data Intensive Engineering and Science, Inaugural Symposium, Johns Hopkins University, Baltimore, ML, August 25-26, 2009.
Habib, S., Hybrid Petacomputing Meets Cosmology: The Roadrunner Universe Project, SciDAC 2009, San Diego, CA, June 14-18, 2009.
Habib, S., The Dark Universe Challenge: Is Theory up to the Task?, Brown University Physics Colloquium, October 5, 2009.
Habib, S., The Dark Universe Challenge: Is Theory up to the Task?, Argonne National Lab, Physics Colloquium, Chicago, IL, December 10, 2009.
Hagberg, A., "Mathematical Challenges in Network Science" DOE Applied Mathematics Program Meeting, Berkeley, CA, May 2010
Hagberg, A., NetworkX: Exploring Network Structure, Dynamics, and Function, SIAM Conference on Computational Science and Engineering, Miami, FL, March 2009.
Hagberg, A., Robust Network Interdiction under Uncertainty, DTRA Basic Research Review, Washington, DC, October 2009.
Hagberg, A., Structure and Dynamics of Cybersecurity Networks, SIAM Annual Meeting, Denver CO, July 2009.
Higdon, D., C.S. Reese, J.D. Moulton, J.A. Vrugt, and C. Fox, Posterior Exploration for Computationally Intensive Forward Models, Technical Report LA-UR 08-05905, Statistical Sciences Group, Los Alamos National Laboratory, 2009.
Jiang, J., Foam, Fly, and Eye: Modeling RPE Morphogenesis, Seminar, Emory Eye Center, Emory University, Atlanta, GA, September 2009.
Jiang, J., Modeling Tumor Growth from Molecule to Tissue, Lecture, Third q-Bio Summer School, Los Alamos, NM, July 2009.

Jiang, J., Multiscale Model of Tumor Angiogenesis, Minisymposium on Cancer Modeling, SIAM Computational Sciences and Engineering, Miami, FL, March 2009.
Jiang, J., Multiscale Model of Tumor Growth and Angiogenesis, Mathematical Modeling in the Medical Sciences, Annual Shanks Conference and Lecture, Vanderbilt University, TN, May, 2009.
Jiang, J., Multiscale Model of Tumor Growth and Angiogensis, Invited Speaker, Minisymposium on Multiscale Modeling, First Joint SMB-CSMB Conference, Hangzhou, China, June, 2009.
Jiang, J., Multiscale Modeling of Tumor Development, Seminar, Cancer Research Center, University of New Mexico, Alburquerque, NM, August 2009.
Jordanova, V.K., Self-consistent Simulations of Plasma Waves and Instabilities in the Ring Current, 11th Scientific Assembly, IAGA, Sopron, Hungary, August 23-30, 2009.
Jordanova, V.K., Y. Miyoshi, R.M. Thorne, and W. Li, Stormtime Dynamics of Ring Current Electrons, International Workshop on Electromagnetic Chorus Plasma Waves, La Jolla, CA, February 10-12, 2009.
Lipnikov, K. A Mimetic Discretization of the Stokes problem with Selected Edge Bubbles, Scientific Computing Seminar, Department of Mathematics, University of Houston, September 10, 2009.
Lipnikov, K. A Mimetic Tensor Artificial Viscosity Method for Arbitrary Polyhedral Meshes, International Conference on Computational Science, Amsterdam, The Netherlands, May 31-June 2, 2010.
Lipnikov, K. A Multilevel Multiscale Mimetic (M3) Method for Two-phase Flows in Porous Media, The SIAM Conference on Mathematical and Computational Issues in the Geosciences, Leipzig, Germany, June 2009.
Lipnikov, K. A Multilevel Multiscale Mimetic (M3) Method for Two-phase Flows in Porous Media, International Conference on The Mathematics of Finite Elements and Applicatios (MAFELAP), Brunel University, London, UK, June 2009.
Lipnikov, K. Mimetic Finite Difference Method for Diffusion Problems, International Conference on Advanced Methods for the Diffusion Equation on General Meshes, Paris, France, July 5-6, 2010.
Lipnikov, K. Mimetic Finite Difference Method for Meshes with Curved Faces, International Workshop on Discretization methods for Viscous Flows, Porquerolles, France, June 2009.
Lipnikov, K. Mimetic Finite Difference Method for Solving PDEs on Polyhedral Meshes, International Conference on Non-Standard Numerical Methods for PDEs, Pavia, Italy, June 29-July 2, 2010.
Lipnikov, K. Optimal and Quasi-optimal Meshes for Minimizing the Interpolation Error and its Gradient, SIAM Conference Conference on Computational Science and Engineering, Miami, FL, March 2009.
Livescu, D., J. Mohd-Yusof, and T. Kelley, Direct Numerical Simulations of Compressible Reacting Turbulence with Type Ia Supernovae Microphysics, 14th SIAM Conf. Parallel Process. Sci. Comput. (PP10), Seattle, WA, February 24-26, 2010.
Livescu, D., J.R. Ristorcelli, and R.A. Gore, Variable-density Rayleigh-Taylor Turbulence, 2nd Int. Conf. Turbulent Mixing and Beyond (TMB09), Trieste, Italy, July 26-August 7, 2009.
Lowrie, R.B., The Structure of Radiative Shocks, Workshop on Computational Kinetic Transport and Hybrid Methods, Institute for Pure and Applied Mathematics (IPAM), UCLA, Los Angeles, CA, March 30-April 3, 2009.
Lowrie, R.B., Tracer Advection for Ocean and Atmospheric Flows, Computer Science and Mathematics Seminar Series, Oak Ridge National Laboratory, Oak Ridge, TN, May 17, 2010.
Lowrie, R.B., Tracer Advection using Characeteristic Discontinuous Galerkin, Frontiers of Geophysical Simulation, National Center for Atmospheric Research, Boulder, CO, August 18-20, 2009.

Mohd-Yusof, J., D. Livescu, and T.M. Kelley, Adapting Compressible Fluid-Flow Solvers to the Roadrunner Hybrid Supercomputer, Center For Computational Science Distinguished Lecture Series, University of Miami, Miami, FL, November 5, 2009.
Mohd-Yusof, J., D. Livescu, and T.M. Kelley, Adapting the CFDNS Compressible Navier-Stokes Solver to the Roadrunner Hybrid Supercomputer, Parallel CFD 2009, Moffett Field, CA, May 18-22, 2009.
Mohd-Yusof, J., D. Livescu, and T.M. Kelley, Fluid Flow Simulation on Roadrunner, SIAM Conference on Computational Science and Engineering (CSE09), Miami, FL, March 2-6, 2009.
Mukherjee, P.P., Electrodics in Electrochemical Energy Systems, Research Seminar NREL; Golden, CO, July 21, 2009.
Mukherjee, P.P., Electrodics, Transport and Materials Design In Polymer Electrolyte Fuel Cells, Invited Seminar, University of California Berkeley, March 2, 2009.
Mukherjee, P.P., Electrodics, Transport And Materials Design In Polymer Electrolyte Fuel Cells Press, Sandia National Laboratories, Albuquerque, NM, April 30, 2009.
Mukherjee, P.P., Multiscale Modeling Of Electrodics And Transport In Polymer Electrolyte Fuel Cells, Symposium On Computational Nanoscience, ASME Intl. Mechanical Engineering Congress and Exposition, Lake Buena Vista, FL, November 13-19, 2009.
Mukherjee, P.P., Polymer Electrolyte Fuel Cells: Transport and Materials Design, Texas A&M University, College Station, TX, March 11, 2009.
Omberg, K, Characterization of the Environmental Fate of Bacillus thuringiensis var. kurstaki (Btk) After Pest Eradication Efforts, 2009 National BioWatch Workshop, Denver, CO, August 17-20, 2009.
Omberg, K, Characterization of the Environmental Fate of Bacillus thuringiensis var. kurstaki (Btk) After Pest Eradication Efforts, Kristin M. Omberg, Invited Speaker, 2009 Biothreat Agent Workshop, Chapel Hill, NC, April 30-May 1, 2009.
Omberg, K, Studying Outdoor Gypsy Moth Suppression Programs as Surrogates for a Biological Attack, 2009 National BioWatch Workshop, Denver, CO, August 17-20, 2009.
Pope, A., Roadrunner Universe Project, Path to Petascale: Adapting GEO/CHEM/ASTRO Applications for Accelerators and Accelerator Clusters, National Center for Supercomputing Applications, Urbana, IL, April 2-3, 2009.
Santhi, N., Y. Guanhua, and S. Eidenbenz, CyberSim: Geographic, Temporal, and Organizational Dynamics of Malware Propagation, invited paper at the WinterSim 2010 (WSC 2010) conference.
Toole G.L, Electric Infrastructure, Local Utilities and ROI of New Infrastructure, presented to Applied Solutions Conference, Santa Fe, NM, 2009.
Toole G.L, Future Electric Grid: Integrating Renewables and Anticipating Change, presentation to Sec. Steven Chu, DOE, 2009.
Urbatsch, T. and B. Carlson, Sn, Supercomputers, and Apple Wine, Presentation in Special Session 'In Memory of Bengt Carlson,' 2009 International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics, Saratoga Springs, NY, May 3-7, 2009 (LA-UR-09-02493).
Urbatsch, T., J. Densmore, R. McClarren, S. Mosher, S.R. Johnson, T. Kelley, P. Henning, G. Rockefeller, M. Buksas, A. Hungerford, and C. Fryer, Jayenne Implicit Monte Carlo Project: Toward Stability, Robustness, Accuracy, Scalability - All Those Good Things, presentation at Oak Ridge National Laboratory, Knoxville, TN, LA-UR-09-03714, June 18, 2009.
Urbatsch, T., Simulating Real X-Ray Transport with Monte Carlo: Numerical Methods, Algorithms, Software, and Totally Juiced Supercomputers, Presentation to the Chemical and Nuclear Engineering Department, University of New Mexico, Albuquerque, NM, LA-UR-09-05744, November 10, 2009.

Zaharia, S., V.K. Jordanova, D.T. Welling, and G.D. Reeves, Interaction between Plasma and Magnetic Fields in the Earth's Inner Magnetosphere: Progress and Challenges, Fall Meeting American Geophysical Union, December 14-18, 2009.

Contributed Talks to Conferences and Workshops

The following list shows 215 contributed talks to conferences and workshops. The list does not show internal meetings or reviews or academic meetings. It reflects the major international involvement of the CPAM capability area staff. The list was compiled via submissions by staff in this capability area.

Abdel-Fattah A., S. Tarimala, E. Garcia, B. Martinez, D. Ware, P. Lichtner, P. Reimus, and R. Roback R, LANL SFA Progress Report: *II Plutonium Transport by Calcite Colloids*, LA-UR-09-01226, Environmental Remediation Sciences Program Science Focus Area Annual Meeting, Lansdowne, VA, April 20-24, 2009.
Abdel-Fattah A.I., *Transport of Pu(VI) in Natural Alluvium by Natural Calcite Colloids*, Migration 09, LA-UR-09-06088, Kennewick, WA, September 21, 2009.
Aluie, H. and G.L. Eyink, *Scale-locality of Energy Transfer in Magnetohydrodynamic Turbulence*, American Physical Society, 51st Annual Meeting of the APS Division of Plasma Physics (APS-DPP09), Atlanta, GA, November 2-6, 2009.
Aluie, H. and G.L. Eyink, *Scale-locality of the Energy Cascade in Turbulence Using Fourier Analysis*, American Physical Society, 62nd Annual Meeting of the APS Division of Fluid Dynamics (APS-DFD09), Minneapolis, MN, November 22-24, 2009.
Ambrosiano, J., and R. Bent, *HCSim: An Agent Model for Urban-scale Healthcare Facility Impact*, Risk Analysis of Complex Systems for National Security Applications, Santa Fe, NM, 2009.
Arcudi, F., G.L. Delzanno, and J.M. Finn, *The Effect of Plasma Flow on Line-tied Magnetohydrodynamic Modes*, International Sherwood Fusion Theory Conference, April 2010.
Arrowsmith, S.J., *Hazardous Release: Acoustic Sensing of Urban Winds*, External Proposal Call/Quad Chart, LA-UR-09-05943.
Batha, S.H., B.J. Albright, D.J., Alexander, C.W. Barnes, P.A. Bradley, J.A. Cobble, J.C., Cooley, J.H. Cooley, R.D. Day, K.A. DeFriend, N.D. Delamater, E.S. Dodd, V.E. Fatherley, J.C. Fernandez, K.A. Flippo, G.P. Grim, S.R. Goldman, S.R. Greenfield, H.W. Herrmann, N.M. Hoffman, R.L. Holmes, R.P. Johnson, P.A. Keiter, J.L. Kline, G.A. Kyrala, N.E. Lanier, E. Loomis, F.E. Lopez, S. Luo, J.M. Mack, G.R. Magelssen, D.S. Montgomery, A. Nobile, J.A. Oertel, P. Reardon, H.A. Rose, D. Schmidt, M.J. Schmitt, A. Seifter, T. Shimada, D.C. Swift, T.E. Tierney, L. Welser-Sherrill, M.D. Wilke, D.C. Wilson, J. Workman, and L. Yin, *Inertial Confinement Fusion Research at Los Alamos National Laboratory*, 7th Symposium on Evaluation of Current Trends in Fusion Research, 20070305-20070309; Washington, DC, AIP Conference Proceedings Vol.1154, 129-147, 2009.
Beckham, R.E., S. Tarimala, P. Roberts, and A.I. Abdel-Fattah, *Enhanced Micromixing in Porous Media Lattice-Boltzmann Modeling and Microfluidic Experimental Results*, LA-UR-09-08087, American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18, 2009.
Bement, M.T., and T.R. Bewley, *Excitation Design for Damage Detection Using Iterative Adjoint-Based Optimization*, Conference on Smart Materials, Adaptive Structures and Intelligent Systems, Ellicott City, MD, USA, October 28-30 2008, 20081028-20081030; SMASIS 2008: Proceedings of the ASME Conference on Smart Materials, Adaptive Structures and Intelligent Systems 2008, Vol 2, 175-183, 2009.
Benage, J., F.J. Wysocki, D.C. Wilson, and G.A. Kyrala, *X-ray Production from a Kilojoule Picosecond Laser Interaction with an Iron Target*, 2009 IEEE 36th International Conference on Plasma Science (ICOPS), San Diego, CA, June 1-5 2009; 2009 IEEE 36th International Conference on Plasma Science (ICOPS), 2009.

Bent, R., B. Daniel, and P. Van Hentenryck, *Randomized Adaptive Decoupling for Large-Scale Vehicle Routing with Time Windows in Disaster Response*, Eleventh INFORMS Computing Society Conference (ICS 2009), Charleston, SC, January 2009.
Bent, R., C. Coffrin, and P. Van Hentenryck, *Vehicle, Location, and Inventory Routing for Disaster Relief*, INFORMS Annual Meeting, San Diego, CA, October 2009.
Bergen, B., *A Compressible Navier-Stokes Solver for Heterogeneous Computing Environments*, SIAM Conference on Parallel Processing for Scientific Computing, Seattle, WA, February 24-26, 2010.
Bergen, B., *Programming Models and Techniques for Iterative Solvers Using OpenCL*, 11th Copper Mountain Conference on Iterative Methods, Copper Mountain, CO, April 4-9, 2010.
Birdsell, K.H., and D. Diaconu, *Overview of the Collaboration between LANL and Romanian Institute for Nuclear Research(ICN) on Radioactive Waste Management*, LA-UR-09-04802, Gulf Cooperation Countries Technical Training Visit, Los Alamos, NM, July 2009.
Booth, T.E., and J.E. Gubernatis, *Improved Criticality Convergence via a Modified Monte Carlo Power Iteration Method*, International Conference on Mathematics, Computational Methods and Reactor Physics 2009, M and C 2009, Saratoga Springs, NY; May 3-7 2009,20090503-20090507; American Nuclear Society - International Conference on Mathematics, Computational Methods and Reactor Physics 2009, M and C 2009 Vol.4, 2466-2476, 2009.
Bowers, K.J., B.J. Albright, L. Yin, W. Daughton, V. Roytershteyn, B. Bergen, and T.J.T. Kwan, *Advances in Petascale Kinetic Plasma Simulation with VPIC and Roadrunner*, J. Phys.: Conference Series vol.180, no.1, 012055, 2009.
Brennan, D.P., M.D. Behlmann, D.P. Flanagan, and J.M. Finn, *On Error Field Penetration Thresholds Near the Resistive MHD Stability Limit*, International Sherwood Fusion Theory Conference, April 2010.
Brown, F.B. *A Review of Monte Carlo Criticality Calculations - Convergence, Bias, Statistics*, International Conference on Mathematics, Computational Methods and Reactor Physics 2009, M and C 2009, Saratoga Springs, NY, May 3-7 2009, 20090503-20090507; American Nuclear Society - International Conference on Mathematics, Computational Methods and Reactor Physics 2009, M and C 2009 Vol.1, 4-15, 2009.
Buyko, A.M., S.F. Garanin, Yu.N. Gorbachev, G.G. Ivanova, A.V. Ivanovsky, I.V. Morozova, V.N. Mokhov, A.A. Petrukhin, V.N. Sofronov, V.B. Yakubov, W.L. Atchison, and R.E. Reinovsky, *Explosive Magnetic Liner Devices to Produce Shock Pressures up to 3 TPa*, 2009 17th IEEE International Pulsed Power Conference (PPC 2009), Washington, DC, June28-July 2 2009; 2009 17th IEEE International Pulsed Power Conference (PPC 2009) 215-220, 2009.
C. Coffrin, P. Van Hentenryck, and R. Bent, *Strategic Planning for Disaster Recovery with Stochastic Last Mile Distribution*, 2010 Health and Humanitarian Logistics Conference, Atlanta, GA, 2010.
Carrington, D.B, Torres, D.J., *T-3 Combustion Modeling and KIVA Development*, Advanced Engine Combustion/Homogeneous Charge Compression Ignition Working Group Meeting, Livermore, CA, February 10, 2009 (LA-UR-09-00553).
Carrington, D.B., Torres, D.J., *T-3 Combustion Modeling KIVA-4mpi and KIVA-hpFE Development*, Advanced Engine Combustion/Homogeneous Charge Compression Ignition Working Group Meeting, Livermore, CA, February 23, 2010 (LA-UR-10-00727).
Chadwick, M.B. *Evaluation of Fission Product Yields from Fission Spectrum n+^{239}Pu Using a Meta Analysis of Benchmark Data*, 4th International Workshop on Nuclear Fission and Fission-Product Spectroscopy, Cadarache, France, October 13-16 2009; AIP Conference Proceedings vol.1175, 71-78, 2009.

Chartrand, R. and B. Wohlberg, *Total-variation Regularization with Bound Constraints*, IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP), Dallas, TX, March 2010.
Chartrand, R. *Total-variation Regularization with Bound Constraints,* IEEE International Conference on Acoustics, Speech, and Signal Processsing (ICASSP), Dallas, TX, March 14-19, 2010.
Chartrand, R., *Fast Algorithms for Nonconvex Compressive Sensing,* DTRA/NSF Algorithms Workshop, Charleston, SC, August 17-19, 2009.
Chartrand, R., *Fast Algorithms for Nonconvex Compressive Sensing: MRI Reconstructions from Very Few Data.*" IEEE International Symposium on Biomedical Imaging (ISBI), Boston, MA, June 28-July 1, 2009.
Chrystal, A.E., J.M. Heikoop, P. Longmire, M. Dale, T.E. Larson, G.B. Perkins, J.T. Fabryka-Martin, A.M. Simmons, and J. Fessenden-Rahn, *Using Isotopes to Define Background Groundwater Nitrate at the Los Alamos National Laboratory in North Central New Mexico USA*, LA-UR-09-08027, American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18, 2009.
Cisneros-Dozal, L.M., J. Fessenden, C. Block, R. Feddema, R. Engel, P. Miller, and R. Wallander, *Evaluating the Carbon Sequestration Potential of Agricultural Fields*, LA-UR-09-02796, 8th Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 4-7, 2009.
Cobble, J.A., M.J. Schmitt, I.L. Tregillis, K.A. Obrey, S.H. Batha, G.R. Magelssen, and M.D. Wilke, *Simulated Neutron Diagnostics of Imploding ICF Targets for the Neutron Imaging System at the National Ignition Facility,* 2009 IEEE 36th International Conference on Plasma Science (ICOPS), San Diego, CA, June 1-5 2009; 2009 IEEE 36th International Conference on Plasma Science (ICOPS), 2009.
Dai, Z., H. Deng, A.V. Wolfsberg, Z. Lu, and P. Reimus, *Upscaling of Reactive Mass Transport in Fractured Rocks with Multimodal Reactive Mineral Facies*, LA-UR-10-00051, 2009 American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18, 2009.
Delzanno, G.L. and J.M. Finn, *Transport and Linear Stability Studies for PPCD Optimization in RFPs*, International Sherwood Fusion Theory Conference, April 2010.
Denli, H., and L. Huang, *Double-difference Elastic Waveform Tomography in the Time Domain*, LA-UR-09-07083, Society of Exploration Geophysicists Annual Meeting 2009, Houston, TX, October 26, 2009.
Denli, H., and L. Huang, *Quantitative Monitoring for Geologic Carbon Sequestration Using Double-Di*, LA-UR-09-08084, American Geopbysical Union Fall Meeting, San Francisco, CA, December 14-18, 2009.
Dillard, S., L. Prasad, and S. Swaminarayan, *Rapid Image Segmentation and Exploitation*, 2009 GEOINT Symposium, San Antonio, TX, Poster and Software Demonstration, Oct 18-21, 2009.
Dixon, P.R., *Program Development Efforts in Advancing DOE-EM Subsurface Simulation and Performance Assessment Capability: The SAFEMAP Project*, SDCLES Briefing, LA-UR-09-03778.
Dixon, P.R., *Status of the Repository at Yucca Mountain*, DOE-EM Performance Assessment Community of Practice Technical Exchange Meeting, Salt Lake City, UT, July 13-14, 2009.
Dixon, P.R., *Status of the Repository at Yucca Mountain*, LA-UR-09-04308, DOE-EM Performance Assessment Community of Practice Technical Exchange Meeting, Salt Lake City, UT, July 13-14, 2009.
Dodd, E.S., and I.L. Tregillis, *Modeling of Possible Hot-hohlraum Targets for Use in High-energy Density Experiments at the NIF,* 2009 IEEE 36th International Conference on Plasma Science (ICOPS), San Diego, CA, June 1-5 2009; 2009 IEEE 36tb International Conference on Plasma Science (ICOPS), 2009.
Dubey, M.K., *Feasibility of Greenhouse Gas Monitoring from Space*, LA-UR-09-05614, LDRD Day Meeting, Santa Fe, NM, September 14, 2009.

Dubey, M.K., K. Costigan, D. Wunch, and P. Wennberg, *Simulations of Los Angeles Region Carbon-dioxide Emissions: Comparisons with Observations*, LA-UR-09-08035, American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18, 2009.
Fabryka-Martin, J.T., A.M. Simmons, and P. Longmire, *Data Reliability for Groundwater Monitoring Wells at Los Alamos National Laboratory*, LA-UR-09-01281, 8th Annual Espanola Basin Workshop, Santa Fe, NM, March 3-4 2009.
Favorite, J.A. *Variational Reactivity Estimates: New Analyses and New Results*, International Conference on Mathematics, Computational Methods and Reactor Physics 2009, M and C 2009, Saratoga Springs, NY, May 3-7 2009; 20090503-20090507; American Nuclear Society - International Conference on Mathematics, Computational Methods and Reactor Physics 2009, M and C 2009 Vol.3, 1868-1882, 2009.
Fernandez, J.C., B.J. Albright, K.A. Flippo, B.M. Hegelich, M.J. Schmitt, L. Yin, and J.J. Honrubia, *Recent Progress on Ion-driven Fast Ignition*, 2009 IEEE 36th International Conference on Plasma Science (ICOPS), San Diego, CA, June 1-5 2009; 2009 IEEE 36th International Conference on Plasma Science (ICOPS), 2009.
Fessenden-Rahn, J., *Standoff Detection of O2-Locating Tunnels*, Quad Chart for potential sponsors, LA-UR-09-05596.
Finn, J.M. and G.L. Delzanno, *Control of Tearing Modes in Reversed Field Pinches above the Ideal-wall Tearing Threshold*, International Sherwood Fusion Theory Conference, joint with APS April Conference, April 2009.
Finn, J.M. and G.L. Delzanno, *Studies of Transport and Stability for Optimized Pulsed Poloidal Current Drive (PPCD) Operation in Reversed Field Pinches*, International Sherwood Fusion Theory Conference, joint with APS April Conference, April 2009.
Finn, J.M., A.S. Richardson, and G.L. Delzanno, *Control of Ideal and Resistive MHD Modes in RFPS above the Ideal Wall Threshold*, International Sherwood Fusion Theory Conference, April 2010.
Finn, J.M., Fichtl, C., and Delzanno, G.L. "Development of an Arbitrary Curvilinear-Coordinate PIC Code," APS Division of Plasma Physics Conference, Nov. 2009.
Finn, J.M., G.L. Delzanno, and J. Sarff, *Transport and Linear Stability Studies for PPCD Optimization in RFPs*, APS Division of Plasma Physics Conference, November 2009.
Flowers, B.A., and M.K. Dubey, *Observations of Aerosol Long-range Transport for Asia Using a New 3-Laser Photoacoustic Spectrometer*, LA-UR-09-07202, Gordon Research Conf on Atmospheric Chemistry, Waterville Valley, NH, August 23-28, 2009.
Francois, M.M, Carlson, N.N., Fuel Cycle Research and Development Separation and Waste workshop meeting, Argonne National Laboratory, April 13-15, 2010.
Francois, M.M. and B.K. Swartz, *Estimating Interface Curvature via Volume Fractions and Mean Values on Nonuniform Rectangular Grids*, 10th US National Congress on Computational Mechanics, Columbus Ohio, July 16-19, 2009.
Francois, M.M., Carlson N.N., NEAMS Safeguards and Separation workshop meeting, Santa Fe, NM, June 25, 2009.
Francois, M.M., E.D. Dendy and R.B. Lowrie, *Eulerian Methods for Multi-material Compressible Flow: Five and Six Equation Models*, Numerical Methods for Multi-material Fluids and Structures Conference, University of Pavia, Italy, September 21-25, 2009.
Francois, M.M., NEAMS Safeguards and Separation workshop meeting, Los Alamos National Laboratory, February 5, 2009.

Garanin, S.F., S.D. Kuznetsov, W.L. Atchison, R.E. Reinovsky, T.J. Awe, B.S. Bauer, S. Fuelling, I.R. Lindemuth, and R.E. Siemon, *Numerical simulations of Thick Aluminum Wire Behavior Under Mega-ampere Current Drive,* 2009 17th IEEE International Pulsed Power Conference (PPC 2009), Washington, DC, June28-July 2 2009; 2009 17th IEEE International Pulsed Power Conference (PPC 2009) 101-106, 2009.
Garimella, R.V., "Conformal Subdivision of Multi-Material Meshes along Reconstructured Interfaces," Trends in Unstructured Mesh Generation Symposium at the 10th US National Congress on Computational Mechanics, Columbus, OH, July 2009.
Garimella, R.V., *Conformal Adaptive Mesh Refinement and Coarsening for Quadrilateral Meshes*, Trends in Unstructured Mesh Generation Symposium at the 10th US National Congress on Computational Mechanics, Columbus OH, July 2009.
Garimella, R.V., *Conformal Adaptive Mesh Refinement and Coarsening for Quadrilateral Meshes*, 18th International Meshing Roundtable, Salt Lake City, UT, October 2009.
Garimella, R.V., *Parallel Subdivision of Unstructured Multi-material Meshes for Accurate Solution of the Diffusion Equation,* in Numerical Methods for Multi-Material Flows 2009, Pavia, Italy September 2009.
Gautier, D.C., D. Kiefer, S. Letzring, L. Yin, J.C. Fernandez, D. Jung, A. Henig, D. Habs, B.M. Hegelich, B. Albright, S.A. Gaillard, B.M. Hegelich, R.P. Johnson, R.C. Shah, T. Shimada, and K.A. Flippo, *Generation of 0.5GEV C6+ Ions from Irradiation of Ultra-thin Foils with High Contrast, High Intensity Laser Pulses,* 2009 IEEE 36th International Conference on Plasma Science (ICOPS), San Diego, CA, June 1-5 2009; 2009 IEEE 36th International Conference on Plasma Science (ICOPS), 2009.
Germann, T.C., G. Dimonte, J.E. Hammerberg, K. Kadau, J. Quenneville, and M.B. Zellner, *Large-scale Molecular Dynamics Simulations of Particulate Ejection and Richtmyer-Meshkov Instability Development in Shocked Copper,* 9th International Conference on Mechanical and Physical Behaviour of Materials under Dynamic Loading, Royal Military Academy, Brussels, Belgium, September 7-11 2009, 20090907-20090911; DYMAT 2009: 9th International Conference on the Mechanical and Physical Behaviour of Materials under Dynamic Loading, 2009.
Gintautas, V., *An Improved Model for Contour Completion in V1 Using Learned Feature Correlation Statistics,* Vision Sciences Society 10th Annual Meeting, Naples, FL, 2010.
Gintautas, V., *Generalized Resonant Forcing of Nonlinear and Chaotic Dynamics*, Dynamics Days, Evanston, IL, 2010.
Gintautas, V., *Identification of Functional Information Subgraphs in Complex Networks,* Eighteenth Annual Computational Neuroscience Meeting CNS*2009, Berlin, Germany, 2009.
Gintautas, V., *Image Categorization through Large-scale Hierarchical Models of the Primate Visual Cortex,* Society for Neuroscience Annual Meeting, Chicago, IL, 2009.
Gintautas, V., *Not So Fast: Optimized Masks Increase Processing Time for Object Detection on Speed-of-sight Tasks,* Society for Neuroscience Annual Meeting, Chicago, IL, 2009.
Gintautas, V., *Preliminary Results from the Comparison of Human Visual Performance to Biologically Inspired Computer Object Categorization,* Decade of the Mind IV, Albuquerque, NM, 2009.
Gintautas, V., *Roughness-dependent Dynamics of a Point Charge Near a Conducting Plane,* Dynamics Days, San Diego, CA, 2009.
Gintautas, V., *When is Social Computation Better than the Sum of its Parts? Social Computing Behavior,* Modeling, and Prediction, Phoenix, AZ, 2009
Gnanakaran, S., *Deconstructing Nature's Biomaterial for Biofuels*, Southwest Biofuels summit, Albuquerque, NM, April 2010.

Goforth, J.H., W.L. Atchison, S.A. Colgate, J.R. Griego, J. Guzik, D.H. Herrera, D.B. Holtkamp, G. Kaul, R.C. Kirkpatrick, R. Menikoff, R.K. Meyer, H. Oona, P.T. Reardon, C. Reinovsky, L. Rousculp, A.G. Sgro, L.J. Tabaka, T.E. Tierney, D.T. Torres, and R.G. Watt, *A New 40 MA Ranchero Explosive Pulsed Power System*, 2009 17th IEEE International Pulsed Power Conference (PPC 2009), Washington, DC, June28-July 2 2009; 2009 17th IEEE International Pulsed Power Conference (PPC 2009) 301-304, 2009.
Grove, J., *Adaptivity and Scientific Computing: From von Neumann to the Stars*, SIAM Conference on Computational Science and Engineering, Miami, FL, 2009.
Gutfraind, A., *Constructing Networks for Cascade Resilience*, International Workshop on Coping with Crises in Complex Socio-Economic Systems, Zurich, Switzerland, June 2009.
Gutfraind, A., *Constructing Networks for Cascade Resilience*, Poster, SIAM Annual meeting, Denver, CO, July 2009.
Gutfraind, A., F. Pan, A.A. Hagberg, and D. Izraelevitz, *Network Interdiction with a Markovian Adversary*, Contributed talk at INFORMS Annual Meeting, San Diego, CA, October 2009.
Gutfraind, A., *Mathematical Terrorism*, Invited talk at Lawrence Berkeley National Laboratory, September 2009.
Gutfraind, A., *Models of Network Interdiction*, Netherlands Defense Academy, The Netherlands, December 2009.
Gutfraind, A., *Resilient Complex Networks*, Risk 2009 conference, Santa Fe, NM, April 2009.
Gutfraind, A., *Understanding Terrorist Organizations with a Dynamic Model*, Minisymposium and introductory talk at SIAM Snowbird Conference on Applications of Dynamical Systems, May 2009.
Hagberg, A., *Wavenumber Locking and Pattern Formation in Spatially Forced Systems SIAM Applications of Dynamical Systems*, Snowbird, UT, May 2009.
Hall, M.L., *Higher-Fidelity Thermal Photon Transport for Time-Dependent Problems*, Numerical Methods for Multi-Material Fluids and Structures, Pavia, Italy, September 21-25, 2009.
Han, J., J.W. Carey, and J. Zhang, *A Water Chemistry Model Applied to CO2 Corrosion under Geologic Conditions*, LA-UR-10-00780, NACE 2010, San Antonio, TX, March 14-18, 2010.
Han, J., J.W. Carey, and J. Zhang, *A Water Chemistry Model Applied to Corrosion under Geologic Conditions*, LA-UR-09-06674, Corrosion Center JIP board meeting Ohio University, Athens, OH, October 19, 2009.
Harp, D.R., V.V. Vesselinov, and K.H. Birdsell, *Hydrogeologic Property Inference Using Spatially-dependent Aquifer Parameters*, LA-UR-09-08028, American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18, 2009.
Harp, D.R., V.V. Vesselinov, *Identification of Hydrostratigraphy: Optimization of Markov-chain Geostatistical Model by Adjusting Facies Conductivity Mean Facies Lengths and Mean Transition Lengths*, LA-UR-09-08029, American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18, 2009.
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Saumon, D., *To See the Inside of a Planet in a Drop of Deuterium*, 7th International Conference on High Energy Density Laboratory Astrophysics, St Louis, MO, April 11-15 1008, 20080411-20080415; Astrophys. Space Sci. Vol.322, iss.1-4, 123-127, 2009.

Schultz-Fellenz, E.S., *Geologic Examination of a Trench Excavated for the Waste Management Risk Mitigation (WMRM) Influent/Effluent Transfer Pipeline*, Technical Area 50, Los Alamos National Laboratory, Memo to ES-PE, LA-UR-09-06469.

Stauffer, P.H., *Numerical Analysis Of The MDA-G Soil-Vapor Extraction Test Material Disposal Area G Technical Area 54*, LA-UR-09-00995.

Stauffer, P.H., R.J. Pawar, B.C. Lettelier, H.S. Viswanathan, D.L. Sanzo, and G.N. Keating, *CO2-PENS: Development of a Spatially Coherent System-level Tool for Performance Assessment of Geologic Carbon Dioxide Sequestration*, LA-UR-09-02596, Hedberg Conference of the American Association of Petroleum Geologists, Vancouver, Canada, August 16, 2009.

Steck, L., M. Begnaud, M. Romero-Yeske, K. Mackey, K. Fujita, and R. Stead, *Seismic Event Relocation in Northeastern Russia*, American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18 2009.

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Teixidor G.T., P.P. Mukherjee, G.Y. Park, and M.J. Madou, *Theoretical Evaluation of Fractal-like Electrode Characteristics for Lithium-Ion Batteries*, 215th Electrochemical Society Meeting, San Francisco, CA, May 24-29 2009.

Tomkins, C.D., B.J. Warthen, H.E. Makaruk, and M.L. Klasky, *Quantifying Errors in Density Reconstructions at DARHT*, LANL report LA-UR-10-01098, 2010.

Toole G.L, et al., *Alternative Electricity Billing Options: Blue Feather Aero., Santa Teresa NM*, report to New Mexico small business, 2009.

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Toole G.L, et al., *Alternative Electricity Billing Options: Monarch Litho Inc., Santa Teresa NM*, report to New Mexico small business, 2009.

Toole G.L, et al., *Alternative Electricity Billing Options: Rogers Inc, Santa Teresa NM*, report to New Mexico small business, 2009.

Toole G.L, et al., *Electric Reliability and Cost Analysis for Santa Teresa Industrial Park*, report to Santa Teresa, New Mexico Industrial Park Association, 2009.

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Toole G.L, et al., *Phase I Report: Task 4a.2 20% Wind Scenario Assessment of Electric Grid Operational Features*, report to National Renewable Energy Laboratory, 2009.

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Toole G.L, et al.,*Electric Service Area Assessment*, report to Joint Warfare Analysis Center J4, 2009.

Trellue, H.R., R.C. Little, M.C. White, R.E. MacFarlane, and A.C. Kahler, ENDF70*: A Continuous-energy MCNP Neutron Data Library Based on ENDF/B-VII.0,* 11th International Conference on Radiation Shielding/15th Topical Meeting of the Radiation Protection and Shielding Division of American Nuclear Society, Pine Mt., GA, April 13-18 2008, 20080413-20080418; Nucl. Tech. Vol.168, iss.3, spec. iss.SI, 832-836, 2009.

Ulrich, T.J., A.K. Van Den, P.-Y. LeBas, B.E. Anderson, M. Griffa, R.A. Guyer, *Three Component Time Reversal Imaging Using Nonlinear Elasticity*, International Congress on Ultrasonics, Santiago Chile, January 11-18 2009.

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Vesselinov, V.V., and D.R. Harp, *Decision Support Based on Uncertainty Quantification of Model Predictions of Contaminant Transport*, LA-UR-09-06553, 2010 Computational Methods in Water Resources Meeting, Barcelona, Spain, June 21, 2010.

Vesselinov, V.V., P.K. Mishra, S.P. Neuman, *Analytical Solution for Flow to a Partially Penetrating Well with Storage in a Confined Aquifer,* LA-UR-09-05668, 2009 American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18 2009.

Viswanathan, H.S., and A.I. Abdel-Fattah, *An Experimental and Theoretical Framework for Reactive Micromixing,* Immigration Exhibit, LA-UR-09-07806.

Vrugt, J.A., *Reconciling Models With Data*, LDRD Day Meeting, Santa Fe, NM, September 14 2009.

Wang, M., and Q. Kang, *Electrokinetic Transport in Realistic Nanochannels,* 62nd American Physical Society Division of Fluid Dynamics, Minneapolis, MN, November 22-24 2009.

Wang, M., and Q. Kang, *Interfacial Electrokinetic and Reactive Transport Phenomena in Micro and Nanopores of Permeable Media,* Journal Article, LA-UR-09-07605.

Wang, M., and Q. Kang, *Ion Transport In Nanofluidic Channels*, 2009 ASME 2nd Micro/Nanoscale Heat and Mass Transfer Conference, Shanghai, China, December 20 2009.

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Wang, Y., and L. Huang, *Reverse-time Migration of Time-lapse Walkaway VSP Data for Monitoring CO2 Injection*, LA-UR-10-00915.

Ward, L., and W.S. Phillips, *Broad Area Yield Estimation Using Regional Phase Data*, NNSA Proposal, LA-UR-09-01839.
Wohlberg, B., *Dictionary Construction in Sparse Methods for Image Restoration*, Report LA-UR 10-00042, Los Alamos National Laboratory; submitted to IEEE Int. Conf. Image Processing; 2010.
Wohletz, K.H., *Constraining the Evolution of Volcanic Hydrothermal Systems by 3d Field-based Thermal Models*, LA-UR-08-07469, 34th Stanford Geothermal Workshop, Stanford, CA, Feb 19-21 2009.
Wohletz, K.H., *Energetics Excavation And Geothermal Significance Of Marr Craters*, LA-UR-08-07543, 3rd Intl Maar Conference, Malargue Mendoza, Argentina, April 14-17 2009.
Xu, H., Y. Zhao, J. Zhang, D.D. Hickmott, S.C. Vogel, L.L. Daemen, and M.A. Harti, *High-P/T Neutron Diffraction Study of Hydrous Minerals*, 2009 American Geophysical Union Joint Assembly, Toronto, Canada, May 24-27 2009.
Yan, X.Q., T. Tajima, M. Hegelich, L. Yin, and D. Habs, *Theory of Laser Ion Acceleration from a Foil Target of Nanometer Thickness*, Spring Meeting of the Quantum Optics and Photonics Section of the German Physical Society 2009, University of Hamburg, Hamburg, Germany, March 2-6 2009; Appl. Phys. B Laser Optic. Vol.98, Iss.4, Spec. Iss.Si, 711-721, 2010.
Yang, X., W.S. Phillips, G.E. Randall, H.E. Hartse, and R.J. Stead, *Developing Frequency Dependent 2d Attenuation Models for Asia*, 2009 Seismological Society of America Annual Meeting, Monterey, CA, April 8-10 2009.
Zajic, D., M. Brown, M. Nelson, and M. Williams, *Description and Evaluation of the QUIC Droplet Spray Scheme: Droplet Evaporation and Surface Deposition*, 16th AMS Conf. Appl. Air Poll. Met., Atlanta, GA, 2010.
Zhang, Z., and L. Huang, *Wave-Equation Migration of Time-Lapse VSP Data for Monitoring CO2 Injection at Aneth Utah*, LA-UR-10-01120, 9th Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 10, 2010.
Zhang, Z., L. Huang, J. Rutledge, and H. Denli, *Source Repeatability of Time-lapse Offset VSP Surveys for Monitoring CO2 Injection*, LA-UR-09-08150, 2009 American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18, 2009.
Zhang, Z., L. Huang, J. Rutledge, and H. Denli, *Source Repeatability of Time-Lapse Offset VSP Surveys for Monitoring CO2 Injection*, 2009 American Geophysical Union Fall Meeting, San Francisco, CA, December 14-18 2009.
Zhou, R., L. Huang, H. Denli, and J. Rutledge, *Double-Difference Tomography Using Microearthquake Data for Monitoring CO2 Injection at Aneth UT*, LA-UR-09-00353, 8th Annual Conference on Carbon Capture and Sequestration, Pittsburgh, PA, May 4-7, 2009.
Zhou, R., L. Huang, J. Rutledge, H. Denli, and H. Zhang, *Double-Difference Tomography of Microseismic Data for Monitoring Carbon Sequestration*, Society of Exploration Geophysicists Annual Meeting, Houston, TX, October 25-30 2009.
Ziock, H.J., and S.A. Colgate, *Is Information Possible Without Life?*, Decade of The Mind IV, Santa Ana Pueblo, NM, January 14-15 2009.
Zou, R., T.E. Larson, D.D. Hickmott, and Y. Zhao, *Hydrogen Storage on Nanoporous Metal-Organic Framework Materials*, LANL-NEDO/AIST Workshop on Hydrogen Storage, Boston, MA, December 4 2009.
Zyvolosk, G., *Calibrating Coupled Heat-Mass-Stress Simulations Constrained with Seismic Data*, Energy Wind And Water Workshop, Auckland University, New Zealand, February 9-12 2009.
Zyvoloski, G.A., *Stress-Dependent Fracture-Aperture Relationships for Geothermal Energy Applications*, 2009 American Geophysics Union Fall Meeting, San Francisco, CA, December 14-18 2009.

Books

Pepper, D.W. and D.B Carrington, *Modeling Indoor Air Pollution*, Imperial College Press Inc, London, UK, April 2009.

Open Source Electronic Contributions and Other Software Contributions

Arrowsmith, S.J., InfraMonitor toolbox (not open source), LA-CC-10-023
CONSIM is a 110,000 line code to simulate satellite instrumentation response to nuclear explosions and backgrounds. It takes weapon outputs, such as those generated by X division, and propagates the signals through the atmosphere, through the detector response, through the satellite computer process, to the generation of the telemetry. It then simulates the ground processing in order to develop analysis techniques. CONSIM handles the neutrons, prompt x-rays, prompt gamma-rays, delayed gamma-rays, and electromagnetic pulses from nuclear weapons. LANL instruments that measure these emissions are placed on every GPS satellite, on the "DSP" series of satellites, and, soon, on a new series of geostationary satellties. This code is used by DoD in an operational system that maintains 24/7 monitoring for nuclear explosions worldwide. The LANL codes provide the simulation ability to test that system and the analysis techniques that are used to analyze any nuclear explosion. LANL also provides codes used to understand the performance of the entire constellation of satellites. A special, unique capability that was developed for this code is the ability for the instrument simulations to be used directly in the flight software executable. This provides a method to test the flight software prior to launch and to generate exact telemetry.
Cubit to KIVA-4 (LA-CC-09-098)
DREAM (Dynamic Radiation Environment Assimilation Model) - LANL developed the science software used by the Burst Alert Telescope (BAT) instrument on NASA's Swift gamma-ray burst explorer satellite. This software maintains operation and calibration of a large detector array (32,768 individual detectors) and analyzes the data for the sudden rate increases that indicate astrophysical transients. It produces images of the events, by the coded aperture method, to accurately locate the transient sources, then autonomously commands the spacecraft to slew to point narrow-field instruments at the new source for follow-up observations, while it notifies observers on the ground to enable their follow-up campaigns. The 'trigger' code that detects rate increases has also been modified and incorporated into the SABRS NUDET system.
Real-Time DREAM (Dynamic Radiation Environment Assimilation Model) installed at the AFRL Space Weather Forecast Lab in Albuquerque, November 2009.
GENIE – Various users outside LANL, including US Government agencies and universities.
Glimmer-Community Ice Sheet Model (Glimmer-CISM)
Grove, J.W., AmhcTools, Solution Verfication Tool
Kang, Q., Publicly available software, 2DLBMMP v 1.0 (LA-CC-07-003), 2007-2009.
Kang, Q., Two dimensional lattice Boltzmann method for multi-phase flow, 2DLBMMP, 2007-2009.
KIVA-4
KIVA-4mpi
KIVA-hpFE
Le Bas, P.-Y., Development of a data acquisition and analysis software for NDE (Resonance Inspection Techniques and Analyses)
Lichtner, P.C., PFLOTRAN v2.0, LA-CC-09-047
Livescu, D., J. Mohd-Yusof, M.R. Petersen, and J.W. Grove, *CFDNS- A computer code for direct numerical simulation of turbulent flows*, LA-CC-09-100.
Los Alamos Sea Ice Model (CICE)

Mohd-Yusof, J., *Direct Numerical Simulation of Fluid Flow on Roadrunner*, Electronic Archive
Parallel Ocean Program (POP)
Pasqualini, D., CLEAR Vers. 2.0 for unconventional fossil fuels, LA-CC-09-064, July 22, 2009
Pasqualini, D., CLEAR Vers. 2.0, LA-CC-09-065, July 22, 2009
The Los Alamos Accelerator Code Group software comes in two groups: • Freely available software packages: Superfish, Trace and Parmila. In 2009 there were a total of 2402 downloads from our website. • Controlled software packages (for some users license bearing): Parmela and Parmteq. In 2009 a total of 40 licenses have been sold or given out to US government laboratory users.
Ulrich, T.J., Development of a data acquisition and analysis software for NDE (Resonance Inspection Techniques and Analyses)

Program Development Initiatives and Programs

Staff in the CPAM capability area are actively engaged in program development initiatives and programs with other federal agencies, national laboratories, universities, and industry. The following list shows descriptions of some programs and initiatives. The list was compiled via selective submissions by staff in this capability area.

Federal Agencies

Smart Grid security with DTRA

Academia

Contract Agreements with Iowa State University, Contract #s 74355-001-09 and Basic Agreement # 74968.000.00 for FY10. This contract is for work related to increasing KIVA-4 modeling capability representing the appropriate physical processes accurately by incorporating the following: appropriate physical modeling of heat transfer with variable and evolving temperatures throughout the engine domain. Iowa State University Department of Mechanical Engineering and Dr. Kong are providing the assistance on this contract.
Contract Agreements with Purdue University, Calument, Contract # 81841-001-10 through FY10 (with some carry-over expected). This contract is for work to increase the capability of KIVA combustion modeling. Model development to address accuracy and robustness by increasing both grid resolution and the spatial accuracy of the model's discretization while at the same time increasing the robustness of the grid evolution. This while minimizing the amount of computational requirements for well-resolved, time-dependent solutions. To accomplish this the development of new discretization is required, known as the characteristic-based split (CBS) method using an hp-adaptive finite element (FE) system for grid and equation/dependent variable representation.
Contract Agreements with University of Nevada, Las Vegas, Contract # 81 840-001 -10 through FY10 (with some carry-over expected).
Purdue's department of Mechanical Engineering and Dr. Wang are providing assistance with the hp-adaptive algorithm development and validations.
Subcontract 57206-001-07 with University of Colorado, Boulder 08/15/2007-08/15/2010 The University will perform Direct Numerical Simulations (DNS) using the Dynamically Adaptive Wavelet Collocation (DAWC) method and analysis of compressible turbulent mixing with applications to the compressible Rayleigh-Taylor instability. This work is the first attempt of DNS of compressible turbulent mixing using adaptive mesh methodologies.
Subcontract 73697-001-09 with Missouri University of Science and Technology 04/01/2009-10/01/2009 The University used a novel experimental setup for studies of large accelerations and geometrical effects on the growth of Rayleigh-Taylor instability, not possible in the context of previous experiments. This research effort has provided experimental results necessary for the development and validation of models for the turbulent growth of a Rayleigh-Taylor unstable fluid system.
Subcontract 75219-001-09 with Ohio State University 04/01/2009-06/30/2009. The University has developed a prototype volume rendering code that can be used to produce movies of turbulent flow from large data sets.
UCOP coding theory with University of California, Santa Barbara.
University of Nevada Los Vegas Department of Mechanical Engineering and Dr. Pepper are providing assistance with general algorithm development and validations.

Multiple Agencies

Hybrid Multicore Consortium, First Annual Workshop, January 19-22, Burlingame, CA. Participated in discussions with vendors and other HPC users on design and provisioning of next-generation computing architectures and software infrastructure. Primary focus was on Applications and Libraries, and Programming Models.	
Sharing graduate students with University of California, Santa Barbara on two different IMMS funded projects • Development of Coarse-Grained Models for Protein Aggregation • A course grained lipid model for studying inhomogeneous membrane interfaces	
Statistical Physics and Computer Science, Cornell University and Massachusetts Institute of Technology.	

Regular Colloquia, Seminars, or Discussion Series Organized by LANL

The following list shows the variety of colloquia, seminars, and discussion series organized at LANL by the CPAM capability area staff. The list was compiled via submissions by staff in this capability.

- Q-Bio Seminar Series. This weekly series of seminars aims to advance predictive modeling of cellular regulation, decision making, and other information processing phenomena. The emphasis is on deep theoretical understanding, detailed modeling, and quantitative experimentation directed at understanding the behavior of particular regulatory systems and/or elucidating general principles of cellular information processing.See http://cnls.lanl.gov/q-bio/seminar-series/index.php/CNLS_q-bio_Seminars. Organizers: S. Gnana Gnanakaran, W. Hlavacek, Y. Jiang, A. Zilman, B. Munsky

- Staff Activity Seminar, CCS-2 Seminar Series, monthly (approx), since 1985.

- The Statistical Sciences Group (CCS-6) hosts a seminar series, which features presentations by speakers on a broad area of statistical topics, with many of the talks of interest to researchers on Monte Carlo methods. Kary Myers, CCS-6, is the current Seminar coordinator.

- Theoretical (T) Division hosts a weekly Phsyics of Algorithms weekly seminar series and Smart Grid weekly seminar series. See http://cnls.lanl.gov/~chertkov/SmarterGrids/seminars.html for a full list of speakers and talks. (POC: Misha Chertkov, Chertkov@lanl.gov)

Conferences and Workshops Organized by LANL

Staff in the CPAM capability area host and/or organize a broad variety of conferences and workshops designed to foster active participation by a wide range of collaborators and potential collaborators in academia, other research laboratories, and industry. This list was compiled via submissions by staff in this capability area.

Ambrosiano, J., participant, contributor, Risk 2009 Workshop, Santa Fe, NM, April 2009.
Annual Santa Fe Cosmology Workshop at St. John's College, July 2009
Bettencourt, L.A.M., *Information Processing in Complex Systems* Seminar series, held at the Center for Non-Linear Science, LANL.
Coblentz, D., 2007-2009, Organizer of the Colorado Rocky Mountain Experiment
Coblentz, D., 2008-2009, Southeast Asian Stress Map Collaboration/Workshop
Coblentz, D., Seismic Transect (CREST) yearly workshop
Energy for the 21th Century, May 18-22, 2009. (http://cnls.lanl.gov/annual29/)
Finn, J.M., co-organizer of CNLS (Center for Nonlinear Studies, Los Alamos) workshop: Monge-Kantorovich Optimal Transport: Theory and Applications", Oct. 2009.
Huang, L., 2009, American Geophysical Union Fall Meeting Union Session, "Geophysical Monitoring, Verification, and Accounting for Geologic Carbon Sequestration"
Huang, L., 2009, Society for Exploration Geophysicists Summer Research Work on Carbon Sequestration Geophysics
Jiang, Y., Minisymposium on *Mathematical Modeling of Cancer Development*, First Joint Society for Mathematical Biology and Chinese Society for Mathematical Biology Meeting, Hangzhou, China, June 14-17, 2009.
Jiang, Y., W. Hlavacek, I. Nemenman, and M. Wall, M., Fourth q-bio Conference: Information Processing in Cellular Signaling and Gene Regulation, Santa Fe, NM, August 11-14, 2009.
Jiang, Y., W. Hlavacek, I. Nemenman, and M. Wall, M., Physics of Cancer Seminar and Lecture Series, Los Alamos, NM, 2009-2010.
Jiang, Y., W. Hlavacek, I. Nemenman, and M. Wall, Third q-Bio Summer School, Los Alamos, NM, July 20 - August 5, 2009.
Jiang, Y., W. Hlavacek, I. Nemenman, M. Wall, and A. Zilman, Third q-Bio Conference: Information Processing in Cellular Signaling and Gene Regulation, Santa Fe, NM, August 5-9, 2009.
Kang, Q, Session Chair, "Pore-scale reactive transport modeling and upscaling to the continuum scale", XVII International Conference on Computational Methods in Water Resources, San Francisco, CA, July 6-10, 2008.
Kang, Q., The 3rd International Workshop on Energy Conversion, Kyoto, Japan, November, 25-27, 2009.
Keating, G., and F. Perry, Technical session, "Climate Change Impacts on Society: Interface Between Earth Systems Science and Policy Making," Geological Society of America fall meeting, Portland, OR, October 18, 2009.

Larmat, C., special session, "Slow Slip and Non-volcanic Tremor in Cascadia and Beyond: Observations, Models and Hazard Implications," Geological Society of America, 2009/
Le Bas, P.-Y., the XIV International Conference on Nonlinear Elasticity in Material was co-organized by LANL in Lisbon, Portugal (http://www-ext.lnec.pt/LNEC/XIVICNEM/index.htm) June 1-5, 2009.
Lipnikov, K., co-organizer: Minisymposium *Advanced Discretization Methods*, International Conference on *Mathematics of Finite Elements and Applications*, Brunel University, London, UK, June 2009.
Maceira, M., and C.A. Rowe, special session, "Slow Slip and Non-volcanic Tremor in Cascadia and Beyond: Observations, Models and Hazard Implications," Geological Society of America, 2009.
Owczarek, R., Special Session, "Subjects in between Pure and Applied Mathematics," 2010 Spring Western Section Meeting, Albuquerque, NM, April 17-18, 2010.
Q-bio Summer School on Cellular Information Processing (2010), July 26-August 11, 2010. (http://cnls.lanl.gov/q-bio/wiki/index.php/The_Fourth_q-bio_Summer_School_on_Cellular_Information_Processing)
Wang, M., Scientific Committee, The 3rd International Symposium on Nonlinear Dynamics, Shanghai, China, Sept. 25-28, 2010.
Wilson, C., and G. Geernaert, Arctic Watershed Evolution Workshop: towards better predictive models of terrestrial arctic change, Sept 15-16 2009.

Educational Programs Organized by LANL

Ambrosiano, J., student mentor, April 2010 to present
Baldridge, W.S., SAGE, the Summer of Applied Geophysical Experience, is a unique educational program designed to introduce students in geophysics and related fields to hands-on geophysical exploration and research. The program emphasizes both teaching of field methods and research related to a variety of basic and applied problems. SAGE is hosted by the Institutes and the Earth and Environmental Sciences Division of the Los Alamos National Laboratory. http://www.sage.lanl.gov/
Coblentz, D., 2007-2009, Organizer of the Colorado Rocky Mountain Experiment
Coblentz, D., 2008-2009, Southeast Asian Stress Map Collaboration/Workshop
Coblentz, D., Seismic Transect (CREST) yearly workshop
Huang, L., 2009, AGU Fall Meeting Union Session, "Geophysical Monitoring, Verification, and Accounting for Geologic Carbon Sequestration"
Huang, L., 2009, SEG Summer Research Work on Carbon Sequestration Geophysics
Organizing a four-part course for Q-bio summer school on "multi-scale modeling of biomolecules" (POC: S. Gnanakaran) (http://cnls.lanl.gov/q-bio/wiki/index.php/Fourth_q-bio_Summer_School:_Multiscale_Modeling_of_Biomolecules)
Schultz-Fellenz, E. and A. Sussman, The Earthwatch Institute engages people worldwide in scientific field research and education to promote the understanding and action necessary for a sustainable environment. Earthwatch believes that teaching and promoting scientific literacy is the best way to systematically approach and solve the many complex environmental and social issues facing society today. I run the Tectonics and Volcanism of the Rio Grande Rift Expedition. http://www.earthwatch.org/
Schultz-Fellenz, E., Earth Sciences Co-Lead (LANL), DOE Academies Creating Teacher Scientists (ACTS) 2009
Sussman, A., DOE Academies Creating Teacher-Scientist (ACTS) Program. The Los Alamos Earth and Space Science Academy program is a professional development experience designed for teachers working at the high school and middle school levels. The program is delivered as one site for the US Department of Energy Office of Science Academies Creating Teacher Scientists (ACTS) program. http://www.scied.science.doe.gov/scied/ACTS/programs/LANL_TAI.html
Sussman, A., Expanding Your Horizons: Like the national network model, Northern New Mexico EYH's mission is to encourage young women to pursue science, technology, engineering and mathematics (STEM) careers. Through Expanding Your Horizons (EYH) Network programs, we provide STEM role models and hands-on activities for middle and high school girls. Our ultimate goal is to motivate girls to become innovative and creative thinkers ready to meet 21st Century challenges. http://www.expandingyourhorizons.org/
Sussman, A., Science Education Institute of the Southwest (SEIS) Summer Course. The mission of the SEIS is to promote advancement in the teaching and learning of science by providing high quality professional development and research opportunities for K-12 educators, building a network of educators to support best teaching practices and intellectual growth, facilitating partnerships and community involvement to promote high quality science education, and collecting data and publishing results on the effectiveness of SEIS activities. I will be running a course called The Valles Caldera: A Tuff Act to Follow. http://www.seisinstitute.org/about/mission.html

Honorary Memberships in Professional Organizations

Ben-Naim, Eli, American Physical Society, Fellow
Ben-Naim, Eli, Institute of Physics, Fellow
Chertkov, Misha, American Physical Society, Member
Dixon, P R., America Chemical Society since 1990
Gubernatis, Jim, IUPAP Computational Physics Chair
Hemez, F., Senior Member, American Institute of Aeronautics and Astronautics
Hyman, J.M., Society for Industrial and Applied Mathematics Fellow
Longmire, P., American Chemical Society
Longmire, P., American Geophysical Union
Longmire, P., Geochemical Society
Longmire, P., International Geochemical Society
Longmire, P., National Ground Water Association
Lookman, Turab, American Physical Society, Member
Mora, C.I., American Geophysical Union
Mora, C.I., Geological Society of America (Fellow)
Mora, C.I., Soil Science Society of America
Rasmussen, Kim, American Physical Society, Member
Reichhardt, Charles, American Physical Society, Member
Wendelberger, J. R., American Statistical Association, Fellow
Wendroff, B., Society for Industrial and Applied Mathematics Fellow

Professorships, Committees, and Editorial and Advisory Board Memberships

Staff in the CPAM capability area are active in the external research community by serving on committees and advisory boards and as adjunct professorships with academic institutions. The list was compiled via submissions by LANL staff in this capability area.

Abdel-Fattah, A.I., International Advisory Board of Electrokinetics, U.S. Representative and Standing Member
Abdel-Fattah, A.I., Technical Advisory Board for International conferences (ELKIN), Member
Albright, B., DOE OFES and SBIR grant proposals reviewer
Albright, B., Guest Editor, Journal of Physics Conference Series
Albright, B., National Science Foundation grant proposals reviewer
Ambrosiano, J., member National Center for Food Safety and Defense (NCFPD) Research Evaluation and Advisory Panel, 2009 to present
Ben-Naim, E, *Europ. J. Phys. B*, Editorial Board
Ben-Naim, E, *J. Phys. A*, Editorial Board
Ben-Naim, E, University of New Mexico, Adjunct Professor
Bent, R., Associate of Brown University Optimization Laboratory
Bent, R., Member of Constraint Programming Society in America
Bettencourt, L.M.A., Editorial Board of Mathematics in Computer Science
Bettencourt, L.M.A., Editorial Board of Sustainability
Bettencourt, L.M.A., Reviewer for Department of Energy
Bettencourt, L.M.A., Reviewer for National Institutes of Health,
Bettencourt, L.M.A., Reviewer for National Science Foundation
Bettencourt, L.M.A., Reviewer for Netherlands Organization for Scientific Research
Bettencourt, L.M.A., Reviewer for Swiss National Science Foundation
Bettencourt, L.M.A., Reviewer for UK's EPSERC
Brown, F., Chair, Advisory Board, Nuclear Engineering and Radiological Science, University of Michigan
Brown, F., Chair, OECD/NEA Expert Group on Monte Carlo Source Convergence and Advanced Monte Carlo Techniques
Brown, F., General Chair, American Nuclear Society PHYSOR-2012 Conference
Brown, F., Technical Program Committee, American Nuclear Society Mathematics and Computation 2009 Conference
Brown, F., Technical Program Committee, American Nuclear Society PHYSOR-2010 Conference
Brown, F., Technical Program Committee, Monte Carlo and Supercomputing for Nuclear Applications 2010 Conference
Brown, M.J., Chair, AMS Committee on Meteorological Aspects of Air Pollution
Brown, M.J., Ph.D. Committee member for Balwinder Singh, University of Utah
Carrington, D.B, Begell House, Inc, *Thermopedia*, Editor

Carrington, D.B., American Society of Mechanical Engineers, K-12 AeroSpace Heat Transfer Technical Advisory Committee, Member
Carrington, D.B., American Society of Mechanical Engineers, K-20 Computational Heat Transfer Technical Advisory Committee, Member
Chartrand, R., Lead Guest Editor, Journal of Selected Topics on Signal Processing vol 4, issue 2, 2010; Special Issue on Compressive Sensing
Coblentz, D., University of New Mexico, Adjunct Professor
Cooper, M.D.; Brookhaven National Laboratory, RHIC Technical Advisory Committee, Member
Dai, Z., Advance in Water Resources, Reviewer
Dai, Z., ChangAn University, China, Adjoint Professor
Dai, Z., Experimental Program to Stimulate Competitive Research (EPSCoR) of the Department of Energy, proposal reviewer
Dai, Z., Florida State University, Adjunct Professor
Dai, Z., Geophysical Research Letters, Reviewer
Dai, Z., Geosphere, Reviewer
Dai, Z., Ground Water, Reviewer
Dai, Z., Hydrogeology Journal, Reviewer
Dai, Z., Hydrological Sciences Journal, Reviewer
Dai, Z., Journal of Contaminant Hydrology, Reviewer
Dai, Z., Journal of Hydrology, Reviewer
Dai, Z., National Science Foundation-Division of Earth Sciences, Hydrologic Sciences Program, proposal reviewer
Dai, Z., Shichuan University, China, Adjoint Professor
Dai, Z., Transport in Porous Media, Reviewer
Dai, Z., Water Resources Research, Reviewer
Daughton, W., Panel member DOE Scientific Grand Challenges: Fusion Energy Sciences and the Role of Computing at Extreme Scale
Deshpande, A., Journal of Infectious Diseases, Reviewer
Dubey, M.K., Atmospheric Chemistry and Physics, Reviewer
Dubey, M.K., Department of Energy, Proposal Reviewer
Dubey, M.K., Geophysical Research Journal, Reviewer
Dubey, M.K., Journal of Geophysical Research, Reviewer
Dubey, M.K., NASA, Proposal Reviewer
Dubey, M.K., National Energy and Technology Laboratory, Proposal Reviewer
Dubey, M.K., National Science Foundation, Proposal Reviewer
Fabryka-Martin, J., National Academies of Science's Waste Form Technology and Performance Committee, Member
Favorite, J., Editorial Advisory Board, Annals of Nuclear Energy
Finn, J.M., NSF-DOE review panel on plasma physics, February 2009

Garimella, R.V., Editor, Special issue of Engineering with Computers based on papers from the 17th International Meshing Roundtable held in Pittsburgh, PA Oct 2008
Grove, J.W., Associate Editor, Computers and Mathematics with Applications, Elsivier
Grove,J.W., Adjust Professor, Stony Brook University
Grove,J.W., Proposal Review Advisor, National Science Foundation
Habib, S., DOE HEP Early Career Program Panel
Habib, S., DOE HEP Graduate Fellowship Committee
Habib, S., Uncertainty Quantification Panel at the joint NNSA/DOE SC Workshop
Haffenden, R., Committee on Disposal of Legacy Nerve Agent GA and Lewisite Stocks at Deseret Chemical Depot, 2009
Haffenden, R., Committee on Review of Chemical Agent Secondary Waste Disposal and Regulatory Requirements, 2007
Haffenden, R., Committee on Review of Secondary Waste Disposal Planning for the Blue Grass and Pueblo Chemical Agent Destruction Pilot Plants, 2008
Haffenden, R., Committee on Review of the Design of the Dynasafe Static Detonation Chamber (SDC) System for the Anniston Chemical Agent Disposal Facility, 2010
Haffenden, R., National Research Council of The National Academies, Board on Army Science and Technology
Hagberg, A.A., DOE Young Investigators Review Panel, Fall 2009
Hartse, H., National Nuclear Security Administration, Proposal reviewer
Hartse, H., National Science Foundation, Proposal reviewer
Hartse, H., of National Academy of Sciences Subcommittee on Seismology, Member
Heitmann, K., NSF Review Panel Member, N-body Simulations
Hemez, F., Funding Proposal Reviewer, Royal Society
Hemez, F., Member, International Modal Analysis Conference Advisory Board
Hemez, F., PSAAP Committee member, University of Michigan, 2009
Higdon, D., Technometrics, Associate Editor
Hoffman, N., DOE HEDLP Joint Program proposal reviewer
Hoffman, N., DOE OASCR ALCC proposal reviewer
Hoffman, N., NNSA ASC PSAAP Academic Alliances Strategy Team
Honnell, K., Industrial Advisory Committee, New Mexico Technical University, Department of Chemical Engineering
Huang, L., Communications in Computational Physics, Associate Editor
Huang, L., Communications in Computational Physics, Guest Editor
Huang, L., SEG CO2 Subcommittee, Member
Huang, L., SEG Conference Proceedings, Reviewer
Huang, L., SEG Publication Committee, Member
Huang, L., SEG Research Committee, Member

Huang, L., Technical Advisory Committee, RPSEA (Research Partnership to Secure Energy for America), Member
Hyman, J.H, Adjunct Professor of Mathematics, University of Arizona
Hyman, J.H, Assoc. Editor for the International Journal of High-Speed Computing
Hyman, J.H, Assoc. Editor for the Journal of Mathematics and Computing with Applications
Hyman, J.H, Assoc. Editor for the SIAM Journal of Scientific and Statistical Computing
Hyman, J.H, Chair Board of Trustees for the Institute of Pure and Applied Mathematics (IPAM)
Hyman, J.H, Chair Nomination Committee for Nonlinear Waves and Coherent Structures SIAM Activity
Hyman, J.H, Chair of the Institute for Pure and Applied Mathematics (IPAM) Board of Trustees
Hyman, J.H, Editor-in-Chief SIAM Frontier Book Series
Hyman, J.H, Member Canadian Mathematics of Information Technology and Complex Systems (MITACS) Board of Trustees
Hyman, J.H, Member of 2011 International Computational, Industrial and Applied Math Conf. proposal team
Hyman, J.H, Member of the Joint Policy Board for Mathematical Sciences
Hyman, J.H, Member of the SIAM Board of Trustees
Hyman, J.H, Member of the SIAM Science Policy Committee
Hyman, J.H, Member Tulane University Science and Engineering Advisory Board
Jiang, Y., Board of Directors for Society of Mathematical Biology, 2007-present
Jiang, Y., Guest Editor, Special Issue on Quantitative Biology for IET Systems Biology, 2008, 2009
Johnson, P.A, University of Paris, Associate professor
Johnson, P.A, Wave Motion, Associate Editor
Jordanova, V.K., LANL, NASA/LWS Committee on Space Computation, Member.
Kang, Q., Advances in Water Resources, Reviewer
Kang, Q., Chemical Engineering Communications Reviewer
Kang, Q., Chemical Geology, Reviewer
Kang, Q., Communication in Computational Physics, Reviewer
Kang, Q., Geophysical Research Letters, Reviewer
Kang, Q., Ground Water, Reviewer
Kang, Q., International Journal for Numerical Methods in Engineering, Computers and Mathematics with Applications, Reviewer
Kang, Q., International Journal of Heat and Mass Transfer, Reviewer
Kang, Q., Journal of Computational Physics, Reviewer
Kang, Q., Journal of Contaminant Hydrology, Reviewer
Kang, Q., Journal of Hydrology, Reviewer
Kang, Q., Physical Review E, Reviewer
Kang, Q., Physics of Fluids, Reviewer
Kang, Q., Review of Geophysics, Reviewer

Kang, Q., SPE Journal, Reviewer
Kang, Q., Transport in Porous media, Reviewer
Kang, Q., Water Resources Research, Reviewer
Kang, Q., Zeitschrift für Naturforschung, Reviewer
Keating, G., Regional Sustainability Working Group, Initiative for Science, Society, and Policy, University of Southern Denmark, Odense, Member
Le Bas, P.-Y., Acta Acustica united with Acustica, Reviewer
Le Bas, P.-Y., Cement and Concrete Research, Reviewer
Le Bas, P.-Y., Geophysical Journal International, Reviewer
Le Bas, P.-Y., Journal of the Acoustical Society of America, Reviewer
Le Bas, P.-Y., Philosophical Magazine, Reviewer
Le Bas, P.-Y., Wave Motion, Reviewer
Lichtner, P. C., DOE-SciDAC organizing committee, Member
Lipnikov, K., Panel member, DOE SciDAC Mid-Term Review of Applied Partial Differential Equations Center (APDEC), Washington DC, April 21, 2009
Livescu, D., Member in the Ph.D. Comprehensive Examination Committee, University of Colorado, Boulder
Lookman, T, University of Toronto, Adjunct Professor
Lowrie, R.B., Texas A&M University, Adjunct Faculty
Mohd-Yusof, J., DOE ASCR Review Panel, Reviewer
Mohd-Yusof, J., DOE EPSCoR Review Panel, Reviewer
Mora, C. I., EAR (Earth Sciences) on AC-GEO committee chair
Mora, C. I., Geoderma, reviewer
Mora, C. I., National Research Council Board of Earth Sciences and Resources, Board Member
Mora, C. I., National Science Foundation Geoscience Directorate Advisory Committee, Board member
Mora, C. I., Nature, Reviewer
Mora, C. I., University of New Mexico, Adjunct Professor
Mora, C. I., University of Tennessee, Adjunct Professor
Moulton, J.D., DOE Young Investigators Review Panel, Fall 2009
Moulton, J.D., DOE/Office of Science ASCR Review Panels
Moulton, J.D., NSERC (Canada) Review Panels
Moulton, J.D., NSF Review Panels
Moulton, J.D., Organizing Committee Member: Copper Mountain Conference on Multigrid Methods, Biennielly in Copper Mountain, CO, member since 2002. Co-editor of the conferences' special issues of Numerical Linear Algebra with Applications since 2003.
Omberg, K., American Chemical Society Committee on Budget and Finance, Associate Member
Omberg, K., American Chemical Society Committee on Chemistry and Public Affairs, Chair
Owczarek, R., Bulletin of the Seismological Society of America, Reviewer
Owczarek, R., Classical and Quantum Gravity, Reviewer

Owczarek, R., Journal of Physics, Reviewer
Owczarek, R., Mathematical Reviews, Reviewer
Owczarek, R., Physical Review E, Reviewer
Owczarek, R., Physical Review Letters, Reviewer
Schultz-Fellenz, E., Geological Society of America Academic and Applied Geoscience Relations Committee, Chair
Schultz-Fellenz, E., Geological Society of America Minorities and Women in the Geosciences Committee, Member
Shaskov, M., Associate Editor SIAM Journal on Numerical Analysis
Sussman, A., Cafe Scientifique Advisory Board, Member
Sussman, A., Crawford Field Prize Committee, Member
Sussman, A., Expanding Your Horizons Board, Member
Sussman, A., Los Alamos Women in Science, Vice President
Sussman, A., University of New Mexico, Adjunct Professor
Swart, P.J.; Institute for Pure and Applied Mathematics, Member, Board of Trustees
T Division: Advisory Group, Southwestern Biofuels Association - involved in New Mexico State Plan for Biofuels
T Division: Involved with New Mexico Alzheimer's association for creating awareness and funding for Alzheimer's disease
T Division: PhD Thesis Committee (2009-), Megan Murphy, Immunology and Molecular Pathogenesis, Emory University
Toole, G.L., University of Missouri, Columbia, College of Engineering, Homeland Security Adjunct Professor
Travis, B.J., NASA, Proposal reviewer
Travis, B.J., National Science Foundation, Proposal reviewer
Urbatsch, T., Member of editorial board, Defense Research Review
Wang, M., Fuels and Energy Science Journal, Editorial Advisory Board
Wang, M., International Journal of Academic Research, Editorial Board Member
Wang, M., International Journal of Non-linear Science and Numerical Simulation, Editorial Board Member
Wang, M., Journal of Materials Science and Engineering, Editorial Board Member
Wang, M., Journal of Physics and Natural Science, Associate Editor
Wang, M., Journal of Porous Media, Editorial Board Member
Wang, M., Multiphase Transport in Porous Media, Thermopedia, Area Editor
Wang, M., Special Topics and Reviews in Porous Media-An International Journal, Editorial Board Member
Wang, M.,Special Issue of Micro/Nanotransport Phenomena in Renewable Energy and Energy Efficiency on Advances in Mechanical Engineering, Guest Editor
Wendelberger, J. R., Technometrics Youden and Wilcoxon Paper Awards Committee
Wendelberger, J. R., Technometrics, Management Committee

Winske, D., Adjunct Professor Boston University
Winske, D., DOE Plasma Physics Panel Review February 2010
Winske, D., DTRA V&V Code Review Committee 2009
Winske, D., NASA Magnetospheric Proposals Panel Review January 2010
Winske, D., National Science Foundation
Wohlberg, B.E., NSF review panels
Wohlberg, B.E., Technical Program Committee member for IEEE International Conference on Image Processing and IEEE International Conference on Acoustics, Speech, and Signal Processing
Woldegabriel, G., Deep Earth Processes Section, National Science Foundation, Program Director
Woldegabriel, G., Journal of Human Evolution , Associate Editor
Woldegabriel, G., Journal of Volcanology and Geothermal Research, Guest Editor
Woldegabriel, G., National Geographic Society, Washington D.C, Grand Reviewer
Woldegabriel, G., Scientific Executive Committee of The Leakey Foundation, California, Proposals Reviewer
Wolfsberg, A.V., Colorado School of Mines –Steering Committee for Oil Shale Symposium 2009.
Wolfsberg, A.V., External Advisory Board – University of Utah Institute for Clean and Secure Energy (ISCE), Member
Wolfsberg, A.V., LANL Energy Security Center Leadership Team, Member
Wolfsberg, A.V., US DOE Fossil Energy Subcommittee for Unconventional Fossil Fuel, Member
Wolfsberg, A.V., US DOE, Nevada Site Office – Technical Working Group (Advisory Committee) for the Underground Test Area Project, Member
Xu, H., American Mineralogist Associate Editor
Xu, H., Neutron Science Review Committee ORNL, Member
Yin, L., APS-DPP 2010 Program Committee
Yin, L., ReNew HEDLP, November 2009, Fredericks, MD
Zaharia, S., LANL, NSF/GEM Program Near-Earth Space and Plasma Focus Group, Chair.
Zaharia, S., NSF Space Weather grant reviewer.
Ziock, H., Alife XII Conference Program Committee, Member
Ziock, H., European Science Foundation Pool of Reviewer
Zyvoloski, G.A., Ground Water, Reviewer
Zyvoloski, G.A., International Journal of Offshore and Polar Engineering (for Methane Hydrate), Reviewer
Zyvoloski, G.A., Journal of Hydrology, Reviewer
Zyvoloski, G.A., Scidac-e proposals, reviewer
Zyvoloski, G.A., Transport in Porous Media, Reviewer
Zyvoloski, G.A., Vadose Zone Journal, Reviewer

Conference Proceedings and Journal Referees

Staff in the CPAM capability area serve the larger scientific community by serving as referees on technical journals. The list was compiled via submissions by LANL staff in this capability area.

Albright, B., IEEE Transactions on Plasma Science
Albright, B., Journal of Computational Physics
Albright, B., Journal of Physics, Conference Series
Albright, B., Physical Review Letters
Albright, B., Physics of Plasmas
Alluie, H., Astrophysical Journal
Alluie, H., Physics of Fluids Letters
Ambrosiano, J., referee, Risk Analysis Journal, October 2009
Bakosi, J., Physics of Fluids
Bent, R., American Association for Artificial Intelligence Conference, 2009
Bent, R., European Journal of Operational Research
Bent, R., INFORMS Journal on Computing
Bent, R., Journal of Heuristics
Bent, R., Operations Research
Bent, R., Transportation Research
Bent, R., Transportation Science
Bettencourt, L.M.A., Annals of Physics
Bettencourt, L.M.A., Complexity
Bettencourt, L.M.A., Journal of Artificial Societies and Social Simulation
Bettencourt, L.M.A., Journal of Statistical Physics
Bettencourt, L.M.A., Physica A
Bettencourt, L.M.A., Physical Review A
Bettencourt, L.M.A., Physical Review D
Bettencourt, L.M.A., Physical Review E
Bettencourt, L.M.A., Physical Review Letters
Bettencourt, L.M.A., Physics Letters A
Bettencourt, L.M.A., Physics of Plasmas
Bettencourt, L.M.A., Proceedings of the National Academy of Sciences (USA)
Booth, T., Nuclear Instruments and Methods in Physics Research B
Booth, T., Nuclear Science and Engineering
Booth, T., Proceedings, American Nuclear Society Radiation Protection and Shielding Division Meeting 2010
Booth, T., Proceedings, PHYSOR 2010 Advances in Reactor Physics to Power the Nuclear Renaissance

Brock, J.:,Scientific Committee, 6th International Conference on Sensitivity Analysis of Model Output, July 2010, Milan, Italy
Brown, F., Journal of Computational Physics
Brown, F., Journal of Nuclear Science and Technology
Brown, F., Nuclear Science and Engineering
Brown, F., Proceedings, American Nuclear Society 2009 Annual Meeting
Brown, F., Proceedings, American Nuclear Society 2009 Winter Meeting
Brown, F., Proceedings, American Nuclear Society 2010 Annual Meeting
Brown, F., Proceedings, American Nuclear Society Mathematics and Computation 2009 Conference
Brown, F., Proceedings, American Nuclear Society PHYSOR 2010 Conference
Carrington, D.B., Computational Thermal Sciences
Carrington, D.B., International Computational Heat Transfer Conference '10
Carrington, D.B., International Journal of Hydrogen Energy
Carrington, D.B., International Mechanical Engineering Congress, 09
Carrington, D.B., Summer Heat Transfer Conference, 09
Chartrand, R., Applied and Computational Harmonic Analysis
Chartrand, R., Computers and Chemical Engineering
Chartrand, R., IEEE Signal Processing Letters
Chartrand, R., IEEE Transactions on Image Processing
Chartrand, R., IEEE Transactions on Information Theory
Chartrand, R., IEEE Transactions on Pattern Analysis and Machine Intelligence
Chartrand, R., IEEE Transactions on Signal Processing
Chartrand, R., Inverse Problems
Chartrand, R., Journal of Mathematical Imaging and Vision
Chartrand, R., Journal on Computational Mathematics
Chartrand, R., Mathematical and Computer Modelling
Chartrand, R., Mathematical Programming A
Chartrand, R., Research Letters in Signal Processing
Chartrand, R., SIAM Journal on Imaging Sciences
Chartrand, R., SIAM Journal on Optimization
Chartrand, R., SIAM Journal on Scientific Computing
Chartrand, R., Signal Processing
Chartrand, R., Transactions on Medical Imaging
Coblentz, D., Earth and Planetary Sciences, referee
Coblentz, D., National Science Foundation, referee.
Coblentz, D., Tectonics, referee
Coblentz, D., Tectonophysics, referee
Daughton, W., Geophysical Review Letters

Daughton, W., Physical Review Letters
Daughton, W., Physics of Plasmas
Dimonte, G., Physical Review E
Dimonte, G., Physics of Fluids
Favorite, J., IEEE Transactions on Nuclear Science
Favorite, J., Transactions of the American Nuclear Society
Francois, M.M, Journal of Fluids Engineering, Reviewer
Francois, M.M., Computer Methods in Applied Mechanics and Engineering, Reviewer
Francois, M.M., International Journal for Numerical Methods in Fluids, Reviewer
Francois, M.M., International Journal of Multiphase Flow, Reviewer
Francois, M.M., Journal of Computational Physics, Reviewer
Fryer, C., Astrophysical Journal, referee
Garimella, R.V., Engineering with Computers
Garimella, R.V., International Journal of Numerical Methods in Engineering
Garimella, R.V., International Journal of Numerical Methods in Fluids
Gnanakaran, S., AIDS Research and Human Retroviruses
Gnanakaran, S., External Reviewer, USDA proposal
Gnanakaran, S., Journal of Theoretical Chemistry
Gnanakaran, S., Proceedings of National Academy of Sciences USA
Gnanakaran, S., Reviewer for Biophysical Journal
Gnanakaran, S., Reviewer for Proteins: Structure, Function, and Genetics
Grove,J.W., Physics of Fluids
Grove,J.W., Computers and Mathematics with Applications
Gutfraind, A., Annals of Operations Research
Habib, S., Astrophysical Journal
Habib, S., Monthly Notices of the Royal Astronomical Society
Hartse, H., Bulletin of Seismological Society of America, Referee.
Heitmann, K., Astrophysical Journal
Heitmann, K., Physical Review D
Heitmann, K., Physical Review Letters
Hemez, F., Proceedings, ICEDYN 2009, Portugal, June 2009
Hemez, F., Proceedings, USD-09 Scientific Committee, Sheffield, UK, June 2009
Hemez, F., Reviewer, Elsevier Journal of Finite Elements in Analysis and Design
Hoffman, N., Physical Review Letters
Hoffman, N., Physics of Plasmas
Honnell, K., Defense Research Review
Huang, L., Advances in Wave Propagation in Heterogeneous Earth, Referee

Huang, L., Bulletin of the Seismological Society of America, Referee
Huang, L., Communications in Computational Physics, Referee
Huang, L., Geophysical Journal International, Referee
Huang, L., Geophysical Prospecting, Referee
Huang, L., Geophysical Research Letters, Referee
Huang, L., IEEE Transactions on Medical Imaging, Referee
Huang, L., International Journal for Numerical and Analytical Methods in Geomechanics, Referee
Huang, L., International Journal of Solids and Structures, Referee
Huang, L., Journal of Geophysical Research -- Solid Earth, Referee
Huang, L., Journal of Geophysics and Engineering, Referee
Hutchens, G., Referee, Journal of Applied Physics
Jiang, Y., Biophysical Journal
Jiang, Y., Bulletin of Mathematical Biology
Jiang, Y., Cancer Research
Jiang, Y., IET-Systems Biology
Jiang, Y., Journal of Mathematical Biology
Jiang, Y., Journal of Theoretical Biology
Jiang, Y., Mathematical Medicine & Biology
Jiang, Y., Nonlinearity
Jiang, Y., Physical Biology
Jiang, Y., Physical Review E
Jiang, Y., Physical Review Letters
Jiang, Y., PLoS Computational Biology
Jiang, Y., Proceedings of National Academy of Science USA
Johnson, P. A., Applied Physics Letters, Referee
Johnson, P. A., Chu, S., Atmospheric Chemistry and Physics, referee
Johnson, P. A., Geophysical Research Letters, Referee
Johnson, P. A., Journal of Geophysical Research, Referee
Johnson, P. A., Journal of the Acoustical Society of America, Referee
Johnson, P. A., Physical Review B, Referee
Johnson, P. A., Physical Review E, Referee
Johnson, P. A., Physical Review Letters, Referee
Johnson, P. A., Science, Referee
Jordanova, V.K., Geophysical Research Letters
Jordanova, V.K., Journal of Geophysical Research
Keating, G., Bulletin of Volcanology, Referee
Kiedrowski, B., Nuclear Science and Engineering

Koo, E., International Journal of Wildland Fires (2007, 2008) and Fire Technology referee.
Lichtner, P. C., Advances in Water Resources, Referee
Lichtner, P. C., Contaminant Hydrology, Referee
Lichtner, P. C., Journal of Contaminant Hydrology, Referee
Lichtner, P. C., Water Resources Research, Referee
Lipnikov, K., Computer Methods in Applied Mechanics and Engineering
Lipnikov, K., IMA Journal of Numerical Analysis
Lipnikov, K., Journal of Computational Physics
Lipnikov, K., Mathematics and Computers in simulations
Lipnikov, K., Numerical Methods for Partial Differential Equations
Lipnikov, K., SIAM Journal on Numerical Analysis
Lipnikov, K., Transport in Porous Media
Livescu, D., International Journal for Numerical Methods in Fluids
Livescu, D., Journal of Computional Physics
Livescu, D., Journal of Engineering Mathematics
Livescu, D., Journal of Fluid Mechanics
Livescu, D., Physics of Fluids
Louis, W. C., Physical Review Letters referee
Lowrie, R.B., International Journal for Numerical Methods in Fluids
Lowrie, R.B., Journal of Computational Physics
Lowrie, R.B., Monthly Weather Review
Lu, Z., Advances in Water Resources, Referee
Lu, Z., Ground Water, Referee
Lu, Z., Hydrological Processes, Referee
Lu, Z., Journal of Contaminant Hydrology, Referee
Lu, Z., Journal of Geochemical Exploration, Referee
Lu, Z., Journal of Hydrology, Referee
Lu, Z., Journal of Porous Media, Referee
Lu, Z., Mathematical Geology, ASCE Journal of Hydrologic Engineering, Referee
Lu, Z., Natural Hazards. Referee
Lu, Z., Society of Petroleum Engineers Journal, Referee
Lu, Z., Stochastic Environmental Research and Risk Assessment, Referee
Lu, Z., Water Resources Research, Referee
Mashnik, S., Annals of Nuclear Energy
Mashnik, S., Journal of Physics A
Mashnik, S., Journal of Physics G, Nuclear and Particle Physics
Mashnik, S., Nuclear Physics A

Mniszewski, S., The Lancet Infectious Diseases
Mohd-Yusof, J., Journal of Computational Physics
Mohd-Yusof, J., Monthly Weather Review
Moulton, J.D., Applied Numerical Mathematics
Moulton, J.D., Numerical Linear Algebra and its Applications
Owczarek, R., Bulletin of the Seismological Society of America, Reviewer
Owczarek, R., Classical and Quantum Gravity, Reviewer
Owczarek, R., Journal of Physics, Reviewer
Owczarek, R., Mathematical Reviews, Reviewer
Owczarek, R., Physical Review E, Reviewer
Owczarek, R., Physical Review Letters, Reviewer
Parsons, D., Nuclear Science and Engineering
Pasqualini, D., Energy Policy, Referee
Pasqualini, D., International System Dynamics Conferences, Referee
Pasqualini, D., Journal of Acoustic Society of America, Referee
Pasqualini, D., Journal of Geophysical Research, Referee
Pasqualini, D., Physics Review B, Referee
Pasqualini, D., Regional Environmental Change, Referee
Pineda-Porras, O., Ecological Economics
Pineda-Porras, O., Journal of Pipeline Systems – Engineering and Practice, American Society of Civil Engineering
Pineda-Porras, O., Journal of Transportation Engineering, American Society of Civil Engineering
Pope, A., Astrophysical Journal
Porch, W., Journal of Atmospheric Chemistry and Physics, Referee
Porch, W., Journal of Optics Letters, Referee
Roytershteyn, V.S., Physical Review Letters
Roytershteyn, V.S., Physics of Plasmas
Saumon, D., Astrophysical Journal
Saumon, D., Physical Review E
Schofield, S.P., International Journal for Numerical Methods in Fluids
Shaskov, M., Communications in Computational Physics
Shaskov, M., Computer & Fluids
Shaskov, M., International Journal for Numerical Methods in Fluids
Shaskov, M., Journal of Computational Physics
Shaskov, M., SIAM Journal on Scientific Computing
Shores, E., Proceedings, American Nuclear Society's Radiation Protection and Shielding Division Topical Meeting, Las Vegas, NV April 2010
Shores, E., Reviewer, Nuclear Technology Journal

Singleton, R., Physical Review E
Singleton, R., Physics of Plasmas
Stauffer P. H., Desalination, referee
Stauffer P. H., ES&T, referee
Stauffer P. H., Ground Water, Referee
Stauffer P. H., IJGGC, referee
Stauffer P. H., Nuclear Technology, referee
Stauffer P. H., Vadose Zone Journal, referee
Stauffer P. H., Water Resources Research, referee
Steck, L. K., Journal of Geophysical Research and Pure and Applied Geophysics. Referee
Tonks, D., Journal of Applied Physics
Tonks, D., Physical Review Letters
Travis, B. J., Geophysical Research Letters, Referee
Travis, B. J., ICARUS, Referee
Travis, B. J., Journal on Math. Modeling, Referee
Travis, B. J., Monthly Weather Review, Referee
Travis, B. J., SIAM (Society of Industrial and Applied Mathematics), Referee
Travis, B. J., Transport in Porous Media, Referee
Urbatsch, T., reviewer, 2009 International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics, Saratoga Springs, NY, May 3-7, 2009
Urbatsch, T., reviewer, Journal of Computational Physics
Urbatsch, T., reviewer, Nuclear Science and Engineering
Urbatsch, T., reviewer, Transactions of the American Nuclear Society
Urbatsch, T., Technical Program Chair, Mathematics and Computation Division, American Nuclear Society
Wang, M., Analytical Chemistry, Referee
Wang, M., Applied Mathematics and Computation, Referee
Wang, M., Chemical Engineering Communications, Referee
Wang, M., Colloids and Surface A: Physicochemical and Engineering Aspects; Referee
Wang, M., Communications in Computational Physics, Referee
Wang, M., Computers & Fluids; Referee
Wang, M., Computers and Mathematics with Applications, Referee
Wang, M., Energy, Referee
Wang, M., Experimental Thermal and Fluid Science, Referee
Wang, M., International Journal for Numerical Methods in Fluids, Referee
Wang, M., International Journal of Heat and Fluid Flow, Referee
Wang, M., International Journal of Heat and Mass Transfer, Referee
Wang, M., Journal of Colloid and Interface Science, Referee

Wang, M., Journal of Composite Materials, Referee
Wang, M., Journal of Enhanced Heat Transfer, Referee
Wang, M., Journal of Fluid Mechanics, Referee
Wang, M., Journal of Nanoparticle Research, Referee
Wang, M., Journal of Physical Chemistry, Physica D, Referee
Wang, M., Journal of Renewable and Sustainable Energy, Referee
Wang, M., Journal of Spacecraft and Rockets, Referee
Wang, M., Langmuir (2008); Referee
Wang, M., Microfluidics & Nanofluidics, Referee
Wang, M., Molecular Physics, Referee
Wang, M., Nanoscale and Microscale Thermophysical Engineering, Referee
Wang, M., Numerical Heat Transfer, Referee
Wang, M., Physica A, Referee
Wang, M., PIME-Journal of Engineering Manufacture, Referee
Wang, M., PIME-Journal of Mechanical Engineering Science, Referee
Wang, M., Sensors and Actuators B, Referee
Wang, M., Transport in Porous Media, Referee
Wang, M., Vadose Zone Journal, Referee
Wang, M., Water Resource Research, Referee
Welling, D., Journal of Geophysical Research
Welling, D., Space Weather Journal
Wendelberger, J. R., Technometrics, American Statistician, Physics Letters A
Winske, D., Journal of Computational Physics
Winske, D., Journal of Geophysics Research
Winske, D., Physical Review Letters
Winske, D., Physics of Plasmas
Winske, D.: Geophysics Research Letters
Wohlberg, B.E., Electronics Letters
Wohlberg, B.E., EURASIP Journal on Advances in Signal Processing
Wohlberg, B.E., IEEE Signal Processing Letters
Wohlberg, B.E., IEEE Transactions on Instrumentation & Measurement
Wohlberg, B.E., IEEE Transactions on Signal Processing
Wohlberg, B.E., Pattern Recognition
Wohlberg, B.E., Transactions on Information Technology in BioMedicine
Zaharia, S., Geophysical Research Letters
Zaharia, S., Journal of Geophysical Research

Classified Reports

The following list shows the classified reports by CPAM capability area staff as submitted by staff.

2/26/2009 Presentation to Secretary of Energy, Washington, DC: 2 classified videos prepared
2008 NECDC Conference Proceedings: 3 LA-CPs submitted
2009 NEDPC 10/26-30, 2009, LLNL: 17 LA-CPs submitted
Boost Fest April 7-10, 2009, Sandia National Laboratories, NM: 2 LA-CPs submitted
JOWOG 42, 6/8-13, 2009, AWE United Kingdon: 11 LA-CPs submitted
LA-CP-09-00119, 2009, SRD, NMR and EPR Studies (U)
LA-CP-09-00142, 2009, OUO, Fate and Transport of Plutonium in Subsurface Environments (U)
LA-CP-09-00171, 2009, SRD, EMP Waveform Calibration and Digitization Project (U)
LA-CP-09-00241, 2009, N/A, Comprehensive Test Ban Treaty Evasion Scenarios and Their Bearing on US Treaty Ratification (U),
LA-CP-09-00247, 2009, OUO, Amplitude Tomography in Eastern Eurasia (U)
LA-CP-09-00259, 2009, SNSI, Ground-Based Nuclear Detonation Detection (U)
LA-CP-09-00325 2009, OUO, Passive Acoustic Detection (U)
LA-CP-09-00501, 2009, FOUO, LANL0800511321 Signatures/SNM Fessenden Task 1 Solvent Signatures in Effluents Leaving LANL Facility (U)
LA-CP-09-00502, 2009, FOUO, LANL0800611321 Signatures/SNM Fessenden Task 2a Solvents in Watershed (Mortandad Canyon) Control and Propagation (U)
LA-CP-09-00503, 2009, FOUO, LANL0800811321 Signatures/SNM Fessenden Task 2b Solvent Signature Propagation in the Environment (U)
LA-CP-09-00504, 2009, FOUO, LANL0800711321 Signatures/SNM Fessenden Task 3 Solvent Signature Development within the LANL PU Facility (U)
LA-CP-09-00536, 2009, SRD, Source to Sensor Simulation of EMP (U)
LA-CP-09-00554 2009, OUO, Full Toss Seismic Collection – LANL (U)
LA-CP-09-01087, 2009, SRD, EMP Yield Scaling (U)
LA-CP-09-01103, 2009, OUO, Patton Howard J Source Model Development: Yield Estimation (U)
LA-CP-09-01104, 2009, OUO, Patton Howard J Source Model Development: 1 Why Is It Important? 2 Outstanding Problem - Shear Wave Generation 3 Approach 4 Important Next Steps (U)
LA-CP-09-01121, 2009(U), OUO, Feasibility Of Terahertz Imaging Of HME (Home Made Explosives): Part I-Do HME Compounds Have Unique Signatures? (U)
LA-CP-09-01443 2009, OUO, Acoustic Time Reversal/Passive Acoustic Detection (U)
LA-CP-09-01540, 2009, OUO, Stable Isotope Signatures of Nuclear Processing (Task 8) Of: LANL Signatures and Observables FY2009 LA-06-SOP-528-PD09 (U)
LA-CP-09-01541, 2009, OUO, LANL 0800811321_Fessenden (U)
LA-CP-09-01629, 2009, OUO, Report on the LANL Seismic Ad-On To the Full Toss Experiment (U)
LA-CP-09-01645, 2009, SNSI, Precise Relative Relocation of the May 25 2009 North Korean Event (U)
Weapon Science Capability Review, LANL 3/25/09: 1 LA-CP submitted

Technology Transfer and Licensing

The following list includes patent disclosures, patent citations, and license and royalty income as submitted by staff.

Ambrosiano, J., ongoing tech transfer effort to commercialize Visual Crosswalk and Analysis Tool (VCAT) copyright assertion and patent application filed April 2010
Bent, R., LA-CC IEISS version 3.x
Bent, R., LA-CC LogiSims version 1.x
Clancy, S., Royalty for licensing PAGOSA export controlled software
Code Name: Cubit to KIVA-4; Classification Review Number: LA-CC-09-098;Export Control Classification Number (ECCN): EAR99; B&R Code: VT0401000
Code Name: KIVA-3V, Version 2 (C10062); Classification Review Number: LA-CC-10-035; Export Control Classification Number (ECCN): EAR99; B&R Code: VT0401000
Code Name: KIVA-4 (C10064); Classification Review Number: LA-CC-10-038; Export Control Classification Number (ECCN): EAR99; B&R Code: VT0401000
Code Name: KIVA-4mpi (C10013); Classification Review Number: LA-CC-09-103; Export Control Classification Number (ECCN): EAR99; B&R Code: VT0401000
Copyright disclosures exist for all codes in the LAACG software repository. Document control numbers are: Parmteq (LA-CC-10-046), ParmteqM (LA-CC-10-047), Parmela (LA-CC-88-030), and additional free software LA-CCs. The controlled software is distributed without charge to US national laboratories and universities. All commercial use or use in foreign countries requires payment of a license fee. The licensing income varies; in recent years we collected approximately $20,000 in fees per year. The controlled software is also export controlled, all foreign requests are going through a customs review.
EES-14, Patent application (2007) 11/894,633
EES-14, Patent application (2007) 60/936,961
EES-17, Patent application (2007) 60/901,903
EES-2, Invention disclosure (2007) S104946/L2005054
GENIE - Licensed to two companies: one for the remote sensing field of use and one for the biomedical field of use.
Greene, R., Pursuing patent for stereoscopic laser pointer
Invention disclosure (2007) S112783/L2007021
Invention disclosure (2007) S112793/L2007034
Invention disclosure (2007) S112875/L2007100
Invention disclosure (2007) S112896/L2007118
Invention disclosure (2007) S112924/L2008021
Invention disclosure (2007) S112924/L2008021
Invention disclosure (2007) S112924/L2008021
Invention disclosure (2007) S112926/L2008023
Invention disclosure (2008) S112936/L2008033
Invention disclosure (2008) S112960/L2008055

Invention disclosure (2008) S116236/L2008107
Invention disclosure (2008) S116236/L2008107
Invention disclosure (2008) S116270/L2009021
Invention disclosure (2008) S116270/L2009021
Invention disclosure (2008) S116270/L2009021
Invention disclosure (2008) S116277/L2009027
Invention disclosure (2009) S104946/L2005055
LA-CC-09-010, 2/9/09, (UCNI), RAM-SCB v1.0
Ortega, F., Assisted Technology Transfer Division to provide an exclusive license for the serial version of the General Mesh Viewer (GMV) to CPFD Software LLC.
Part of the PCT Patent (S-112,799) filed by Duke University: Acute Transmitted HIV Envelope Signatures
Patent application (2007) 7179602
Patent application (2008) 12/033,789
Patent application (2008) 12/033,841
Patent application (2008) 12/249,953
Patent application (2008) 12/249,953
Patent application (2008) 61/126,299
Patent application (2008) 61/130,938
Patent application (2009) 12/463,796
Patent application (2009) 12/463,802
Patent application (2009) 12/476,081
Patent application (2009) 61/170,070
Toole, L., Software disclosure: RCME (Renewable Capacity Mix Estimator) issued 2009

External Awards

The following list includes R&D 100s, National Academies memberships, and other external (non-LANL) awards.

American Statistical Association SPAIG Award (Statistical Partnerships among Academe, Industry, and Government) in recognition of collaboration between the Los Alamos National Laboratory Statistical Sciences Group and the Iowa State University Statistics Department.
Brown, F., Best Paper, American Nuclear Society Nuclear Criticality Safety 2009 Conference
Haruta, Amon, DOE Award, Outstanding efforts in the China Deployment (ARM - Atmospheric Radiation Measurement), 05/09
Hemez, F., 2010 Society of Experimental Mechanics Dominick DeMichele Award
Maskaly, K., 2009 R&D 100 Award (Artificial Retina Project)
Meyer, Clif, DOE Award, Outstanding efforts in the China Deployment (ARM - Atmospheric Radiation Measurement), 05/09
Nitschke, Kim, DOE Award, Outstanding efforts in the China Deployment (ARM - Atmospheric Radiation Measurement), 05/09
Roybal, Louella, DOE Award, Outstanding efforts in the China Deployment (ARM - Atmospheric Radiation Measurement), 05/09
Sanchez, Tania, DOE Award, Outstanding efforts in the China Deployment (ARM - Atmospheric Radiation Measurement), 05/09
Team, 2008 Defense Programs Awards of Excellence, National Nuclear Security Administration (NNSA), CMR Consolidation/Risk Mitigation - 30 Team Members, 2009
Travis, Bryan, R & D 100 Award, R & D Magazine, Artificial Retina, 11/09
Vrugt, Jasper, 2010 Young Scientist Award, European Geophysical Union (EGU), Recognizes young scientists who have made significant contributions to any field of geosciences within seven years of completing their Ph.D, 10/08

ISTC CPAM Statistics

FY10 Metrics Template
ISTC CPAM relevant

A. Graduate Level Courses and Participation

CAO Category: Education Programs

CAO Description: Graduate level courses offered at LANL, jointly with partner Universities, and the number of students participating in them

Directions/Definitions: Enter ALL courses offered (Student listing will show which courses "Took").
QTR (1,2,3,4); Academic Semester (Fall, Winter, Spring, Summer); Org (University or LANL Group)

Institute/ Center	Qtr	Academic Semester	Course Number	University	Course Title	Student Names/Org	CAO Report	Place on Web	Date on Web
EI	fall	2009		UCSD	Detection Theory				
EI	fall	2009		UCSD	Array Processing				
ISTI	Fall	2009		UCSC	Sensor Networks				
ISTI	fall	2009		UCSC	Knowledge Systems and Data Analytics				
ISTI	fall	2009		UCSC	Machine Learning				
ISTI		Tutorial 2009			Learning Task specific Object location				

B. Participation in Research Collaborations

CAO Category: University Technical Collaborations

CAO Description: Students and LANL staff participating in research collaborations

Directions/Definitions: University (List University research project is associated with)
Org (University or LANL Group)

Institute/ Center	Qtr	Name/Title of Research Project	University	STUDENT Names/Org	LANL Staff Names (mentor)/Org	CAO Report	Place on Web	Date on Web
		Extensive list of collaborations in IST areas including modeling and simulation, HCP, machine learning etc....						

C. Technical Papers

CAO Category: University Technical Collaborations

CAO Description: Technical papers published

Directions/Definitions: May include date of submittal for internal data, but only actual publications will be reported
Date of Publication: include citation (Volume, Issue and Page Numbers)

Institute/ Center	Qtr	Title of Technical Paper	Authors/Org	Publication Title	Date Submitted (for internal use only)	Date of Publication (include Citation)	CAO Report	Place on Web	Date on Web
		Not Applicable to this request							

D. Conference (and Workshop) Presentations

CAO Category: University Technical Collaborations

CAO Description: Presentations at national or international conferences

Directions/Definitions: Type of presentation (Poster, Presentation, Panel)

Note: List NON-national or international conferences or workshops, seminars, meetings, lectures below in "G"

Institute/ Center	Qtr	Type of Presentation	Title of Presentation	Name of Presenter/Org	Conference Name/Location/Date (National or International ONLY)	CAO Report	Place on Web	Date on Web
ISTC	1	Presentation	Equation-Free Implementation of Statistical Moment Closures	Frank Alexander, LANL/INST-OFF	Center for Computational Science Seminar Boston University Boston, Massachusetts November 13, 2009	Yes	Yes (D1)	11/13/09

E. Conferences and Workshops (Organized, Funded or Supported)

CAO Category: Science and Engineering Development

CAO Description: Conferences and workshops organized or sponsored by PADSTE Institutes

Directions/Definitions: Type of Event (Conference or Workshop)

Type of Involvement (Organized, Sponsored, Funded, Supported)

Institute/ Center	Qtr	Type of Event	Event Name/Location/Date	LANL Involvement	Names of LANL Attendees/Org (if list is extensive, include summary information only and attach list/sign-in sheet as backup)	CAO Report	Place on Web	Date on Web
ISTC	1	Conference	Los Alamos Computer Science Symposium (LACSS) 2009 La Fonda Hotel, Santa Fe, NM October 13-14, 2009	Organized, Sponsored, Supported	LANL and external participants. List not available. Committee members: Adolfy Hoisie, Chair, Los Alamos National Laboratory; Frank Alexander, Los Alamos National Laboratory; Ben Bergen, Los Alamos National Laboratory; Jack Dongarra, University of Tennessee; Salman Habib, Los Alamos National Laboratory; William Harrod, DARPA; Thuc Hoang, NNSA; Fred Johnson, SAIC; Doug Kothe, Oak Ridge National Laboratory; Stephen Lee, Los Alamos National Laboratory; Osni Marques, Office of Science; Al McPherson, Los Alamos National Laboratory; Jose Munoz, NSF; Dan Reed, Microsoft; Stephen Scott, Oak Ridge National Laboratory; Horst Simon, Lawrence Berkeley National Laboratory; Andy White, Los Alamos National Laboratory	Yes	No (E3)	
ISTC	1	Workshop	Information Science for Materials Design & Discovery LARP, Room 203A &B November 9-10, 2009	Organized, Sponsored, Funded	Turab Lookman, LANL/T-4; Joanne Wendelberger, LANL/CCS-6; Ed Kober, LANL/INST-OFF; Xiangdong Ding, LANL/T-4; Virginie Dupont, LANL/T-1; Marcel Porta, LANL/T-4; Hari Dahal, LANL/T-4; Stephen Sintay, LANL/CCS-2; Prasanna V. Balachandran, Iowa State University; Hari Narayanan, MIT; Rodney McCabe, LANL/MST-6; Chang Sun Kong, Iowa State University; Katharine Page, LANL/LANSCE-12; Jim McGuffin, Case Western Reserve University; Volker Eyert, Augsburg University; Frank Alexander, LANL/INST-OFF	Yes	Yes (E1)	11/19/09

ISTC	1	Workshop	FY-11 LDRD-DR Information Science and Technology Grand Challenge Town Hall LANL/Study Center, Cochiti/Jemez Conference Room November 24, 2009	Organized	Doug Berning, LANL/IAT-1; Malcolm Boshier, LANL/P-21; Paul Dotson, LANL/ADTSC; Joanne Wendelberger, LANL/CCS-6; Lawrence Cox, LAN:/ CCS-DO; William Hlavacek, LANL/T-6; Jared Dreicer, LANL/PADSTE; William Priedhorsky, LANL/LDRD-PO	Yes	Yes (E2)	11/16/09
ISTC	4	workshop	Data Fusion Workshop Challenges in Data Fusion I: Methods & Algorithms Study Center, Jemez Conference Room 8/27/2009	Organized	FISK MIKE ACS-PO; SHLACHTER JACK ADEPS; BISHOP ALANADTSC; DOTSON PAUL ADTSC; DJIDJEVA TATIANA CCS-3; EIDENBENZ STEPHAN CCS-3; KASIVISWANATHAN SHIVA CCS-3; GRAVES TODD CCS-6; HAMADA MICHAEL CCS-6; COX LAWRENCE CCS-DO; THORP JOHN CCS-DO; LEISHMAN DEBORAH D-6; SENTZ KARI D-6; ROMAN JORGE HPC-1; SPEARING ANDREA "SHELLY" HPC-1; CONNOR CAROLYN HPC-5; LONCARIC JOSIP HPC-5; ALEXANDER FRANK INST-OFF; SAUER NANCY INST-OFF; GEORGE JOHN P-21; SCHMIDT DAVID P-21; COLLINS MARY LINN SPBPO-RL; POWELL JAMES SPBPO-RL; WARREN MICHAEL T-2; HAGBERG ARIC T-5; REDONDO ANTONIO T-DO			
ISTC	4	workshop	Data Fusion Workshop,ÄìChallenges in Data Fusion II. Applications Study Center, Jemez Conference Room 9/17/2009	Organized	SHLACHTER JACK ADEPS; BISHOP ALAN ADTSC; DOTSON PAUL ADTSC; CHALLACOMBE JEAN B-6; STRAUSS CHARLIE B-9; BLANCHARD SEAN CCS-1; DJIDJEVA TATIANA CCS-3; EIDENBENZ STEPHAN CCS-3; MNISZEWSKI SUSAN CCS-3; GRAVES TODD CCS-6; BENT RUSSELL D-4; CASH LEIGH D-4; DAUELSBERG LORI D-4; JENSEN MARK D-4; SKOUSEN BENJAMIN D-4; SENTZ KARI D-6; LOWE RICK HPC-1; SPEARING HELLY HPC-1, CONNOR CAROLYN HPC-5; FIELDS PARKS HPC-5; TOMLINSON BOB HPC-DO; NEIL JOSHUA IAT-2; ALEXANDER FRANK INST-OFF; BEWLEY THOMAS INST-OFF; FARRAR CHUCK INST-OFF; FLYNN ERIC INST-OFF; HARVEY DUSTIN INST-OFF; MORO ERIK INST-OFF; SAUER NANCY INST-OFF; TAYLOR STUART INST-OFF; FRASER ANDY ISR-2			
ISTC	4	workshop	Physics of Algorithms Chaco Ballroom, Inn at Loretto, Santa Fe 8/31/2009	Organized				

CBSS		workshop	Quantitative Models to assess infectious bacterial Disease Stages (Dec 7-12 2009)					
IGPP		workshop	Climate Science Challenges and its systems dynamics coupling with infrastructure design. Transport and mesh adaption 10/20/2009					
ISTC		Conference	Los Alamos Computer Science Symposium	A. Hoisie chair				
ISTI		workshop	Parallel Data retreat	CMU/LANL organizers				
IGPP	2009	workshop	Permafrost modeling strategy	LANL led Multiple universities and nat. labs				
IGPP	2009	workshp	Ice sheet modeling	LANL led Multiple				
Quantum CNLS	2009 and 2010	workshp	Quantum Information processing	LANL led, southwest constorium				

F. Joint Research Proposals

CAO Category: Science and Engineering Development

CAO Description: Joint research proposals submitted

Directions/Definitions: Internal (i.e. LDRD)

Proposals should not be put onto web unless Leader authorizes distribution/release of information. Should have LA-UR

Institute/ Center	Qtr	Internal or External	Proposal Title	Authors/Org *(list all)*	Organization Proposal Submitted To	Date of Submittal	Funding Requested (Internal Info Only)	Funding Awarded (Internal Info Only)	CAO Report	Place on Web	Date on Web
			NA to this request								

G. Seminars, Lectures, Meetings, Summer Schools, Outreach, Other Activities

Category: Internal only

Description: Summer Schools, Seminars, lectures and meetings, other activities

Directions/Definitions: Include activities, including Conferences and Workshops, NOT included as National or International Conferences and Workshops above in "E"
Include activities that are Non-Institute that we provide Admin Support for – list Institute as "Admin", type of participation as "Admin"
Type of Activities (Seminar, Lecture, Meeting, Conference, Workshop, Summer School, Outreach, Other)
Type of Participation (Presentation, Poster, Organized, Supported, Funded, Sponsored, Admin)

Institute/ Center	Qtr	Type of Activity	Type of Participation	Title of Activity/ Location/Date	Name of Contact/Org	Names of Participants/Org (if list is extensive, include summary information only and attach list/sign-in sheet as backup)	CAO Report	Place on Web	Date on Web
ISTC	3	Seminar	LANL	ISTC Seminar: "Epistemology of Small-Sample Classification" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 4/14/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	3	Seminar	LANL	ISTC Seminar: "Robustness and Plasticity in RNA" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 4/21/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	3	Seminar	LANL	ISTC Seminar: "Scheduling for Small Delays in Multi-channel Wireless Networks" TA-3, Bldg. 123, Room 121 (T-DO Conference Room) 4/8/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	3	Seminar	LANL	ISTC Seminar: "Statistical Inference for Dynamical Structural Biology" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 5/19/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	3	Seminar	LANL	ISTC Seminar: "Time Series of Attributed Graphs" TA-3, Bldg. 123, Room 102 (CNLS Conference Room) 5/12/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			

G. Seminars, Lectures, Meetings, Summer Schools, Outreach, Other Activities

Category: Internal only

Description: Summer Schools, Seminars, lectures and meetings, other activities

Directions/Definitions: Include activities, including Conferences and Workshops, NOT included as National or International Conferences and Workshops above in "E"
Include activities that are Non-Institute that we provide Admin Support for – list Institute as "Admin", type of participation as "Admin"
Type of Activities (Seminar, Lecture, Meeting, Conference, Workshop, Summer School, Outreach, Other)
Type of Participation (Presentation, Poster, Organized, Supported, Funded, Sponsored, Admin)

Institute/ Center	Qtr	Type of Activity	Type of Participation	Title of Activity/ Location/Date	Name of Contact/Org	Names of Participants/Org (if list is extensive, include summary information only and attach list/sign-in sheet as backup)	CAO Report	Place on Web	Date on Web
ISTC	3	Seminar	LANL	ISTC Seminar: "Understanding Cyberattack as an Instrument of U.S. Policy" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 4/23/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Presentation: "Memory at Different Timescales" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 1/19/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: "Accounting for Robustness in Optimization-Based Identification of Nonlinear Models" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 1/13/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: "Bayesian Image Reconstruction for Muon Tomography" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 2/3/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: "Group Lifting Structures for Wavelet Transforms and Multirate Filter Banks" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 2/10/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			

G. Seminars, Lectures, Meetings, Summer Schools, Outreach, Other Activities

Category: Internal only

Description: Summer Schools, Seminars, lectures and meetings, other activities

Directions/Definitions: Include activities, including Conferences and Workshops, NOT included as National or International Conferences and Workshops above in "E"
Include activities that are Non-Institute that we provide Admin Support for – list Institute as "Admin", type of participation as "Admin"
Type of Activities (Seminar, Lecture, Meeting, Conference, Workshop, Summer School, Outreach, Other)
Type of Participation (Presentation, Poster, Organized, Supported, Funded, Sponsored, Admin)

Institute/ Center	Qtr	Type of Activity	Type of Participation	Title of Activity/ Location/Date	Name of Contact/Org	Names of Participants/Org (if list is extensive, include summary information only and attach list/sign-in sheet as backup)	CAO Report	Place on Web	Date on Web
ISTC	2	Seminar	LANL	ISTC Seminar: "Iterative Bias Reduction for Multivariate Smoothers" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 3/31/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: "Quantum Key Distribution: Longer Ranges and Stronger Security with Superconducting Detectors and Decoy States" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 1/6/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: "Radial Kernels in Learning Theory" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 3/3/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: "Statistical Anomaly Detection with Applications in Cybersecurity" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 3/24/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: ‚ÄúState and Parameter Estimation in Models of Nonlinear Systems" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 2/24/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			

G. Seminars, Lectures, Meetings, Summer Schools, Outreach, Other Activities

Category: Internal only

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Directions/Definitions: Include activities, including Conferences and Workshops, NOT included as National or International Conferences and Workshops above in "E"
Include activities that are Non-Institute that we provide Admin Support for – list Institute as "Admin", type of participation as "Admin"
Type of Activities (Seminar, Lecture, Meeting, Conference, Workshop, Summer School, Outreach, Other)
Type of Participation (Presentation, Poster, Organized, Supported, Funded, Sponsored, Admin)

Institute/ Center	Qtr	Type of Activity	Type of Participation	Title of Activity/ Location/Date	Name of Contact/Org	Names of Participants/Org (if list is extensive, include summary information only and attach list/sign-in sheet as backup)	CAO Report	Place on Web	Date on Web
ISTC	2	Seminar	LANL	ISTC Seminar: On a Sturm-Liouville Framework for Continuous and Discrete Frequency Modulation TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 2/22/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: "Information, A New Approach" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 3/10/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: "Search and Classification Decision-Making for Mobile Sensor Coverage of Large-Scale Domains" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 1/20/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar: "Use of Blur in Neural Networks for Vision" TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 1/27/2010	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	1	Seminar	LANL	Large- Scale Functional Models of Visual Cortex for Computer Vision and Remote Sensing LANL/CNLS Conf. Room 10/07/2009	Steven Brumby, Speaker, LANL/ISR-2 Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar. (G1)		Yes	10/01/09

G. Seminars, Lectures, Meetings, Summer Schools, Outreach, Other Activities

Category: Internal only

Description: Summer Schools, Seminars, lectures and meetings, other activities

Directions/Definitions: Include activities, including Conferences and Workshops, NOT included as National or International Conferences and Workshops above in "E"
Include activities that are Non-Institute that we provide Admin Support for – list Institute as "Admin", type of participation as "Admin"
Type of Activities (Seminar, Lecture, Meeting, Conference, Workshop, Summer School, Outreach, Other)
Type of Participation (Presentation, Poster, Organized, Supported, Funded, Sponsored, Admin)

Institute/ Center	Qtr	Type of Activity	Type of Participation	Title of Activity/ Location/Date	Name of Contact/Org	Names of Participants/Org (if list is external, include summary information only and attach list/sign-in sheet as backup)	CAO Report	Place on Web	Date on Web
ISTC	1	Seminar	LANL	Predicative Maturity: A Quantitative Metric for Optimizing Complex Simulations via Systematic Experimental Validation LANL/CNLS Conf. Room 10/14/2009	Huriye Atamturktur, Speaker, LANL/X-3 & Clemson University Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar. (G2)		Yes	10/07/09
ISTC	1	Seminar	LANL	Numerical Aspects of Image Segmentation LANL/CNLS Conf. Room 10/21/2009	Anna Matsekh Speaker, LANL/ISR-2 Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar. (G3)		Yes	10/14/09
ISTC	1	Seminar	LANL	Measurement Selection and Receiver Operating Characteristics LANL/CNLS Conf. Room 11/04/2009	Andy Fraser, Speaker, LANL/ISR-2 Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar. (G4)		Yes	10/28/09
ISTC	1	Seminar	LANL	Using Neurophysiological Markers to Measure Conceptual Integration between Mathematical and Semantic Information LANL/CNLS Conf. Room 11/18/2009	Amy Guthormsen, LANL/IAT-2 Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar. (G5)		Yes	11/13/09

G. Seminars, Lectures, Meetings, Summer Schools, Outreach, Other Activities

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ISTC	1	Seminar	LANL	Coarse-Graining Agent-Based Computations: Equation-Free and Variable-Free Computations LANL/CNLS Conf. Room 12/02/2009	Professor Yannis Kevrekidis, Speaker, Princeton University Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar. (G6)		Yes	11/26/09
ISTC	1	Seminar	LANL	Learning Task-Specific Object Location Predictors with Boosting and Grammar-Guided Feature Extraction LANL/CNLS Conf. Room 12/16/2009	Damian Eads, Speaker, LANL/ISR-2 & University of California-Santa Cruz Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar. (G7)		Yes	12/07/09
ISTC	4	Seminar	LANL	Frontopolar Cortex and Complex Thought TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 9/23/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	4	Seminar	LANL	Science in an Exponential World TA-3, Bldg. 1690, Room 102 (CNLS Conference Room) 8/5/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			

G. Seminars, Lectures, Meetings, Summer Schools, Outreach, Other Activities

Category: Internal only

Description: Summer Schools, Seminars, lectures and meetings, other activities

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Institute/ Center	Qtr	Type of Activity	Type of Participation	Title of Activity/ Location/Date	Name of Contact/Org	Names of Participants/Org (if list is extensive, include summary information only and attach list/sign-in sheet as backup)	CAO Report	Place on Web	Date on Web
ISTC	3	Seminar	LANL	ISTC Adv Stu Seminar-Direct Neural Imaging using Ultra-Low Field MRI CNLS Conf Rm 5/13/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	3	Seminar	LANL	ISTC Seminar - Prof Mikhail Belkin - Learning Using Laplace Operations Cnls Conf Rm 4/1/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	3	Seminar	LANL	ISTC Seminar - Using Analogy with Pictures- Prof Melanie Mitchell CNLS Conf Rm 4/15/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	3	Seminar	LANL	ISTC Seminar-Dynamic Data Analysis for Homeland Security-Prof Fred Roberts CNLS Conf Rm 4/22/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	3	Seminar	LANL	Software Engineering Institute Presentation: The Team Software Process Study Center, Jemez Room 5/27/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar - Prof David Gamarnik, MIT - Algorithms for Graph Counting Problems CNLS Conf Rm 3/4/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			

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Institute/ Center	Qtr	Type of Activity	Type of Participation	Title of Activity/ Location/Date	Name of Contact/Org	Names of Participants/Org (if list is extensive, include summary information only and attach list/sign-in sheet as backup)	CAO Report	Place on Web	Date on Web
ISTC	2	Seminar	LANL	ISTC Seminar - Prof Don Johnson - Neural Information Processing CNLS Conf Rm 3/11/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar Speaker Prof Rex Jung CNLS Conf Rm 2/25/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar-Closed -Loop Simulation for Parkinson's Disease Quantum Room, TA3,Sm40,RmN101 3/10/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	2	Seminar	LANL	ISTC Seminar-Fundamental Limitations of Networked Decision Systems Quantum Room, TA3,Sm40,RmN101 3/10/2009	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			
ISTC	1	Seminar	LANL	Intelligent Computation with CMOL CNLS Conference Room (TA-3, SM1690, Rm. 102) 10/22/2008	Frank Alexander, Institutional Host, LANL/INST-OFF Garrett Kenyon, Technical Host, LANL/P-21	No roster taken at CNLS per Garret Kenyon and Frank Alexander. Sixty attendees maximum can attend the seminar.			

LANL Org Chart


Institutional Leaders
Michael R. Anastasio
Laboratory Director
Isaac E. Richardson
Deputy Laboratory Director
Executive Director
Rich Marquez
Executive Office Manager
Peggy Gonzales
Audits & Ethics Director
Community Programs Office
Chief Prime Contracts
Office of Equal Opportunity & Diversity
Ombuds Office
Comm. & Gov. Affairs
Contractor Assurance Officer
Chief Information Security Officer
Chief Information Officer
General Counsel
Chief Financial Officer
LANS, LLC Executive Staff Director
Terry Wallace
Principal Associate Director
Science, Technology & Engineering
Charles McMillan
Principal Associate Director
Weapons Programs
William Rees, Jr.
Principal Associate Director
Global Security
Mike Mallory
Principal Associate Director
Operations & Business
Chemistry, Life, & Earth Sciences
Assoc. Director
Mary Neu
Engineering & Engineering Sciences
Assoc. Director
Experimental Physical Sciences
Assoc. Director
Theory, Simulation, & Computation
Assoc. Director
Alan Bishop
Stockpile Manufacturing & Support
Assoc. Director
Carl Beard
Weapons
Assoc. Director
Bret Knapp
Nuclear & High Hazard Operations
Assoc. Director
Project Management & Site Services
Assoc. Director
Environment, Safety, Health, & Quality
Assoc. Director
Chris Cantwell
Safeguards & Security
Assoc. Director
Michael Lansing
Business Services
Assoc. Director
Mark Barth
Environmental Programs
Assoc. Director
Michael Graham
Chemistry
Earth & Environmental Sciences
Applied Engineering & Technology
Engineering Services
Physics
Theoretical
Computer & Computational Sciences
Weapons Systems
Dynamic and Energetic Materials
Applied Physics
Manufacturing Quality
Safety Basis
Operations Support
CMR Facility Operations
TA-55 Facility Operations
Weapons Facility Operations
Project Projects
Construction Management
Cost & Schedule
Infrastructure Planning
Maintenance & Site Services
Radiation Protection
Occupational Medicine
Environmental Protection
Quality Assurance
Security
Safeguards
Emergency Operations
Human Resources
Central Training
Acquisition Services
Waste Services
TA-21 Closure
Science Program Office
Technology Transfer

08/28/09

Acronym List

Poster Session

Computational Physics and Applied Math Capability Review
Poster Session

Study Center, Santa Clara Gallery, June 9, 2010, 4:30 – 6:30 PM

Poster Position	Poster Title	Presenter*
	Theme Area: Monte Carlo Methods	
1	Comparative Monte Carlo Efficiency by Monte Carlo Analysis	Jim Gubernatis, T-4
2	Finite State Projection Methods for the Analysis of Continuous Time, Discrete State Markov Processes	Brian Munsky, CCS-3
3	Statistically Exact Monte Carlo Probability of Initiation Calculations	Thomas Booth, XCP-4
4	MCNP - Monte Carlo for Nuclear Reactor Analysis	Brian Kiedrowski, XCP-3
	Theme Area: Molecular Dynamics	
5	Atomistic Simulations of Oxide Nuclear Fuel Behavior	Chris Stanek, MST-8
6	Pushing the Envelope of Biomolecular Dynamics Simulation: large system size and long time scale simulations of the ribosome	Karissa Sanbonmatsu, T-6 Paul Whitford, T-6
7	Accelerated Molecular Dynamics Methods for Long Time Atomistic Simulation	Art Voter, T-1
8	Spatio-Temporal Frontiers of Atomistic Simulations in the Petaflop Computational World	Tim Germann, T-1
9	Nonequilibrium Phenomena at the Interface Between Hard and Soft Matter	Cynthia Reichhardt, T-1
	Theme Area: Descrete Event Simulation	
10	Multi-scale Integrated Information and Telecommunications System (MIITS)	Stephan Eidenbenz, CCS-3
11	Agent Framework for Simulations	Dennis Powell, D-4
12	FastTrans: Scalable, Discrete-event Microsimulations for Transportation Networks	Sunil Thulasidasan, CCS-3
13	CyberSim: Malware Propagation in Online Social Networks	Nandaksihore Santhi, CCS-3
14	BotSim: Understanding Propagation, Command, and Control in BotNets	Guanhua Yan, CCS-3
15	Epidemic Simulation System	Sara Del Valle, D-4
16	ActivitySim: Large-scale Agent-based Activity Generation for Infrastructure Simulation	Sue Mniszewski, CCS-3
17	SimCore: A Scalable Discrete-event Simualtion Design Framework	Lukas Kroc, CCS-3

Computational Physics and Applied Math Capability Review
Poster Session

Study Center, Santa Clara Gallery, June 9, 2010, 4:30 – 6:30 PM

Poster Position	Poster Title	Presenter*
Theme Area: Integrated Codes		
18	ASC Programs Urban Nuclear Consequences Project	Randy Bos, XCP-4
19	Utilization of a Multi-Phase Particle Model to Develop Self-Consistent Bulk Microphysical Paramaterization of Hurricane Models	Jon Reisner, EES-16
20	The Roadrunner Universe Project	Salman Habib, T-2
21	Roadrunner, Quasars, and a Message from the Big Bang	Katrin Heitmann, ISR-1
22	Leveraging Massively Parallel Computing: PFLOTRAN Scalability, Uranium Migration, and CO2 Sequestration	Peter Lichtner, EES-16
Theme Area: Computational Fluid Dynamics		
23	Astrophysical Applications of Computational Fluid Dynamics	Chris Fryer, CCS-2
24	Application Support for Material Tension and Real Equations of State	John Grove, CCS-2
25	Establishing a Technology Integration Path for Advanced Computing Architectures	Ben Bergen, CCS-7
Theme Area: Partial Differential Equations		
26	Advances in the Material Point Method for Nonlinear Mechanics	Duan Zhang, T-3
27	Solvers Development Supporting Subsurface Applications	David Moulton, T-5
28	Mesh Generation Capabilities at LANL	Rao Garimella, T-5
29	Mimetic Finite Difference Methods: Theory and Applications	Konstantin Lipnikov, T-5
*Only the on-site presenter is listed; a full set of poster authors is listed on each poster.		

Updated: 26 May 2010

McBranch

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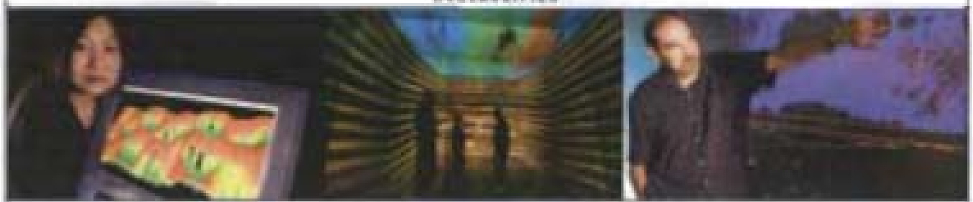

Los Alamos National Laboratory

Duncan W. McBranch

Deputy Principal Associate Director for
Science, Technology and Engineering

Charge to the Computational Physics and Applied Math Capability Review

June 8, 2010

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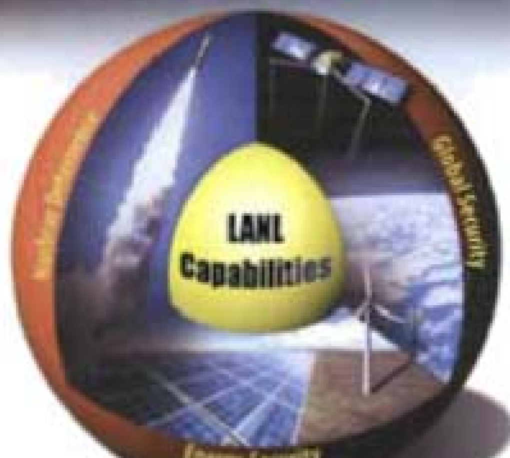
The Laboratory's capabilities support national security missions and national needs.



Scientific Credibility   Delivery of Product   Agility and Innovation

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Los Alamos science in the 21st century

The Premier National Security Science Laboratory:

- Integrates theory, simulation, and experiments
- Uses multidisciplinary science, technology, and engineering
- Solves problems that are large scale, complex, and high impact
- Utilizes unique, multifaceted, or experimental and computational facilities
- Develops technology that is highly complex, and sensitive or classified nature.

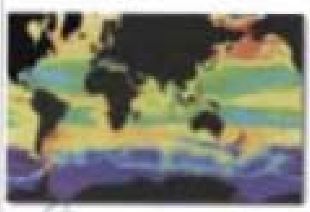
High performance computing

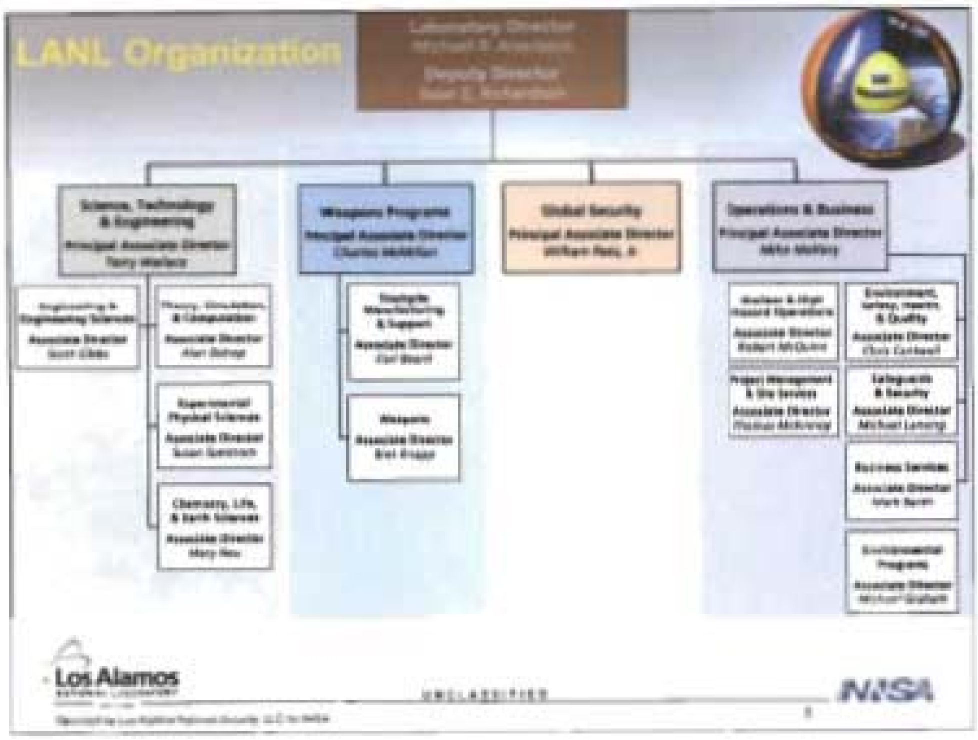
Studies of materials under extreme conditions

Raptor "thinking" telescopes

LANL is a capabilities-based laboratory.

- Capabilities are strategic areas where LANL needs to excel.
- Capabilities are chosen to be cross-cutting.
- Capabilities are led by an Associate Director.
- Capabilities do not reside in one organization.
- Strategies and plans are being developed for each capability.





Capability Reviews

- LANL uses external reviews to measure and continuously improve the quality of its science, technology and engineering (STE).
- Capability reviews are chartered by the Director and PADSTE.
- LANL uses capability reviews to assess the STE quality and institutional integration and to advise Laboratory Management on the current and future health of the STE.
- The capability reviews are cross-cutting across directorates. They provide a holistic view of STE quality, integration to achieve mission requirements, and mission relevance.
- The principal product of the capability review is a report that includes the Committee's assessments, commendations, and recommendations for the capability.

Laboratory Management will use this report for capability planning and provide it to DOE as part of LANL's annual performance plan.

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Charter for the Computational Physics and Applied Math Capability Review Committee

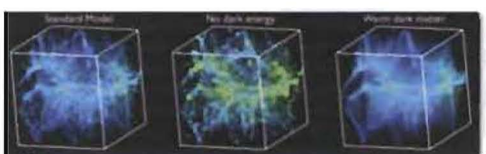
Specifically, the Committee will:

- ***Assess the quality of science, technology and engineering*** within the capability in the areas defined in the agenda. Identify issues to develop or enhance core competencies in this capability.
- ***Evaluate the integration of this capability*** across the Laboratory organizations that are listed in the agenda in terms of joint programs, projects, proposals, and/or publications. Describe the integration of this capability in the wider scientific community using the recognition as a leader within the community, ability to set research agendas, and attraction and retention of staff.
- ***Assess the relevance*** of this capability's science, technology and engineering contributions to current and emerging LANL programs, including Nuclear Weapons, Global Security, and Energy Security.
- ***Advise the Laboratory Director/Principal Associate Director for Science, Technology and Engineering on the health of the capability*** including the current and future (5 year) science, technology and engineering staff needs, mix of research and development activities, program opportunities, environment for conducting science, technology and engineering.

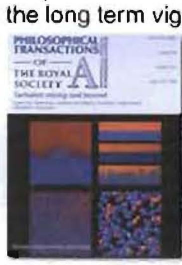
Capability Assessment Evaluation

Evaluation of topics in the agenda must address the following criteria:

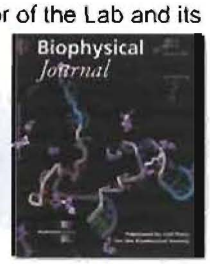
- ***Comparison to peers:*** State how this work compares to similar or related work conducted by others.
- ***Sustainability:***
  - State the extent to which the contribution strengthens or weakens LANL capabilities.
  - How does this activity/contribution build core competencies or other resources that contribute to the vitality of the activity itself and the long term vigor of the Lab and its ability to meet the needs of the nation?



Roadrunner simulation of the universe



Model of turbulent mixing



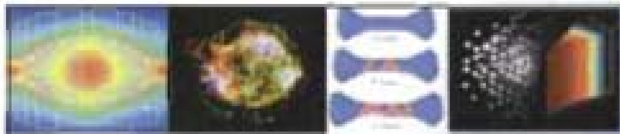
All-atom riboswitch simulation

Communicating Conclusions with Management

- The review committee presents their findings to LANL management in an out-brief.
- The committee must prioritize its assessment and advice for the out-briefing and the report.
- Specifically, the Committee should identify and prepare for presentation:
  - Assessment of STE topics covered in the agenda.
  - Between 3 and 7 prioritized most notable contributions observed in the review.
  - Between 3 and 7 prioritized most important "actionable" recommendations.
- The Committee must submit its assessment and advice via written report within 30 days of the end of the review.

Out-brief and report templates are available for the Committee's use.

Bishop



CPAM Overview

Computational Physics and Applied Mathematics (CPAM)
Capability Review June 8-10, 2010

Alan Bishop
Associate Director for
Theory, Simulation, and Computation

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Computational Physics and Applied Mathematics
Capability Review, June 8-10, 2010

Review Committee

- William Martin, University of Michigan–Committee Chair
- David Brown, Lawrence Livermore National Laboratory
- David Nichol, University of Illinois at Urbana-Champaign
- Wayne Pfeiffer, University of California-San Diego
- Steven Plimpton, Sandia National Laboratories
- Anil Prinja, University of New Mexico
- John Turner, Oak Ridge National Laboratory
- Mark Christon, Dassault Systémes SIMULIA

- Sidney Karin, University of California-San Diego–S&T POC

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List of Materials Provided to Committee

- Materials sent in advance
  - Charter
  - Instructions to the Committee
  - Theme Area Self-Assessments
  - Selected Statistics
- On-site materials
  - Agenda
  - LANL Organization Chart
  - Acronym List
  - Poster and Poster Presenters List
  - Presentations (only unclassified summaries for classified presentations)
  - Roadrunner Petascale Open Science Application Article Summaries

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Outline

- About Los Alamos and Capability reviews
- CPAM @ Los Alamos: some statistics
- CPAM application exemplars
- Our "Co-Design" future
- Summary and Charge

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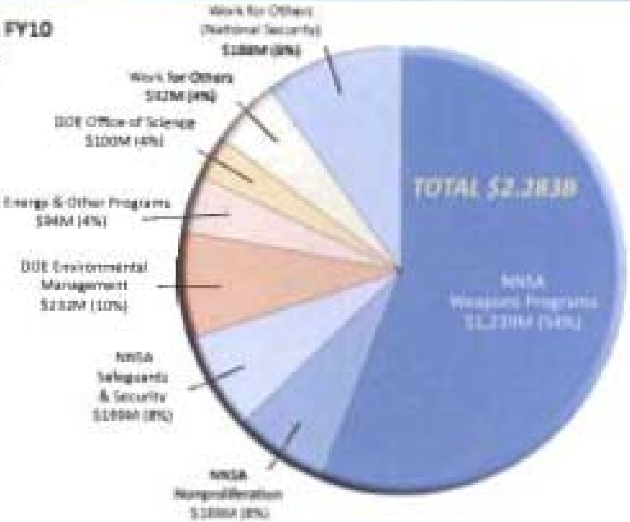
Computational Physics and Applied Mathematics

Los Alamos is the Nation's Largest Multi-program Laboratory

The Laboratory's FY10 annual budget is approximately $2.3 billion.



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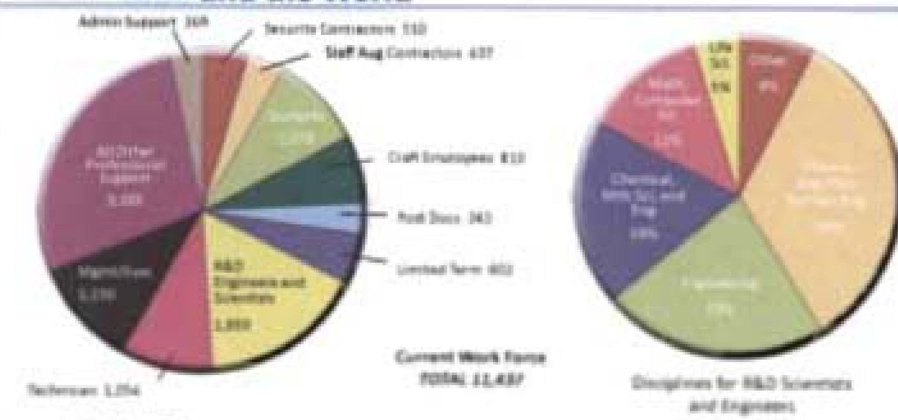
Computational Physics and Applied Mathematics

Los Alamos has Broad and Deep Science Capabilities, drawn from around the Nation and the World



- 2,171 PhDs
- One quarter of workforce started as students or postdocs – pipeline!

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Computational Physics and Applied Mathematics
The Institutional Management Challenge in a Large Multi-Program National Security Science Laboratory — Delivering the Best S&T to Current Programs and being Prepared for Future National Needs
LANL Capabilities and Programs
Global Security
Energy Security
The S&T Manager's Challenge:
Balancing
• Individual entrepreneurs and teams
• Program delivery and capability maintenance/development
• Multiple customers
• Core disciplines and interdisciplinary capabilities
■ Optimizing the LANL intellectual/business advantages for addressing compelling, complex national security S&T missions
■ Over time, most staff spend time working on a spectrum of basic and applied programs
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Computational Physics and Applied Mathematics
CPAM Participating Divisions Span Three Principal Directorates in LANL (C, CCS, D, EES, IAT, ISR, MST, T, TT, XCP, XTD)
Institutional Leaders
Michael R. Anastasio
NNSA

Computational Physics and Applied Mathematics
Capability Review, June 8-10, 2010

Cross-Laboratory Capability Reviews

- Lab-wide Capability oversight is to emphasize communication/agility/ response to Mission need/Opportunity – present to future
  - Technical divisions/groups remain the line-program management nexus – capability not an organizational structure
- Input on S,T&E Quality is primary interest
  - People, facilities, use of integrated skills, training the next generation,...
- Not a traditional line organization review
  - but views on leverage opportunities very helpful
- Not a Program/Mission review
  - but understanding how capability supports mission is essential

*See "Voice-of-Customer" session Thursday morning

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Computational Physics and Applied Mathematics
Capability Review, June 8-10, 2010

Outline

- About Los Alamos and Capability reviews
- CPAM @ Los Alamos: some statistics
- CPAM application exemplars
- Our "Co-Design" future
- Summary and Charge

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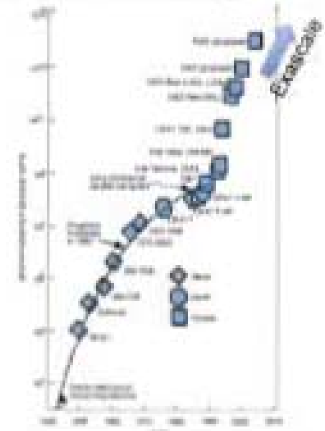
Computational Physics and Applied Mathematics Capability Review

Los Alamos has a Rich History of CPAM Capabilities

Iconic examples include

- MC and MD methods & codes
- Climate
  - Work at Los Alamos has roots in work in nuclear winter
- Nuclear theory and data
- Materials at extremes
- Astrophysics and Cosmology
- Pre-conditioning algorithms
- Multiscale approaches
- Uncertainty quantification
- ....

Just as the history of computational power and technology was intimately tied to the history of nuclear weapons, so has been CPAM – not a static capability



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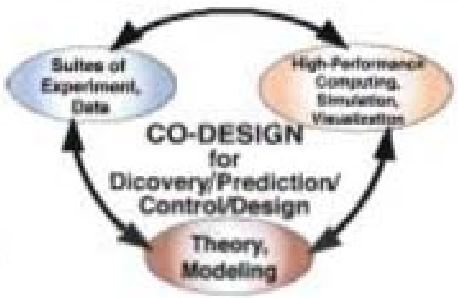
Computational Physics and Applied Mathematics Capability Review

The Overarching CPAM Strategy is Centered on Co-Design

The present and future offer exciting, unprecedented new science, technology, and engineering opportunities to accelerate accuracy and timeliness of mission impacts

- Agile and modular code structures
- Use of distinct levels of parallelization to exploit multiscale opportunities
- Exascale strategy and partnerships
- Training tomorrow's scientists today



See A. White presentation

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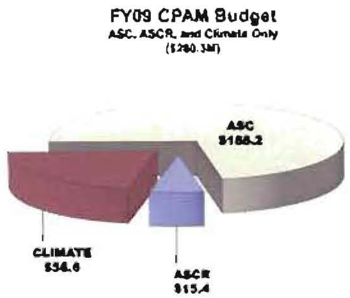
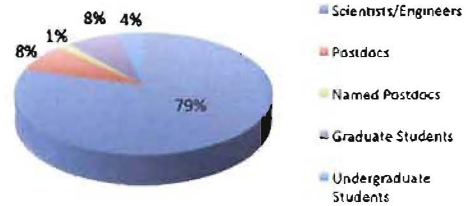
Capability Review, June 8-10, 2010

The CPAM Capability Slice through Los Alamos is Complex



Current CPAM Capability Employee Profile



(Approx. 591 FTEs)

Funding for CPAM is extremely diverse and embedded. Only large funding sources shown that directly support CPAM.

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Capability Review, June 8-10, 2010

CPAM is Critical to all Los Alamos LDRD Grand Challenges!

- Beyond the standard model
- Materials: discovery science to strategic applications
- Complex biological systems
- Information science and technology
- Earth and energy systems
- Nuclear performance
- Sensing and measurement science for global security
- Intelligent, adaptive, engineered systems

See exemplar LDRD presentation (D. Livescu) and supplementary slides

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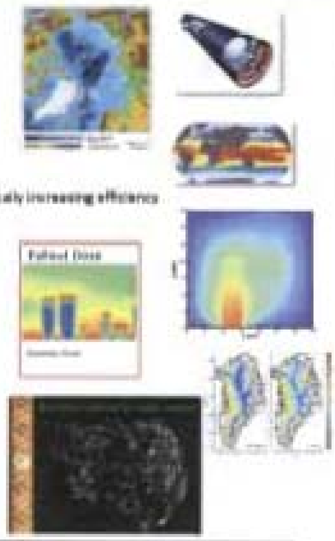
Capability Review
June 8-10, 2010

Capability and Mission/Program

(See Presentations and posters)

- Long History of Powerful Leverage/Pull/Push
  - e.g. Nuclear Weapons Stewardship
    - Climate
    - Energy
    - Biology
    - Astrophysics and Cosmology
    - Materials science
    - Nuclear theory/data
    - Radiochemistry
- Current Mission impacts include:
  - Plasma physics: self-focusing laser in plasma interactions, laser speckles
  - New hybrid methods developments maintain IMC accuracy while dramatically increasing efficiency
  - Turbulence/Mix modeling
  - a-model and discovery of slow, non-hydrostatic dynamics in the Arctic
  - IND impact modeling for urban environments
  - Power Grid/Communication Network modeling
  - Epidemiology modeling
  - Cosmic explosions and Supernovae
- Future Mission directions include:
  - Nuclear Weapons Stewardship and Non-proliferation, DHS
  - Nuclear energy
  - MaRIE
  - Environmental Remediation
  - Other energy security (e.g., CO_2 capture and management)



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Capability Review
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Capability and Mission/Program (cont.)

- History of Strong connections to DOE-SC/SciDAC/Industry
  - Leveraged with LDRD projects
- History of Strong (International) Partnership
  - Industry and Tech Transfer
    - 432 software disclosures (intent to share) since FY05
    - 129 separate copyrighted codes since FY05; from a few to tens of thousands of users worldwide (copyrights vary from commercial to open source distribution)
  - Extensive Collaboration/Visitor/Student/Postdoc Programs
  - LANL Workshops/Summer Schools
- History of Strong Staffing Pipeline for Sustained Capability
  - Students – Postdocs – Staff – Associates/Visitors

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CPAM Technical Scope is vast, Covering Multiple Activities: *First Cross-Lab Look*

- Review organized into 6 technical "themes" to make scope tractable
- Themes covered in presentations (and posters, self assessment)
  - Computational Fluid Dynamics (CFD)
    - Historical strength, vast array of capabilities: fluids under shocks, low-speed flow, turbulence, ...
  - Partial Differential Equations (PDE)
    - Pre-conditioners, particle transport, solvers, plasma physics, ...
  - Monte Carlo (MC)
    - Invented at Los Alamos, vital for particle transport, condensed matter, biology, ...
  - Integrated Codes (IC)
    - Climate and Nuclear Weapons covered in this review
- Themes covered in posters (and self-assessment)
  - Molecular Dynamics (MD)
  - Discrete Event Simulations (DES)
- CPAM complements many capability reviews See supplementary slides
  - LANL technical AD's meet to discuss the set of all reviews

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DOE Deputy Secretary (Science) Koonin's Views Align with our Practice

presentation to ASCAC (8/09)

Computation as a tool in science

Required Ingredients:
Theorists
Computational Scientists
Experimentalists
Applied Mathematicians
Computer Scientists

Successful Program:
Guides experiments
Quantifies uncertainties
Yields solutions/insights
Eliminates tunable parameters

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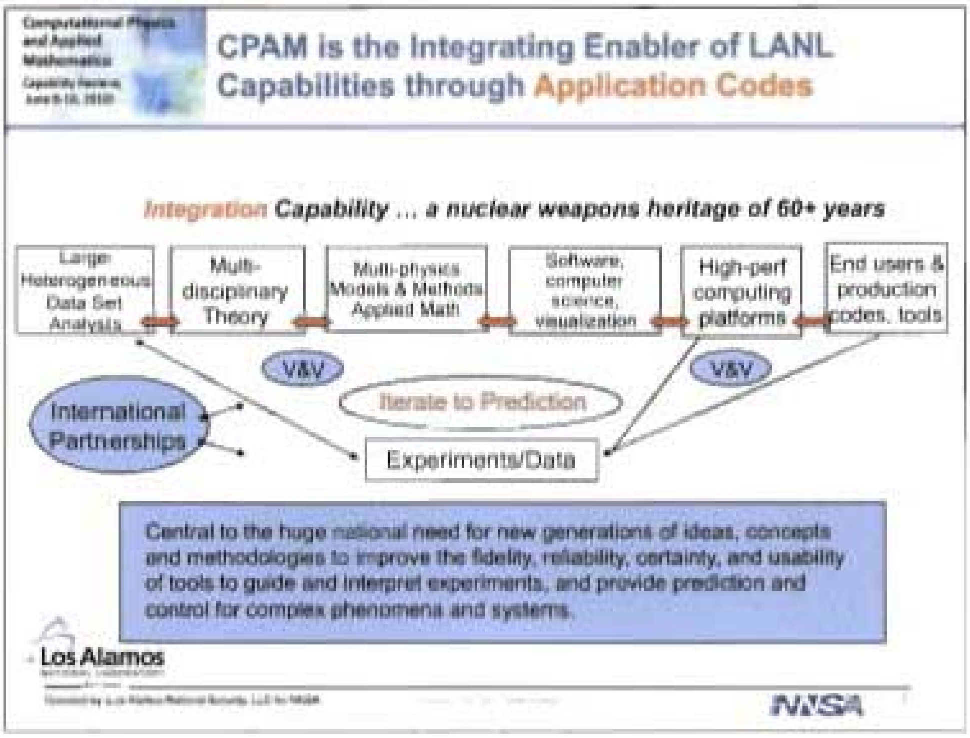
Computational Physics and Applied Mathematics
CPAM is the Integrating Enabler of LANL Capabilities through Application Codes
Integration Capability … a nuclear weapons heritage of 60+ years
Large Heterogeneous Data Set Analysis
Multi-disciplinary Theory
Multi-physics Models & Methods Applied Math
Software, computer science, visualization
High-perf computing platforms
End users & production codes, tools
V&V
V&V
International Partnerships
Iterate to Prediction
Experiments/Data
Central to the huge national need for new generations of ideas, concepts and methodologies to improve the fidelity, reliability, certainty, and usability of tools to guide and interpret experiments, and provide prediction and control for complex phenomena and systems.
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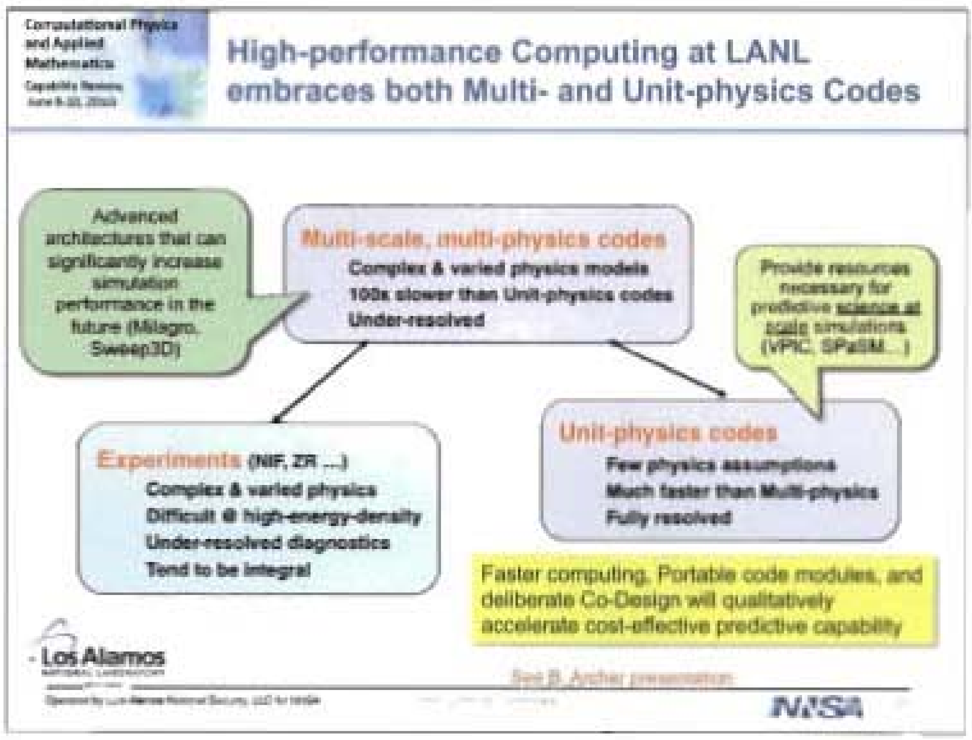
Computational Physics and Applied Mathematics
High-performance Computing at LANL embraces both Multi- and Unit-physics Codes
Advanced architectures that can significantly increase simulation performance in the future (Milagro, Sweep3D)
Multi-scale, multi-physics codes
Complex & varied physics models
100x slower than Unit-physics codes
Under-resolved
Provide resources necessary for predictive science at scale simulations (VPIC, SPaSM…)
Experiments (NIF, ZR …)
Complex & varied physics
Difficult @ high-energy-density
Under-resolved diagnostics
Tend to be integral
Unit-physics codes
Few physics assumptions
Much faster than Multi-physics
Fully resolved
Faster computing, Portable code modules, and deliberate Co-Design will qualitatively accelerate cost-effective predictive capability
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See B. Archer presentation
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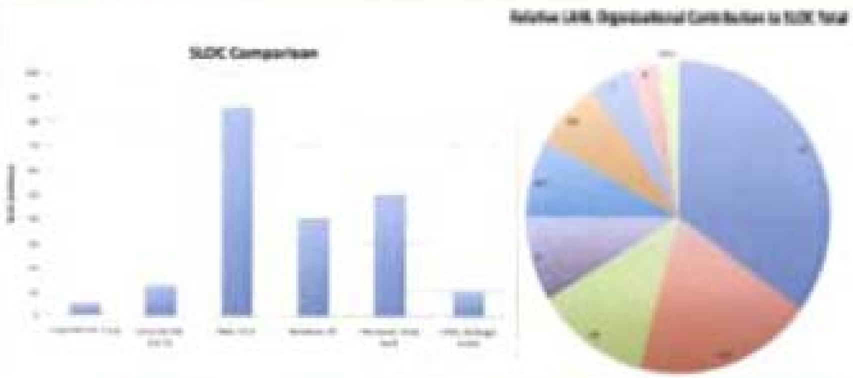
LANL has Created a Significant Set of Strategic Application Codes



Los Alamos has over 100 strategically important codes with about 10 million total single lines of code. Licensed codes have generated $1.6M in revenue for Los Alamos since FY07.

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LANL CPAM capabilities address problems of national concern...

Senator Bingaman press release stating work of LANL and SNL on the Gulf of Mexico oil leak problem, something not publically known until now.

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Outline

- About Los Alamos and Capability reviews
- CPAM @ Los Alamos: some statistics

CPAM application exemplars

- Our "Co-Design" future
- Summary and Charge

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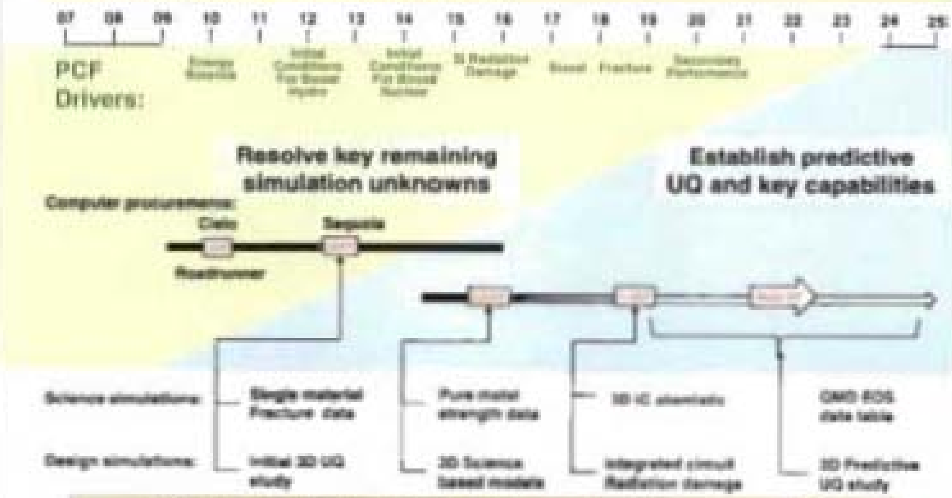
Nuclear Weapons Strategic Planning: Requirements are Driving Greater Understanding, Requiring Exascale to Establish Predictive 3D UQ



ASC plan to deliver the first Exascale platform by 2018

Provide Mission Responsive Computational Environments

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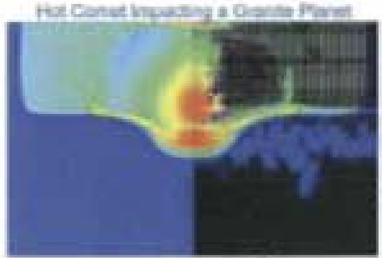
Capability Review
June 8-10, 2010

e.g., Neutronics and Radiation Transport: The 65-year-old Multiscale Grand Challenge

- Applications:
  - Nonproliferation
  - Nuclear Weapons
  - Nuclear Power
  - Astrophysics
  - Fusion
  - Radiography
  - Isotope Production
  - Medical Diagnostics and Treatment
  - Oil Exploration
  - Food Irradiation
- In the majority of cases, there is not enough compute power for high fidelity simulations of the 7+ Dimensional Problem:
  - 3 in space (1000s of cells per dimension)
  - 2 in angle (1000s of angles in 3D)
  - 1 in energy/frequency (up to a 1000 groups or more)
  - 1 in time (1000s of time steps)
  - + thermal radiation => nonlinear dependence on material temperature
  - *Clearly a Petascale to Exascale... problem!*
- *The necessary leap forward requires new algorithms targeted to advanced architectures*
  - Efforts have already begun on developing IBM-Cell-Based kernels that represent the core of Neutronics and Radiation transport software

Hot Comet Impacting a Granite Planet



Radiation Temperature   Density

Asymmetric Supernova Explosion

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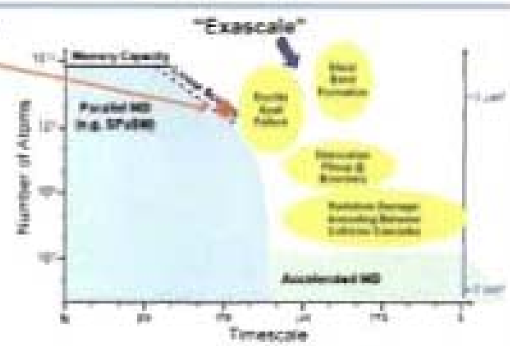
e.g., Los Alamos MD Simulations on Roadrunner - Nearing Access of Phenomena at the Micron Scale: Relevant to both Nuclear Stewardship and MaRIE*

e.g., 2D MD simulations of shock-induced ejecta and Richtmyer-Meshkov instability, showing bubbles and spike growth. (RR, 361 TF/s)



Future ejecta modeling challenges:
- 3D modeling of conical etching pits
- Polycrystal 3D ejecta (role of solid phase ejecta production)
- Use of more sophisticated atomic potentials

Our MD simulations of ejecta mass and velocity distributions, together with experimental data, have helped develop an ejecta source model in our codes

*MaRIE: LANL's Signature Materials Facility plan

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Computational Physics and Applied Mathematics Capability Review

Outline

- About Los Alamos and Capability reviews
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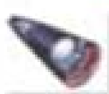
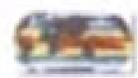
Computational Physics and Applied Mathematics Capability Review

The Promise and Challenge of Science in the 21st Century

- **Isolating complicated phenomena to "understand" them not always sufficient**

science of prediction & **uncertainty quantification** for **complex systems/networks**





- NW: e.g., nuclear stewardship; non-proliferation ...
- homeland security: cyber; IND; borders; Infrastructure; ...
- energy & environment: climate; carbon seq; grids; EM; nuclear...
- complex matter: nano S&T; extreme conditions...
- biological systems: disease spread; vaccination; cognition...
- ...

- **Quantitative tools for decision makers/risk assessment**
  - (coupled) socio, economic, humanities, physical sciences, ...
  - from observation to prediction and uncertainty quantification

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Global Partnership: Community Climate System Model

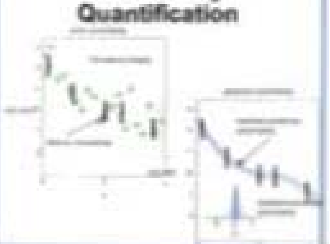
~ 50/50 (Parallel) Architecture/Algorithm history: Co-Design

LANL is Bringing Key Assets to Bear in a Larger Sense of Co-Design: Energy and Climate Science

Measurements & Analysis (Microbes to Satellites!)

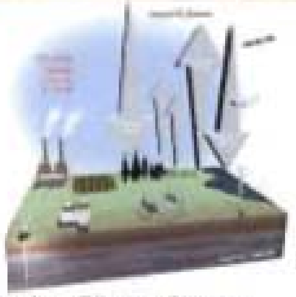
Climate and Modeling

Uncertainty Quantification



Social, Energy, and Infrastructure Modeling

Global Climate Science: Tools for Policymakers



- Los Alamos developed the Coupled Sea-Ice Model: *the global standard used by the Intergovernmental Panel on Climate Change*
- Los Alamos makes key contributions to the DOE/NSF Community Climate System Model: *the first interactive model of molecular to planetary scale*
- National Challenge: *Science-based policies for energy use, regional infrastructure investments, and resource allocation*

Understanding climate change as a global system is required to develop predictive tools for mitigating regional impacts

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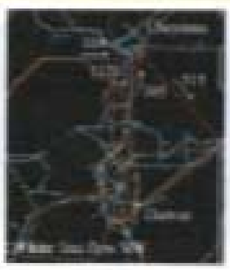
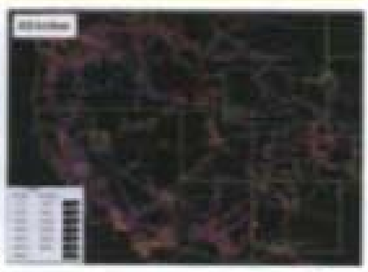
Energy Grid Challenges of the Future

- Requires predictive simulation and rapid integration of new technologies for renewable generation, transmission, and storage.
- Integration is needed to maintain grid stability.
- Cost-effective investment requires predictive simulation.

LANL develops energy infrastructure models to understand impacts and address power options for insertion of renewable and nuclear energy.





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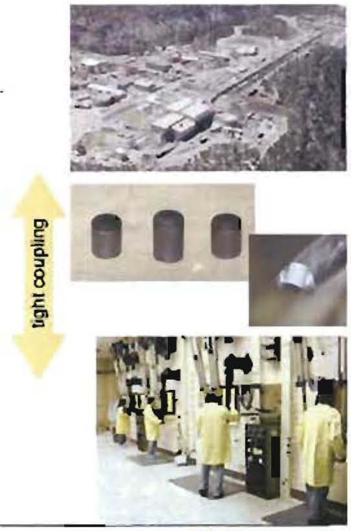
LANL Developing Materials for Sustainable Nuclear Energy

- **Experimental**
  - Design advanced fuels and structural materials.
  - Develop, test, and characterization of new waste forms.
  - Develop new materials for safeguards instrumentation.
  - Develop selective, cost-effective separation technologies.
- **Modeling & Simulation**
  - Perform multiscale modeling of fuel and cladding behavior.
  - Design stable waste forms.
  - Process development for ultra efficient casting of metal fuels.
- **Infrastructure**
  - Use unique experimental facilities and capabilities.



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The Winding DOE Path to Exascale/Co-Design: Fascinating(!) Last 18 months for CPAM Nationally and at LANL

- New Administration and DOE Leadership
  - Impacts on Agency, Labs, Industry dynamics
  - High expectations for S&T impact, and increased cross-cut leveraging of assets
- ASC funding at LANL on path to zero, then restored, and then increased!
  - Tri-Lab "Right Sizing" planning with HQ (3/09)
    - part of NW Budget Uplift for FY11 and beyond (Nuclear Posture Review)
- National Exascale Initiative: ASCR *and* ASC (2009→)
  - Science & Application Frontier workshops
  - CS/App. Math Workshops
  - Architecture/Industry workshop
  - Briefings to D'Agostino, Brinkman, Koonin, Trivelpiece Commission Chu

  } Strong LANL involvement and Leadership
- Hybrid Multicore Consortium (HMC) with ORNL/LBNL (http://computing.ornl.gov/HMC/)
- LANL a key partner in successful (!) CASL, the DOE-NE M&S Hub proposal lead by ORNL

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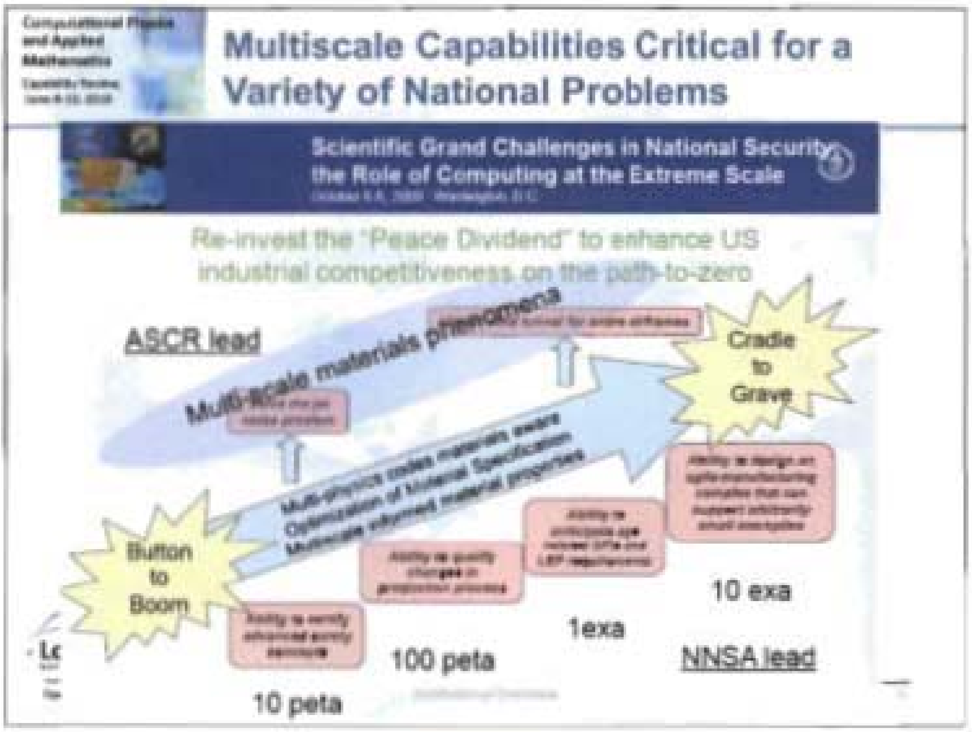
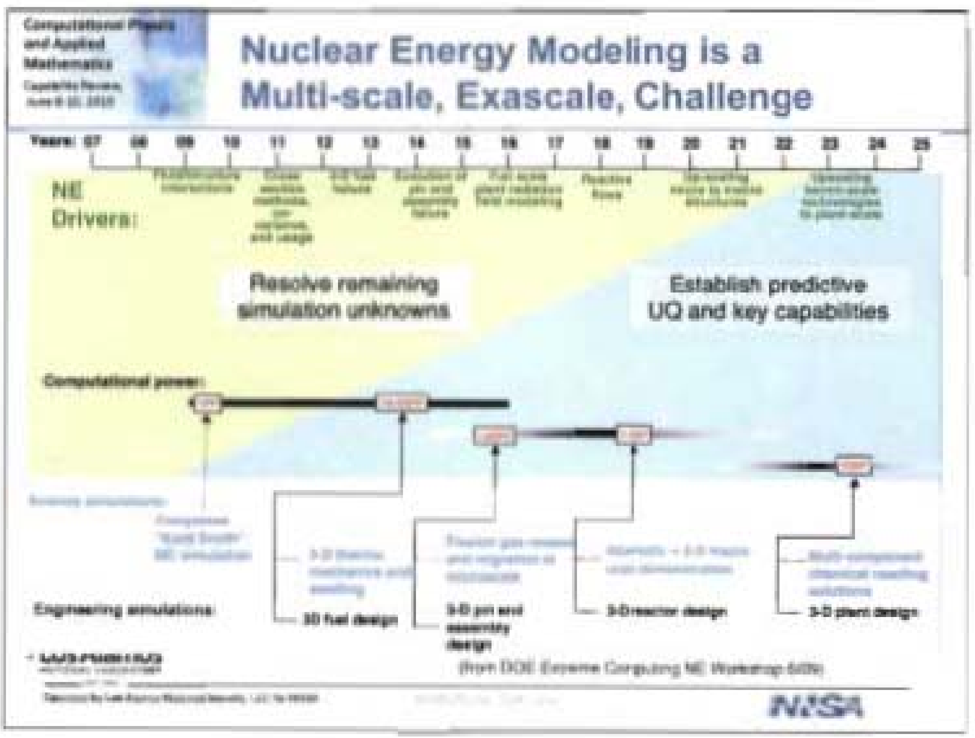

Multiscale Capabilities Critical for a Variety of National Problems
Scientific Grand Challenges in National Security: the Role of Computing at the Extreme Scale
Re-invest the "Peace Dividend" to enhance US industrial competitiveness on the path-to-zero
ASCR lead
Multi-scale materials phenomena
Cradle to Grave
Button to Boom
10 exa
1exa
100 peta
10 peta
NNSA lead


Nuclear Energy Modeling is a Multi-scale, Exascale, Challenge
NE Drivers:
Resolve remaining simulation unknowns
Establish predictive UQ and key capabilities
Computational power:
Engineering simulations:
3D fuel design
3-D pin and assembly design
3-D reactor design
3-D plant design
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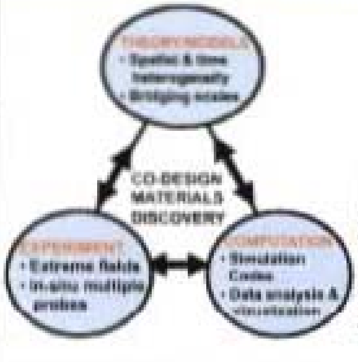
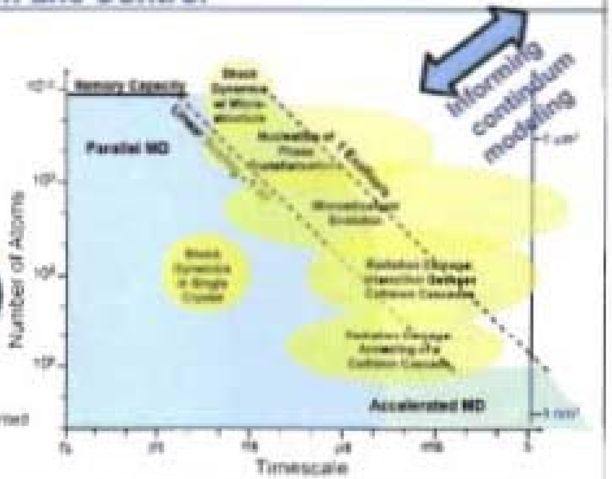
A Decadal Opportunity for Materials Science: Removing Key Scientific Barriers to Discovery, Prediction and Control



Anticipated advances in petaflop – exaflop computing, experimental tools with unprecedented resolution, modeling put us on the verge of accessing critical phenomena at the meso (micron) scale



MaRIE: Matter-Radiation Interactions in Extremes
LANL Signature Facility plan (NW, NE, Fission-Fusion ...)

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Environmental Sciences Challenges Require CPAM

- Development of predictive capability
  - contaminant migration
  - geologic sequestration
    - CO_2
    - Nuclear Waste
- Requirements include:
  - Multi-scale modeling of reactive flows
    - Fluid Flow
    - Physical and chemical processes
  - Subsurface environment characterization
  - Dealing with orders of magnitude in time (sub-second to epoch) and space (pore-size to kilometers)

simulation showing migration of geologically sequestered CO_2 at an elapsed time of 300 years

simulation showing a 3D model of the Hanford 300 Area uranium plume

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Major Themes from DOE-ASCR Exascale Application Workshops (2008-10)

- **Need computational algorithms/codes for relevant physical phenomena, *optimized* for extreme-scale computing architectures (hybrid/multicore...)**
  - Robust, Portable, "O(N)" scaling, modular code approach...
  - Discrete and continuous phenomena, data, models
  - Theory-and (heterogeneous) data-driven modeling and simulation
  - Vast space-time ranges (multiscale, multi "physics")
  - Complex realities
    (far from equilibrium, nonlinear, nonadiabatic, metastable, heterogeneous, stochastic, importance of
    "rare events"/"anomalies,"/long-tails/intermittency, defects, interfaces, clusters, hotspots, extreme conditions, ...)

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Major Themes from DOE-ASCR Exascale Application Workshops (2008-10)

- **Need modeling and simulation for multiscale (space, time)**
  - "Systems" of **functional** scales
  - "Mesoscale" gaps between "atomistic" and "continuum"
  - Atomistic to engineering scales
  - Hybrid simulation approaches (quantum/classical, discrete/continuous, short/long range)
  - Data-management S&T (Is there a "middle way" for compute-and data-intensive HPC?)
  - Need for advances in use of UQ, error analysis, optimization tools, inverse methods
  - Need for use of advanced IS&T tools (image analysis, machine learning, intelligent coarse graining and stochastic modeling, training models/hypothesis discovery...)
- **Timeliness**
  - National security imperatives: Need for early S&T impact
  - Generational technology changes for HPC compared to 15 years ago
    - Speed-up solution unlikely
    - Even more need (& opportunity) for "Co-Design" of National Assets
      ➡ Discovery Prediction, control raised to qualitatively higher level

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LANL's Response: Recent Actions Supporting and Guiding CPAM

- Team assessing Co-Design opportunities for LANL
- New Group in CCS Division "Applied Computer Science"
  - Agile codes for future architectures (NW, NE, EM, Climate, ...); Training next generation
- XCP division created; aligned with CPAM for weapons program
- Multi-division leader planning team for ASC Program balance
- Roadrunner Open Projects; FY10 LDRD investment in "Comp Co-Design"
- Los Alamos Computer Science Symposium Series
  - Themes: "Data Intensive Architectures and Applications"; "Heterogeneity for Future Applications"
  - 2011: plan to evolve into a LANL, ORNL, SNL collaborative effort

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LANL's Response: Recent Actions Supporting and Guiding CPAM

- Major progress in Mod & Sim, HPC roles in MaRIE; synergy with NW, NE
- New ECI, EM, EERE teaming across Lab and in multi-Lab consortia
- Extensive use of LANL Centers, Institutes, NM Consortium (collaborations, students)
- ASC support for Metropolis Postdoctoral Fellow, and Computational Astrophysics Initiative
- Positioning for SciDAC & Co-Design Centers. (Dedicated DOE-ASCR POC's for AM, CS, SciDAC)

Full engagement and leadership roles in DOE exascale decadal planning (NNSA & SC)

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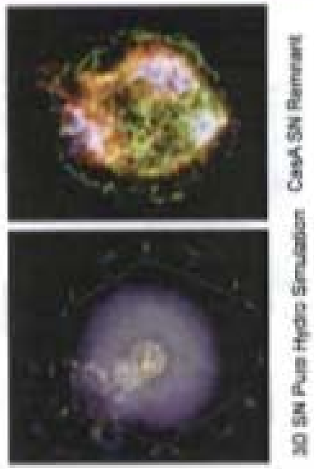
Science @ Roadrunner: e.g., CASSIO (IMC-Hydro) –Simulation of Core Collapse Supernovae

(See C. Fryer poster)

- Core collapse supernovae are an ideal cosmic laboratory for studying high energy density physics (HEDP)
- Supernovae diagnostics of the HEDP regime come primarily from the optical spectra of supernovae
- Modeling these spectra requires higher order radiation hydro codes
  - LANL has built an IMC-Hydro code (CASSIO) to simulate an asymmetric supernova
  - The RR cells are being used to accelerate the most expensive part of the calculation, IMC
- Positions LANL as part of DOE-ASCR End Station and SciDAC initiatives



(Hungerford et al.)

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Selected (from dozens) Recent Conferences and Educational Activities

- Los Alamos Computer Science Symposium (LACSS, Santa Fe, annual event)
- Workshops
  - Scientific Grand Challenges in National Security: the Role of Computing at the Extreme Scale (10/09) (Joint DOE – ASCR & NNSA)
  - ISTC: Uncertainty Quantification (2008)
  - Ice Sheet Modeling (2009)
  - UQ (Fall 2010)
- Graduate level courses (2009 – 2010)
  - Finite Element Methods in Solid Mechanics I, II, III
  - Verification and Validation of Computer Models I, II
  - Digital Signal Processing II
  - Computational Systems Biology
  - Parallel Processing
- Seminars/lectures/tutorials (2009 – 2010)
  - "Roadrunner Tutorial Series" (series of 5 sessions)
  - "Models and Simulations for Energy"
  - "Coarse-graining agent-based computations: equation-free and variable-free computations"
  - "Predictive Maturity: a Quantitative Metric for Optimizing Complex Simulations via Systematic Experimental Validation"
  - "Equation-free Implementation of Statistical moment Closures"

A few recent Honors
- 3 SIAM Fellows
- Chair, IUPAP Commission on Computational Physics
- Editor, ASME J. Fluids Eng
-
-

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Summary: We are Focused on Foundations for Discovery and Progress in the 21st Century.
➢Computational Science and Applied Math critical to science and engineering: *must provide effective resources.*
➢Computational technology is undergoing a transformation: *must prepare for the future.*
➢Information and knowledge discovery will open exciting new opportunities: *must develop the science and technology base.*
Ocean Vorticity Simulation
Cell Broadband Engine Chip
Long Wavelength Array
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Co-Design can Define a Future with Maximum Impact: A Sociological and Scientific Challenge
Models/ Algorithms
Codes
National Missions
Architectures
Experiments/Data/ Facilities
CO-DESIGN for Prediction/ Control/Design
Theory, Modeling
What should a next-generation user facility look like? Beyond "cottage industries"?
• Resetting integration and collaboration framework for transformational S,T & E: Science & Mission Frontiers (SciDAC, End Stations, Hubs, Cloud,... Co-Design Centers)
• LANL opportunities being developed: NW Predictive Capability Framework, Energy–Climate, NE, EM, Cyber... MaRIE...
(Interdisciplinary teams, agile codes, IS&T tools, Analysis & Visualization of massive (streaming) data...)
See A. White presentation: Applications; Community CS/AM activities; Multi-Lab Associations
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The National Setting: The Next Decade will be a Perfect Storm of Opportunity: Understanding, Prediction, & Management

(See A. White presentation)

Summary of Requests for CPAM Review

- Quality of the science, technology and engineering
- Views on strategic directions
- Opportunities, Partnerships overlooked?
- Gaps

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Computational Physics and Applied Mathematics
Capability Review

Supplementary Slides

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Computational Physics and Applied Mathematics
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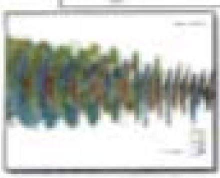
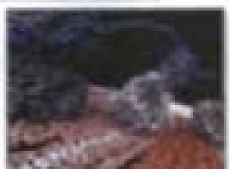
In This Time of National Transition & Opportunities, Los Alamos is Committed to Continuing Excellence in Computer and Computational Sciences and Applied Math


HIV epidemiology


Formation of nanomaterials


Laser-plasma interactions


Breakdown of cellulose

- Delivering to the nuclear weapons program:
  - Support for Predictive Capability (certification, SFIs, 3-D baselines, Knob resolutions ...)
- Open science
  - Reliable and deep capability base for weapons
  - Enabling new science and mission frontiers
- Institutional computing
  - Supporting scientific innovation and technology development
  - Partnership with climate (DOE-SC) and weapons (ASC) programs
- Investing in the future
  - Right-sizing/Balancing ASC Program
  - Centers/Institutes
  - Exascale planning! (Joint DOE-SC/NNSA)
    - "Codesigning" codes, architectures, applications
  - Hybrid/Multicore consortia

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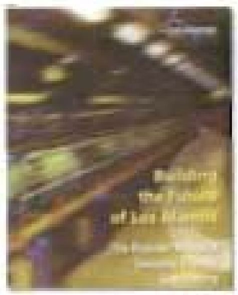
Laboratory Goals – http://int.lanl.gov/goals/

- Safe, Secure Workplace
- Exemplary Information Security
- Environmental Stewardship
- Reliable Nuclear Deterrence
- The Future Weapons Complex
- Global Threats and energy Security
- Be the National Security Science lab
- Response Infrastructure
- Performance-Based Management
- Business Excellence
- Effective Communications and Community Programs
- Successful Workforce



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Capabilities Reviewed at LANL

Capability	Organizing Associate Directorate
Nuclear and Particle Physics, Astrophysics and Cosmology	ADTSC
Computational Physics and Applied Math	ADTSC
Computer and Computational Sciences	ADTSC
Information and Knowledge Sciences	ADTSC
Biosciences	ADCLES
Chemical Sciences	ADCLES
Sensors, Remote Sensing and Sensor Systems	ADCLES
Earth and Space Sciences	ADCLES
Accelerators and Electrodynamics	ADEPS
High-energy Density Plasmas and Fluids	ADEPS
Materials	ADEPS
Nuclear Engineering and Technology	ADE
Advanced Manufacturing	ADW
Weapons Science	ADW

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Los Alamos LDRD Grand Challenges: CPAM Critical to all of them!

Beyond the Standard Model

Advances in nuclear and astrophysics at extremes, dynamics and composition of the universe and fundamental symmetries and force

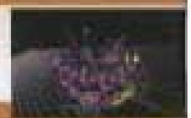
Mission Impact: Sensitive instrumentation and tools to manipulate massive data volumes, in support of national security missions

Materials: Discovery Science to Strategic Applications

Advances in prediction and control of performance, extreme environments and emergent phenomena

Mission Impact: Energy sources, efficiency and storage; sensing for threat reduction; materials underpinnings of stockpile security

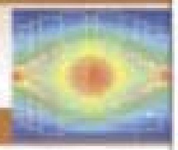
Complex Biological Systems



Advances in protection from pathogens, biology by design, understanding of the human brain and energy and climate impacts

Mission Impact: Energy, national security, health and the environment

Information Science & Technology

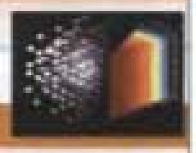


Advances in data intensive computing, inference/prediction, quantum information science and computing in extremes

Mission Impact: Overarching capability supporting all Laboratory missions

Los Alamos LDRD Grand Challenges

Energy & Earth Systems



Advances in energy storage, new fuels, nontraditional sources, sustainable nuclear power and managing energy byproducts

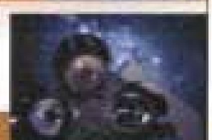
Mission Impact: Energy and climate security

Nuclear Performance

Advances in performance of heterogeneous explosives, degradation of thermonuclear performance, feedback between nuclear and thermonuclear performance and effects of off-normal conditions

Mission Impact: Stockpile safety, surety and reliability

Sensing & Measurement Science for Global Security



Advances in detection, forensics, signatures and movement/network characterization

Mission Impact: Nuclear weapons of mass destruction, space situational awareness, global environmental treaty monitoring and emerging threats

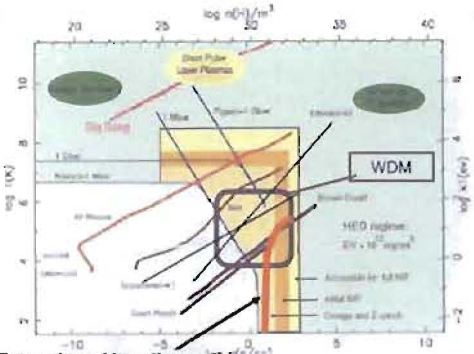
Intelligent, Adaptive Engineered Systems

Advances in validated models and simulations, intelligent sensor systems and information collection

Mission Impact: Overarching capability supporting all Laboratory mission

Matter Interaction in Extremes (HED, WDM)

- Research Directions
  - Predict, characterize, control performance of matter between solids and plasmas
  - Control transport of energy, momentum, mass at extreme density and T.
  - Exploit chemistry at extreme P, T.



Examples of Loading path
(out of equilibrium path-dependence)

Isochoric pre-Heating (ions)

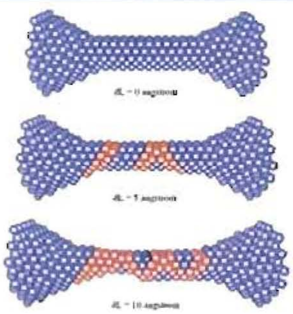
Isentropic compression

Probing with x-ray pulse & ion beam

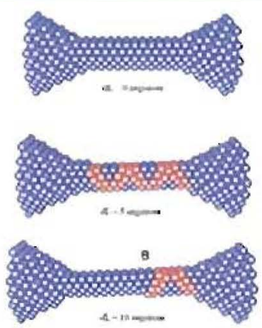
X-ray TS, & dE_0 / dx measurement

(See A. Voter poster)

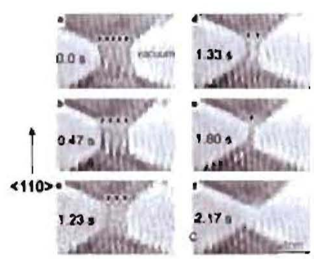
Science @ Roadrunner: Stretching Metallic Nanowires



High strain rate (10^7 s^{-1}) simulation shows necking



Lower strain rate (10^3 s^{-1}) simulation thins uniformly



(note rotated orientation)

Gold nanowire experiment can be compared with Roadrunner simulations

New with Roadrunner: atomistic simulations long enough to be directly validated by experiment

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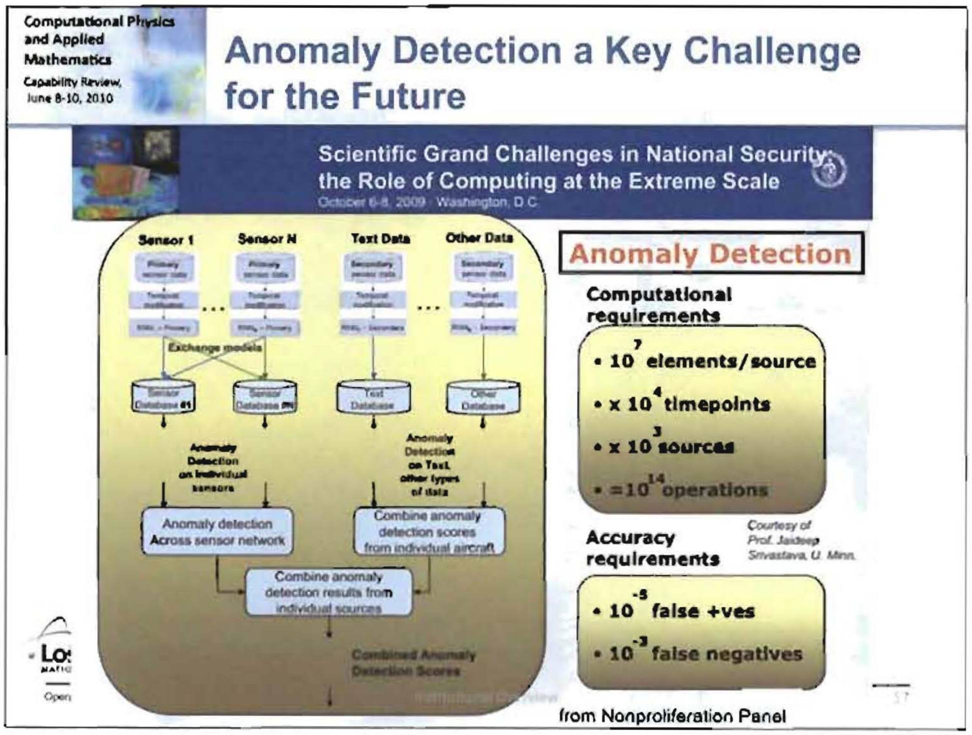
Courtesy Pao, Perez, Swaminarayan and Voter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Anomaly Detection a Key Challenge for the Future
Scientific Grand Challenges in National Security: the Role of Computing at the Extreme Scale
October 6-8, 2009 · Washington, D.C.
Sensor 1
Sensor N
Text Data
Other Data
Exchange models
Anomaly Detection on individual sensors
Anomaly Detection on Text, other types of data
Anomaly detection Across sensor network
Combine anomaly detection scores from individual aircraft
Combine anomaly detection results from individual sources
Combined Anomaly Detection Scores
Anomaly Detection
Computational requirements
• 10^7 elements/source
• x 10^4 timepoints
• x 10^3 sources
• =10^14 operations
Accuracy requirements
Courtesy of Prof. Jaideep Srivastava, U. Minn.
• 10^-5 false +ves
• 10^-3 false negatives
from Nonproliferation Panel

Lowrie

Overview of Computational Fluid Dynamics Research at Los Alamos

Robert B. Lowrie / CCS-2

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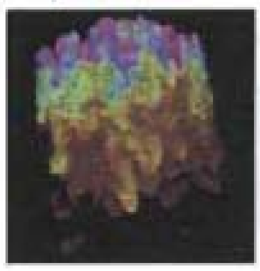
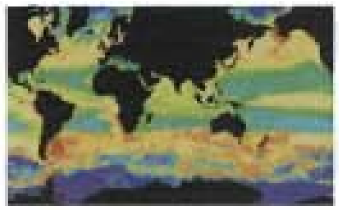
LANL missions drive CFD to be a core capability

- Computational Fluid Dynamics (CFD) at LANL is supported primarily by DOE NNSA (60%) and Office of Science (20%), LDRD (15%), and others (5%: DTRA, NSF, NASA).
- Supports our missions in stockpile stewardship, environmental management, national security, climate prediction, and energy security.
- Staff primarily from XCP, T, CCS, EES, and WX Divisions
- A critical component is our collaborations with other labs and universities



Coupling CFD with other physics is a significant focus

This CFD theme will highlight our efforts in:



- Weapons modeling
- Climate modeling
- Turbulence research
- Subsurface flow modeling
- Astrophysics research
- Urban consequences
- CFD on heterogeneous multicore architectures

In collaboration with many others, LANL is a leader in coupling other physics with CFD and applying it to complex problems on the most advanced computer architectures

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LANL's CFD Capability is Critical to its Nuclear Deterrent Mission

- DOE Advanced Simulation and Computing (ASC) Program supports two major code projects at LANL
- Shavano Project:
  - Lagrangian/ALE hydro on general polyhedral meshes
  - See Shashkov talk
- Crestone Project:
  - Eulerian-Godunov hydro on Cartesian meshes with cell-by-cell AMR

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Crestone Project Capabilities are Unique in NNSA Complex

- Godunov-based, high-resolution method, Eulerian
  - Dominant method in CFD, particularly for flows with large vorticity
- Cell-by-cell adaptive mesh refinement (AMR)
  - Ability to resolve features not seen before in Lagrangian/ALE code simulations
- Very easy problem set-up
- Cell-centered: when coupling to other physics, easy to conserve mass, total momentum, total energy
- There remain significant technical challenges, such as excessive artificial mixing at immiscible material interfaces
- Crestone codes also support other science missions (astrophysics, urban consequences, ICF)

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AMR is critical to attain a predictive capability

- LLNL and AWE are now developing AMR codes as well
- As an example, consider the radiative shock verification problem of Lowrie & Edwards 2008
  - First-of-kind, full rad-hydro verification problem, used also by LLNL, AWE, and university codes
- Mach 5 shock into a hydrogen gas (1 g/cc, 100 eV), Bremsstrahlung absorption, Thomson scattering
- Produces Zel'dovich spike (multiscale feature)
- RAGE shown to converge roughly first-order to exact solution (Lowrie & McClarren 2008)

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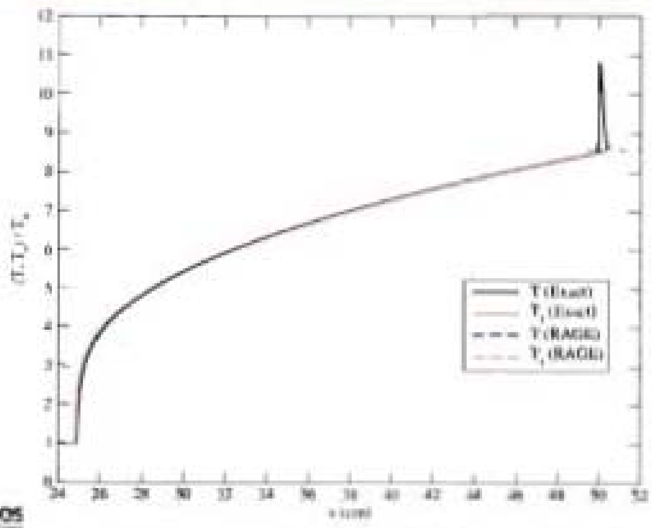
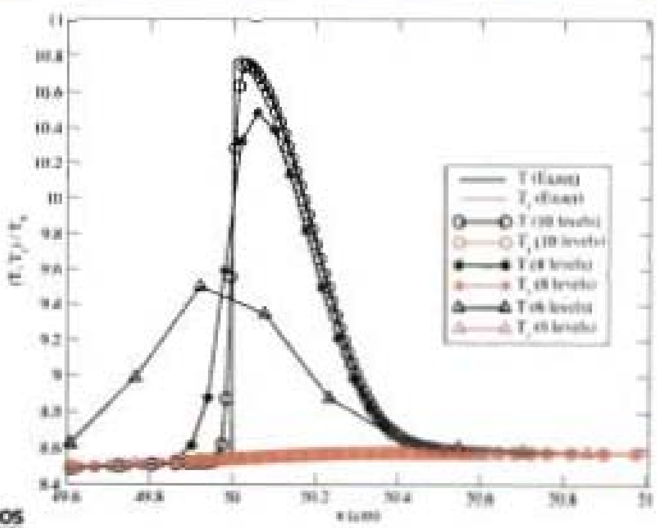
RAGE converges to exact radiative shock solution



AMR required 10 levels of refinement to resolve spike



AMR offered significant savings for radiative shock problem

- 528 cells vs. 51,200 cells (equally spaced mesh)
- Problem is relatively simple, yet spike is rarely resolved in engineering calculations
  - Most AMR calculations use only 4 or 5 levels (unless they have sub-cycling)
- Spike can result in a ~30% overshoot in temperature
  - Resolving spike may be critical for reactive flows
- Spike does NOT move at the flow speed
  - No Lagrangian/ALE code can currently compute the spike accurately without unreasonable meshing

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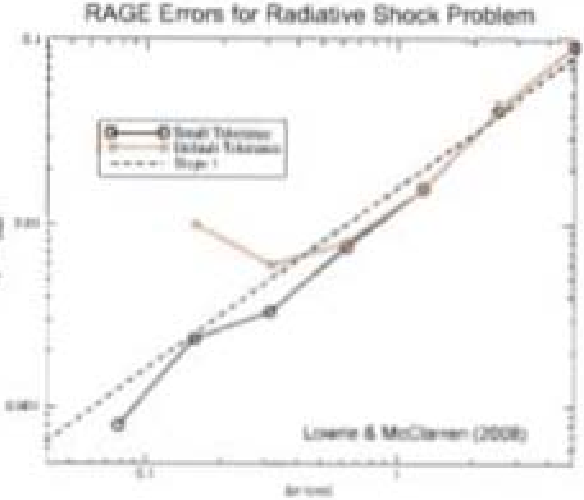
LANL multiphysics verification efforts impact community codes

- A robustness "fix-up" was causing convergence to stall
- Undetected without exact solution
- This problem has also uncovered issues in LLNL and AWE codes
- Multiphysics verification is an ongoing challenge

RAGE Errors for Radiative Shock Problem



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Astrophysics helps drive mission-relevant R&D

- Astrophysics R&D is directly relevant to stockpile stewardship and national security missions
- Allowed LANL to produce the first detailed spectra of supernovae from a coupled rad-hydro simulation
- Helped drive development of Roadrunner accelerated code (product of ASC Crestone Project)
- Also leverages on LANL's expertise in atomic physics

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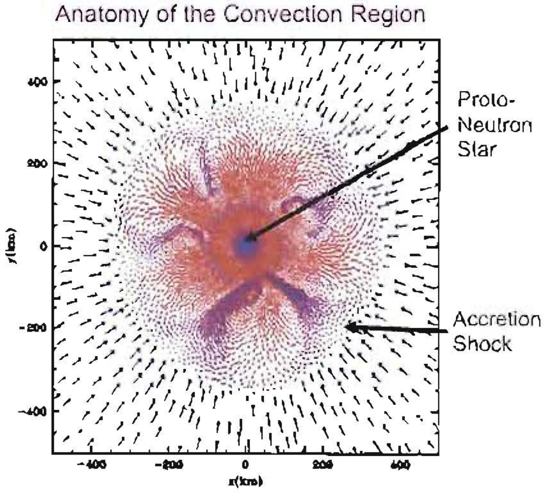
LANL at cutting edge of multi-physics supernovae simulations

- We model a wide spectrum of problems:
  - Core-collapse engine (neutrino transport)
  - Ejecta and nucleo-synthesis (nuclear networks)
  - matching spectra to observations (thermal transport)
- See Fryer's poster

Anatomy of the Convection Region



Fryer et al.: convection in the SN engine

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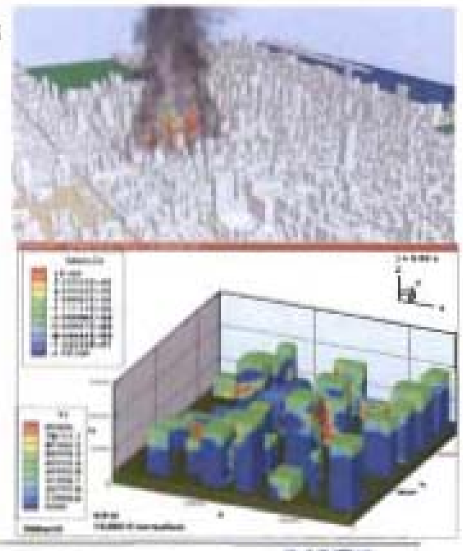
LANL CFD *R&D 100* winners used for urban consequences

- ASC Crestone Project provides source calculations
- R&D 100 winners modified for these applications:
  - Firetec forest-fire code (2003 winner; EES-16) models fire storm, on Roadrunner
  - CartaBlanca code (2005 winner, T-3) models flow and building damage
- Program development stage:
  - $500K ASC; $250K DTRA
- See Bos' poster



LANL a leader in HPC for environmental management

- Major Projects:
  - SciDAC-2 *Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows using Advanced Computing* (Lichtner PI, EES-16)
    - $800K / year for 5 years + INCITE
  - DOE-EM *Advanced Simulation Capability for Environmental Management* (Dixon PM, EES-DO)
    - LANL funding: FY10: ~$3M, FY11: ~$4-6M (anticipated)
- Targeted at energy security and environmental management missions

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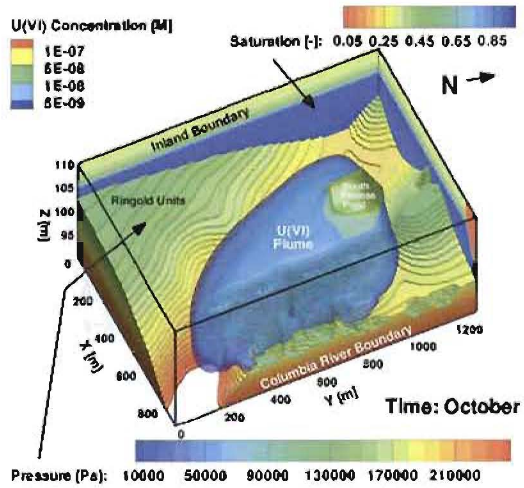
PFLOTRAN state-of-the-art modeling of Hanford waste site

- SciDAC-2 PFLOTRAN: next-generation reactive flow and transport code
- Joint with PNNL, EGI/UU, ORNL, UIUC
- Demonstrated good scaling on various architectures up to 131,072 cores
- On right are results of uranium plume as it impacts the Columbia River
- See Lichtner's poster



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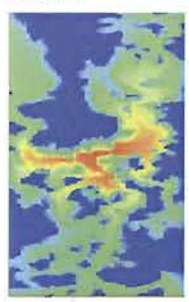
LANL leads effort to develop HPC Environmental Management code

- DOE-EM initiated Advanced Simulation Capability for Environmental Management (ASCEM) project
- Joint effort with LBNL, PNNL, ORNL, LLNL
- LANL leads critical tasks (PM Paul Dixon)
  - HPC Simulator (core framework, geo-chem reactions, nonlinear solvers, multi-process coupling)
  - Spatial discretizations (see Lipnikov's poster)
  - UQ and decision support
- Staff from EES, T, and CCS Divisions.
- See Moulton's poster



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LANL world leadership in heterogeneous multicore advances our CFD capability

- *Cassio* astrophysics code:
  - Hydro on Opterons ("unaccelerated")
  - Thermal transport (implicit Monte Carlo) accelerated
  - Product of the ASC Crestone Project
  - See Fryer poster
- DNS simulation of turbulence (Livescu talk)
- Wohlbier, Lowrie, Bergen rad-hydro ASC project (2009-, unsplit Eulerian hydro)
- Woodward (U. of Minnesota) PPM simulations of fluid mixing

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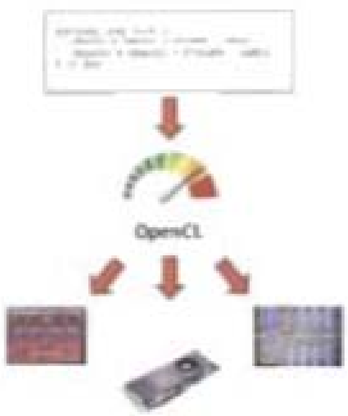
OpenCL used as a programming model for CFD development

OpenCL is a framework for applications development on multicore, manycore and accelerated architectures

- Runtime Environment
  - Work distribution, dynamic kernel compilation
- Application Programming Interface
  - Process launch, communication, synchronization
  - Topology interrogation (resource detection)
- OpenCL C Kernel Language
  - Low-level computational kernel language
  - Subset of C with extensions
  - Abstract vector types and intrinsics



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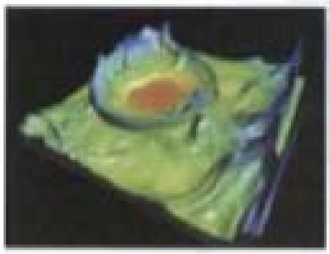
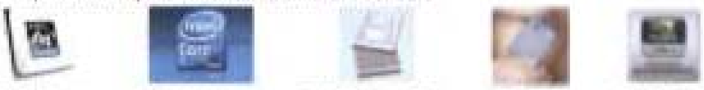
Our goal is portable code on heterogeneous architectures

Demonstration:

- High-resolution direct Eulerian hydrodynamics solver
  - MUSCL-Hancock Godunov method
  - Solves two-dimensional Euler equations
  - Structured grid with reflecting boundaries
  - Surface plot shows density on z-axis
- Distributed-memory parallel with MPI
- Implemented with C++ and OpenCL
  - Same source implementation runs on all architectures
  - SC09 Demo ran on five different architectures using OpenCL compilers form three different vendors





AMD Multicore | Intel Multicore | IBM Multicore (P6) | IBM Cell | NVIDIA GPU

See Bergen's Poster

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Significant challenges remain for heterogeneous multicore

- Thus far, Roadrunner codes accelerate only a subset of algorithms:
  - single physics
  - small amount of constitutive data
  - particle methods, or Cartesian meshes for PDEs
- Porting production-level MPI code remains a significant challenge
  - unstructured meshes, AMR, sparse c[illegible] material data storage
  - training, programming models

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Issue: UCNI designation limits our collaborations and science

- The Unclassified Controlled Nuclear Information (UCNI) designation is given to codes with very limited capability
- Example UCNI code: Perfect gas, single-material hydro coupled with P_N radiation
- But if code written at a U.S. university, then typically *not* treated as UCNI
- Severely limits our collaborations, peer review, and recruitment in astrophysics and HEDP.

Future Directions: Algorithmic Challenges

- AMR will be required for *multiphysics* predictive capability
  - refinement criteria and error control (multiphysics)
  - subcycling other physics to allow increased levels of refinement
  - code performance and scaling
  - AMR on a fully-unstructured (e.g., used in Lagrangian/ ALE) base mesh
- Material mixed-cell treatments and other subgrid models

Future Direction: Multiscale

- In our application space, the era of developing CFD capability as an isolated physical process is coming to an end
  - Early on, must account for other physical processes
  - Account for tight coupling (stiffness)
- DNS of coupled physics processes
- Kinetic descriptions for fluids / plasmas
- Molecular dynamics for constitutive data
- Non-LTE effects for radiation
  - population of bound states a local calculation

Future Direction: Exascale

- Exascale requires two major focus areas:
  1. Port existing algorithms. But current algorithms generally do not scale, so...
  2. Develop new algorithms and physical models to take advantage of the extra computing power
- #1 has been our initial focus
- #2 will be our future focus on <u>*co-design*</u>:
  - a close collaboration between theorists, numerical analysts, and computer scientists,
  - across NNSA, Office of Science, and universities

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LANL's long history in developing and applying CFD continues today

- In collaboration with many others, LANL is a leader in coupling other physics with CFD and applying it to complex problems on the most advanced computer architectures
- CFD is ubiquitous across our results-driven missions in stockpile stewardship, environmental management, climate prediction, national security, and energy security

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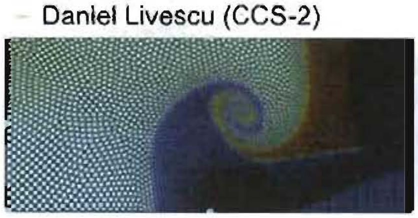
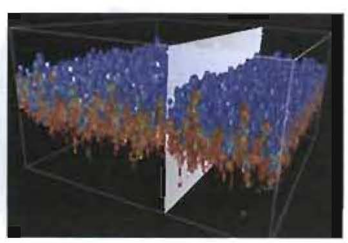
Upcoming CFD Talks

- *Discretizations and Closures for Climate Applications*
    - Todd Ringler (T-3)
- *Numerical Methods and Algorithms for High-speed Multimaterial Compressible Hydrodynamics*
    - Misha Shashkov (XCP-4)
- *Direct Numerical Simulations of Fluid Turbulence*
    - Daniel Livescu (CCS-2)





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Ringler

5/27/10

Discretizations and Closures for Climate Applications

Todd Ringler, Theoretical Division

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History of climate modeling at LANL

Climate modeling got its start at LANL in 1979 with the participation of Bob Malone in the development of the first version of the NCAR Community Climate Model (CCM0).

In 1983 this grew into a small project directed toward the modeling of nuclear winter.

In 1990 DOE started the Computer Hardware, Advanced Mathematics, and Model Physics (CHAMMP) program. Out of this program, the LANL Climate, Ocean and Sea-Ice Modeling (COSIM) project was born.

COSIM now includes about 20 staff/postdoc members focused on ocean, sea-ice and land-ice model development. FY10 budget ~$6M

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Climate modeling is a computational grand challenge of nation importance.

Modeling the Earth's climate as the concentrations of greenhouse gases rise is a grand challenge in many different respects:

1. Unresolved scales are of O(1) importance
2. Incomplete understanding of O(1) processes
3. Complexity
4. Limited data that is representative of future conditions.

This talk is focused how we might tackle #1 and #2 in a computationally-tractable manner.

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Climate modeling is an important component of LANL's and DOE's mission

Climate modeling aligns with LANL's Earth and Energy Systems Grand Challenge to "....develop the capability to measure, model, and predict, in a quantifiable manner, the impacts of energy choices on climate and their cascading effects on the environment and society."

Within DOE BER, the Climate and Environmental Science Division supports fundamental research to "achieve a predictive, systems-level understanding of climate change."

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Within the DOE, climate modeling is spread broadly across the complex.

Within LANL, the Climate, Ocean and Sea-Ice Modeling (COSIM) activity related to global climate modeling.

LANL, LBNL, LLNL, ORNL, PNNL and SNL all make substantial contributions to the DOE climate modeling activity.

The Community Climate System Model (CCSM) hosted by the National Center for Atmospheric Research (NCAR) the the integrating activity for the majority of the DOE climate effort.

is

The CCSM is used broadly, ranging from hypothesis-driving experimental design to IPCC assessment reports.

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Computational Physics and Applied Mathematics
Capability Review
June 8-10, 2010

Working toward a comprehensive multi-scale modeling capability for climate simulation

The points I would like to leave you with today:

1. The scientific community would benefit greatly through the creation of a comprehensive multi-scale modeling capability.

2. We have taken the first steps along this path 1) by deriving the first multi-resolution finite-volume method applicable to climate system modeling, 2) by developing a high-order transport scheme applicable to multi-resolution grids, and 3) by developing dispersive closure models.

3. This new approach to climate system modeling has the potential to change, in a very fundamental way, how we build and use climate system models.

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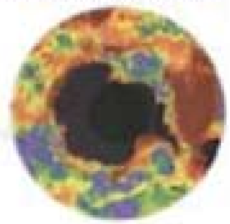
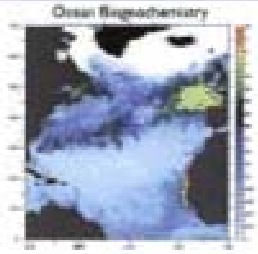
Global climate modeling will always be an under-resolved endeavor.

Cloud Processes

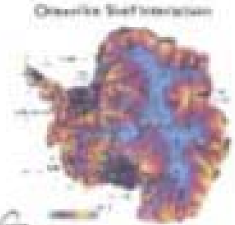
Ocean/Atmosphere Interaction



Ocean Biogeochemistry



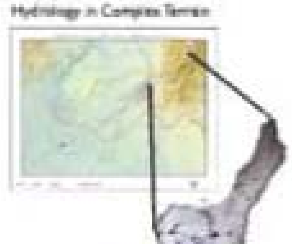
Ocean/Ice Shelf Interaction



Each of these examples demonstrate scale-sensitive processes that might impact the climate system in a fundamental and important way.

The length scale of these processes is O(km). Resolving all of these processes, everywhere, all the time is not an option due to computational limitations.

Hydrology in Complex Terrain



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A multi-scale modeling approach allows the simulations of key processes in specific regions with conforming, variable resolution meshes.

The goal is to resolve specific processes in specific regions, while maintaining a global modeling system.

The approach allows us to explore the influence of resolving new processes on both the regional (downscale) and global (upscale) climate system.

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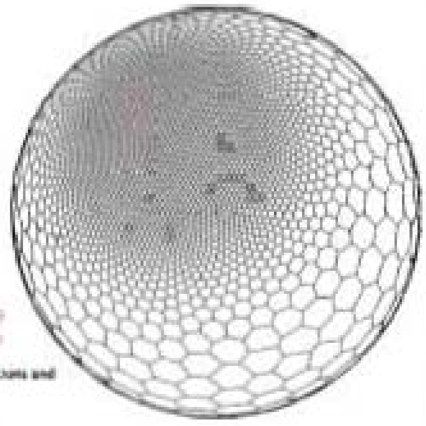
Modeling based on Spherical Centroidal Voronoi Tessellations (SCVTs).

The approach is flexible; the user specifies the mesh density field.

The approach has a theoretical foundation; the cell size is inversely proportional to the user-supplied density field.

The approach is extensible; Gersho's conjecture (now proven in 2D) states that all cells will be perfect hexagons regardless of the density field in the limit if infinite grid cells.

Here are?



X ?

Du, Faber and Gunzburger: 1999: Centroidal Voronoi Tessellations: Applications and Algorithms. SIAM Review.

Ringler, Ju and Gunzburger, 2008: A Multi-Resolution Approach to Climate System Modeling. Ocean Dynamics.

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A finite-volume solver for SCVTs that is robust for climate applications.

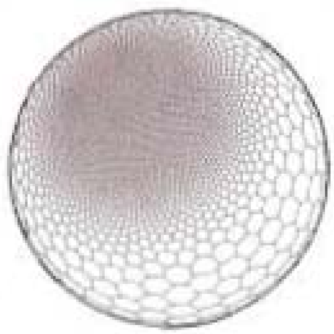
Computational fluid dynamics solvers for atmosphere and ocean climate applications have several special requirements.

1. Conserve total energy and accurately model the flow of energy between its different forms.

2. Conserve potential vorticity while respecting the Lagrangian nature of this quantity.

It is essential that finite-volume solvers respect a set of conservation principles founds in the underlying continuous system.

This has been the hallmark of robust finite volume methods used in climate applications for the last 40 years.



Ringler et al. 2010 (A unified approach to energy conservation and potential vorticity dynamics on arbitrarily structured C-grids in JCP) describes how to conserve energy and potential vorticity on arbitrary SCVTs.

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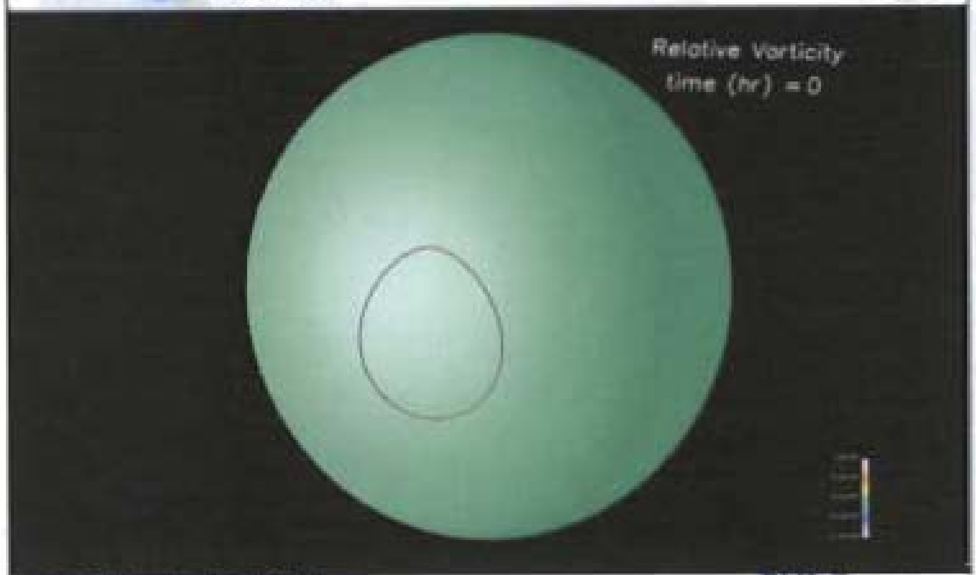
The method can accurately simulate highly rotating flows, even with variable resolution meshes.



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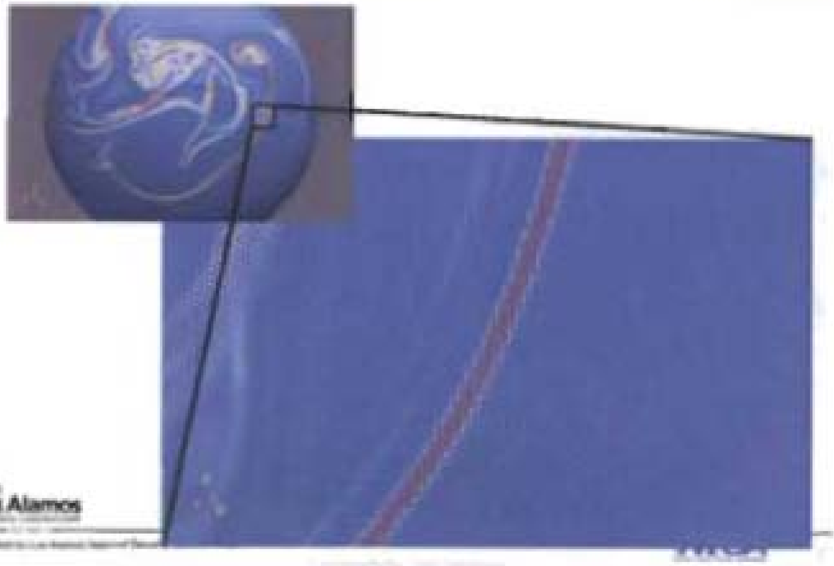
Idealized baroclinic eddy test case (i.e. weather systems) in a global 3D atmosphere model.

Global 30 km mesh, relative vorticity at surface, day 16

Grid-scale features are long-lived.



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Idealized ocean basin simulations show high levels of eddy activity and long-lived features.

Potential Vorticity, one frame per day

Ocean Double-Gyre Problem

forced by surface wind stress
5 km mesh
5000 km x 2500 km domain
No bottom drag
Laplacian mixing on velocity at 1.0 m^2/s
no-slip boundary conditions

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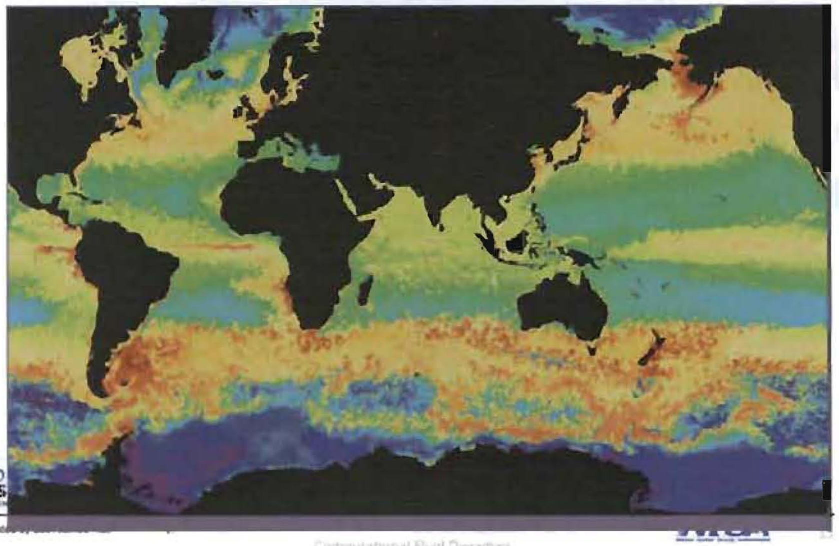
Transport is one of the most fundamental and important processes in global climate modeling.

Chlorophyll concentration from LANL's Parallel Ocean Program.



Computational Fluid Dynamics

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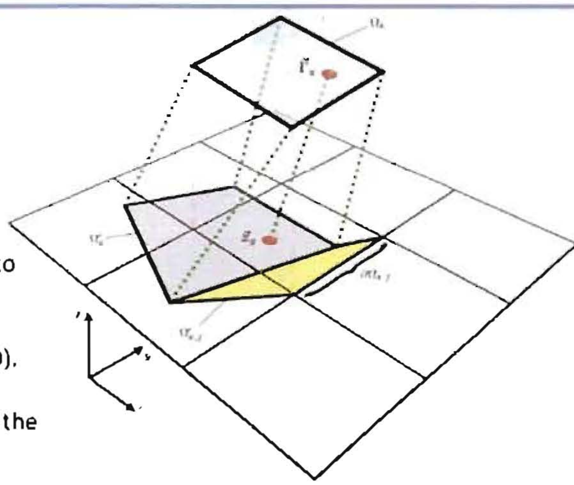
We have developed a high-order transport scheme to complement the finite-volume solver.

The Characteristic Discontinuous Galerkin (CGD) method takes advantage of the Lagrangian nature of transport while maintaining a static mesh. (Lowrie, 2010)

The method has been extended to arbitrary convex polygons and to arbitrary order of accuracy. (Buonoi, Lowrie and Ringler 2010).

The method has also illuminated the connection between CDG and Prather's Method-of-Moments.



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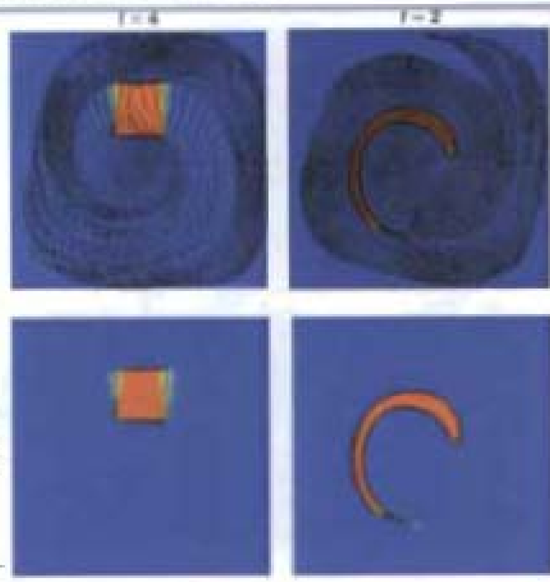
Computational Fluid Dynamics

16

Solid body rotation of a square bump with and without limiting.

High-order advection is prone to producing dispersive error (ripples) in regions of strong gradients.

These ripples are not physical, but are numerical error. In this method, we limit the flux calculation to insure that new extrema are not produced, thus removing the ripples.



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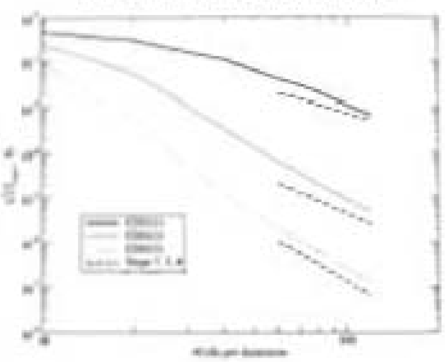
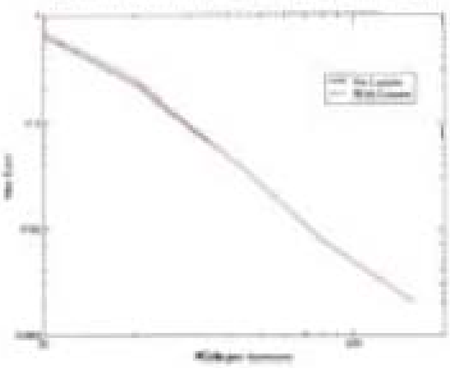
Error norms for solid body rotation of a (smooth) Guassian bump.

Order of accuracy increases with order of CDG reconstruction



The flux-limit algorithm does not impact accuracy when the function is smooth.



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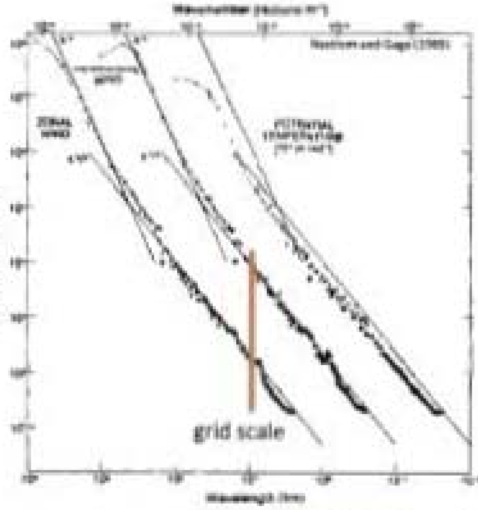
Even with a robust multi-scale approach, we still have to deal with unresolved scales.

Spectra of the atmosphere and ocean are typical of a system dominated by nonlinearity.

While the net energy transfer is toward higher wave number, the net is the small difference between large upscale and downscale energy fluxes.

A robust closure needs to capture the net impact of the truncated scales and be scale-aware.



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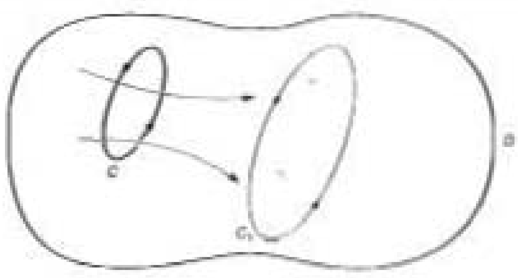
LANL has developed the Lagrangian-Averaged Navier Stokes (LANS-α) model.

LANS-α model is based on the following premise:

1. the system is best characterized by two velocities
a. a rough velocity from which vorticity is derived
b. a smooth velocity that transports this vorticity
2. the smooth velocity can be determined from the rough velocity
3. the rough and smooth velocities are related through a length scale



Also see presentation by Wingate.

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The power of the LANS-α model stems from the closures respect of energy and vorticity dynamics.

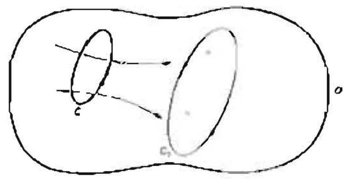
Even though the LANS-α model contains two velocities, it retains Kelvin's Circulation Theorem.

$$\mathbf{u} = Filter(\mathbf{v})$$

$$Filter = (1 - \alpha^2\nabla^2)^{-1}$$

$$\frac{d}{dt}\oint_{\gamma(\mathbf{u})} \mathbf{v}\cdot dr = \oint_{\gamma(\mathbf{u})} \nu\nabla^2\mathbf{v} + \mathbf{F}$$

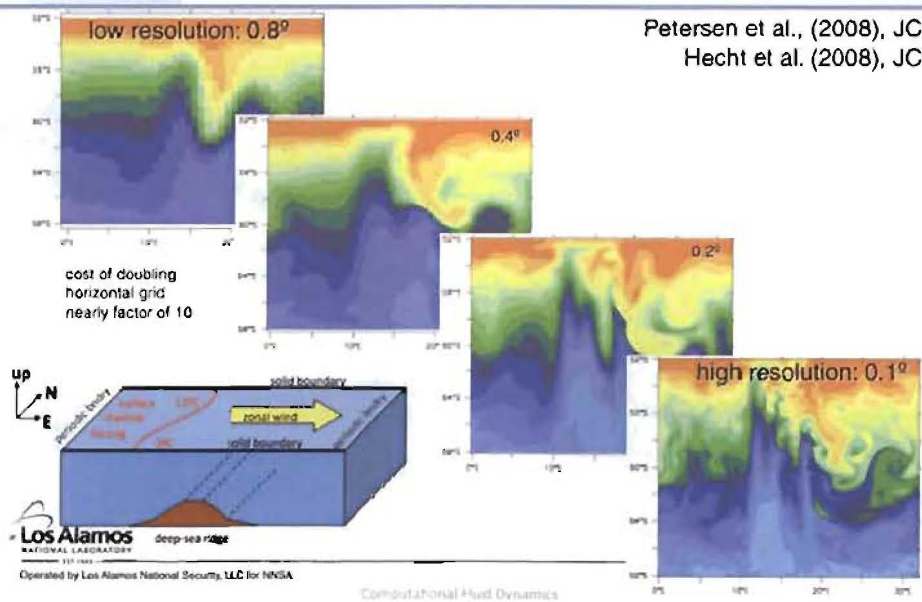
$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{v} + \nabla\mathbf{u}^T\cdot\mathbf{v} + \nabla\pi = \nu\nabla^2\mathbf{v} + F$$



Note: The finite-volume scheme discussed previously is the first implementation of the LANS-α model that preserves the LANS-α circulation theorem after discretization.

Evaluating the LANS-α model as a turbulence closure for ocean simulations

Petersen et al., (2008), JCP
Hecht et al. (2008), JCP



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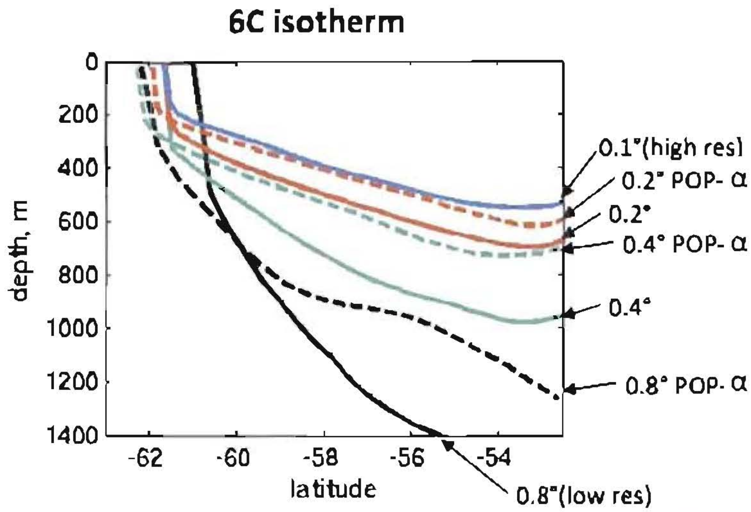
The LANS-α closure doubles the effective resolution of the simulation.



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Computational Fluid Dynamics

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We have taken the first steps toward the construction of a multi-scale climate model.

1) by deriving the first multi-resolution finite-volume method applicable to climate system modeling,

2) by developing a high-order transport scheme suitable for use on multi-resolution meshes, and

3) by developing LANS-a model as a turbulence closure.

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Computational Fluid Dynamics

The next decade will be an exciting period for global climate modeling at LANL.

1. A global atmosphere model based on the finite-volume solver is currently being tested as a dynamical core within the NCAR Community Climate System Model.

2. A global ocean model based on this same approach is currently under development with anticipated completion of prototype by end of 2010.

3. We expect to be testing a multi-scale climate system model (i.e. coupled atmosphere, ocean, ice system with variable resolution) within the next three to five years.

Shashkov

Numerical Methods and Algorithms for High-speed Multi-material Compressible Hydrodynamics

Mikhail J. Shashkov, XCP-4 Methods and Algorithms

Computational Physics and Applied Mathematics
Capability Review June 8-10, 2010

Connection to the Goals and Mission of the Laboratory

- LANL's primary responsibility is to develop and apply science and technology to ensure the safety, security, and reliability of the US nuclear deterrent.
- Under Advanced Simulation and Computing (ASC), computer simulation capabilities are developed to analyze and predict the performance, safety, and reliability of nuclear weapons and to certify their functionality.
- The Integrated Codes (IC) subprogram of ASC at LANL comprises laboratory code projects that develop and improve the weapons simulation tools, physics, engineering, and specialized codes.
- The core of the ASC codes is high-speed, multimaterial, compressible hydrodynamics.

Therefore, development of new numerical methods and algorithms for high-speed multi-material compressible hydrodynamics is absolutely critical for the mission of the Laboratory.

Numerical methods for high-speed multi-material compressible hydrodynamics from *ART* to Science

- Conservative discretization of Lagrangian equations on general polyhedral meshes
  - Artificial viscosity
  - Control of parasitic grid motion (hourglass)
  - Closure models for mixed cell
- Mesh rezoning: untangling, smoothing, adapting, reconnecting
- Remapping; conservative, accurate, bound-preserving interpolation
- Multi-material interface reconstruction

us (:)

Development of new methods and algorithms based on solid mathematical foundation allow to improve predictiveness and robustness of ASC codes.

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Funding, People Involved, Peers-Competitors

- Funding:
  - ASC Integrated Codes
    - Code Projects: Implementation and short-term research
    - Focused Research Innovation and Collaboration: Mid-term research and prototyping;
  - ASCR DOE Office of Science
    - ASCR Projection Mimetic Methods for PDEs-long term research and proof of principles.
  - LANL LDRD: ER, DR
    - Theoretical foundation
- LANL People Involved:
  - XCP-1, XCP-2, XCP-4, CCS-2, T-3, T-5
- Peers-Competitors:
  - US (LLNL,SNL), UK (AWE), French (CEA), Russian Labs
  - The Predictive Science Academic Alliance Program (PSAAP) centers at the Universities

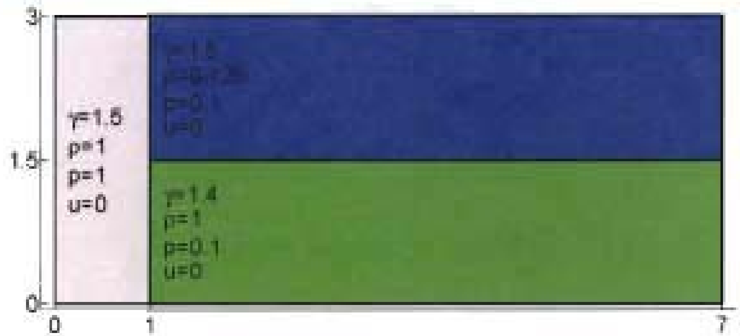
Context–Multi-material Arbitrary Lagrangian-Eulerian (ALE) Methods

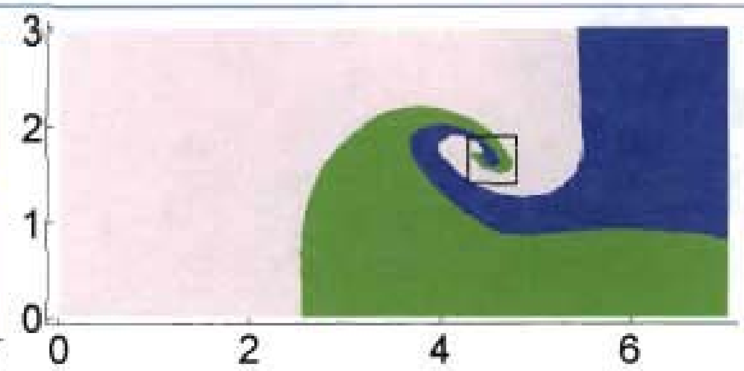
- Explicit Lagrangian (solving Lagrangian equations) phase—grid is moving with fluid
- Rezone phase changing the mesh (improving geometrical quality, smoothing, adaptation)
- Remap phase (conservative interpolation)—remapping flow parameters from Lagrangian grid to rezoned mesh

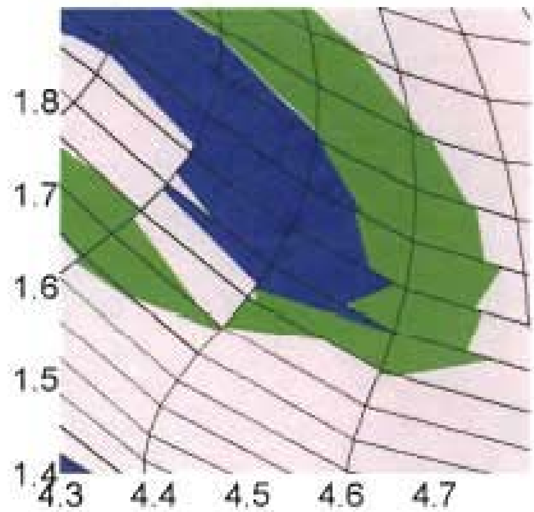
Accurate Interface Reconstruction is Critical for Multi-material ALE

- Multimaterial flows - immiscible materials
- Mesh is not moving with fluid
- Mixed cells containing several materials
- Interface reconstruction is needed to identify where the materials are in mixed cells
- Inverse problem-recover interface from multimaterial data
- PLIC – Piece-wise Linear Interface Construction
  Interface in each cell is represented by a segment of straight line

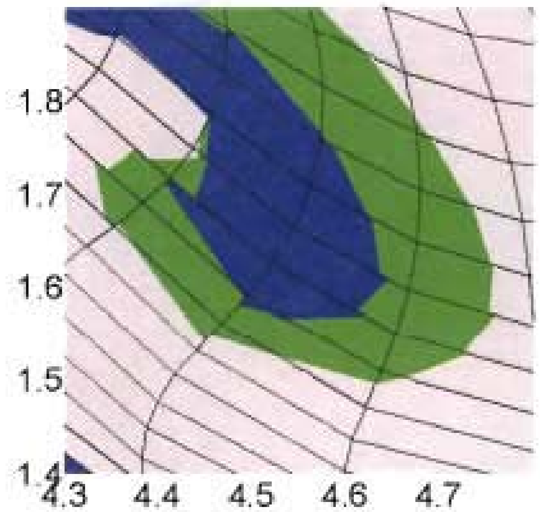
Interface Reconstruction-Vorticity Generation Why better methods are needed?





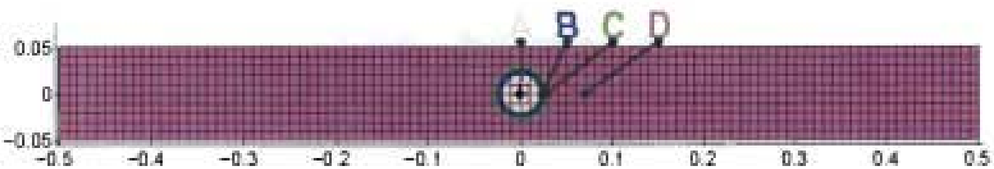


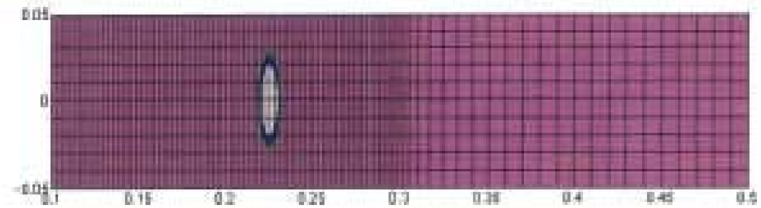
Conventional Interface Reconstruction – Integrity of Vortex is Broken

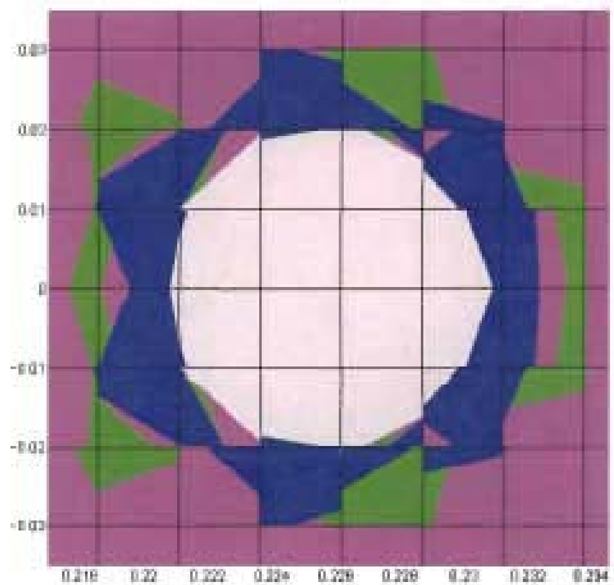


Moment of Fluid Interface Reconstruction – Integrity of Vortex is Preserved

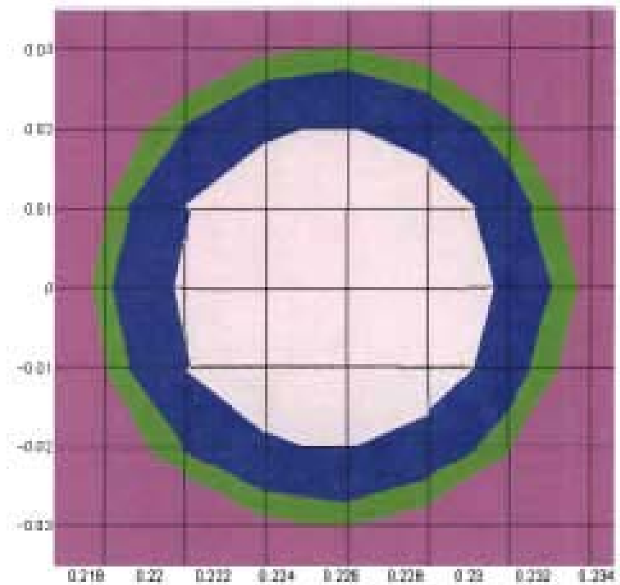
Interface Reconstruction-Shock/Bubble Interaction Why better methods are needed?







Conventional Interface Reconstruction – Integrity of Vortex is Broken



Moment of Fluid Interface Reconstruction – Integrity of Vortex is Preserved

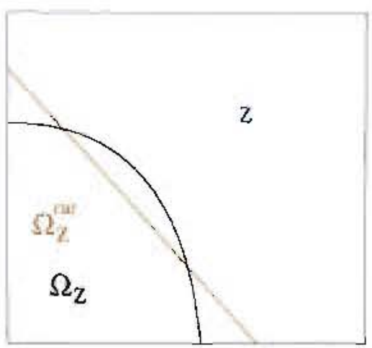
Moments of Fluid (MoF) Interface Reconstruction – Motivation

- Interface Reconstruction - Approximation of the Material Domain Ω

  Pure zone - $\Omega \bigcap Z = Z$, Mixed zone - $\Omega \bigcap Z \neq Z$, Z - zone of the mesh

  In standard interface reconstruction methods we are only given volume $|\Omega \bigcap Z|$ of the material in mixed zone - zeroth moment of $\Omega \bigcap Z$

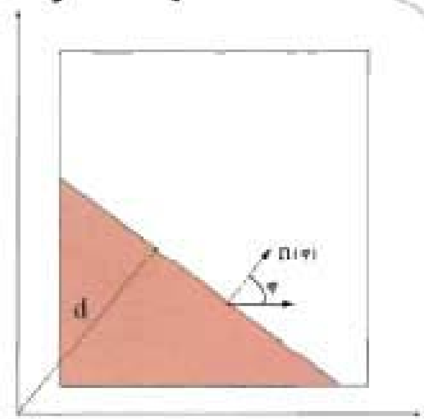
- In PLIC methods $\Omega_Z = \Omega \bigcap Z$ is approximated by Ω_Z^{cut} - cutout, piece of mixed zone.



Requirement is that zeroth moments of Ω_Z and Ω_Z^{cut} are the same $|\Omega_Z| = |\Omega_Z^{cut}|$

Moments of Fluid (MoF) Interface Reconstruction - Motivation

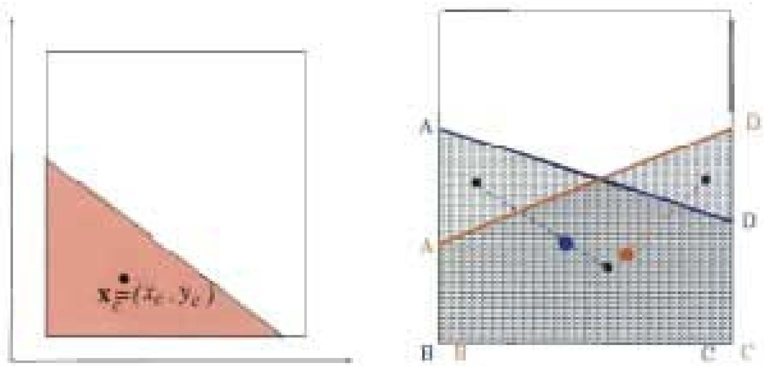
- There is infinite number of cutouts with given volume - one parameter
- How to chose one cutout, Ω_Z^{cut}, that is "best" approximation for Ω_Z?
- Cutout is uniquely defined by two parameters: $\varphi \rightarrow \mathrm{n}(\varphi)$ and d



- In standard PLIC methods normal is chosen using volume fractions at neighboring zones, volume fraction in zone Z itself defines d

  Problems with standard PLIC methods: material ordering, computation of normals

Moments of Fluid (MoF) Interface Reconstruction - Motivation



- **Cutout is also uniquely defined by its centroid = ratio of the first and zeroth moments of** Ω_Z^{cut}
  $\mathbf{x}_c\left(\Omega_Z^{cut}\right) = \int_{\Omega_Z^{cut}} \mathbf{x}\, dV \Big/ \left|\Omega_Z^{cut}\right|$
- **Now assume that we know centroid of** $\Omega_Z \longrightarrow \mathbf{x}_c\left(\Omega_Z\right)$.
- **We can construct unique cutout** Ω_Z^{cut}**, such that** $\mathbf{x}_c\left(\Omega_Z^{cut}\right) = \mathbf{x}_c\left(\Omega_Z\right)$
- **However, in general, for such cutout:** $\left|\Omega_Z^{cut}\right| \neq \left|\Omega_Z\right|$

Moments of Fluid (MoF) Interface Reconstruction - Statement

- Given: volume fractions of materials and their centroids (reference volume fraction, reference centroid)
- In each zone find: cutout which has the reference volume fraction, and which centroid is close as possible to reference centroid
- Properties:
  - Accuracy-recover cutouts exactly (in particular, half-plane),
  - One-cell consideration no information from neighboring cells is needed

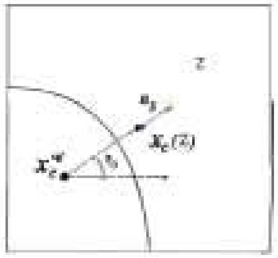
Moments of Fluid (MoF) Interface Reconstruction - Algorithm

$$F_{V^{ref}}(\Omega_Z^{cut}) = |\mathbf{x}_c\left(\Omega_Z^{cut}\right) - \mathbf{x}_c^{ref}|^2, \quad \Omega_Z^{cut} : |\Omega_Z^{cut}| = V^{ref}$$

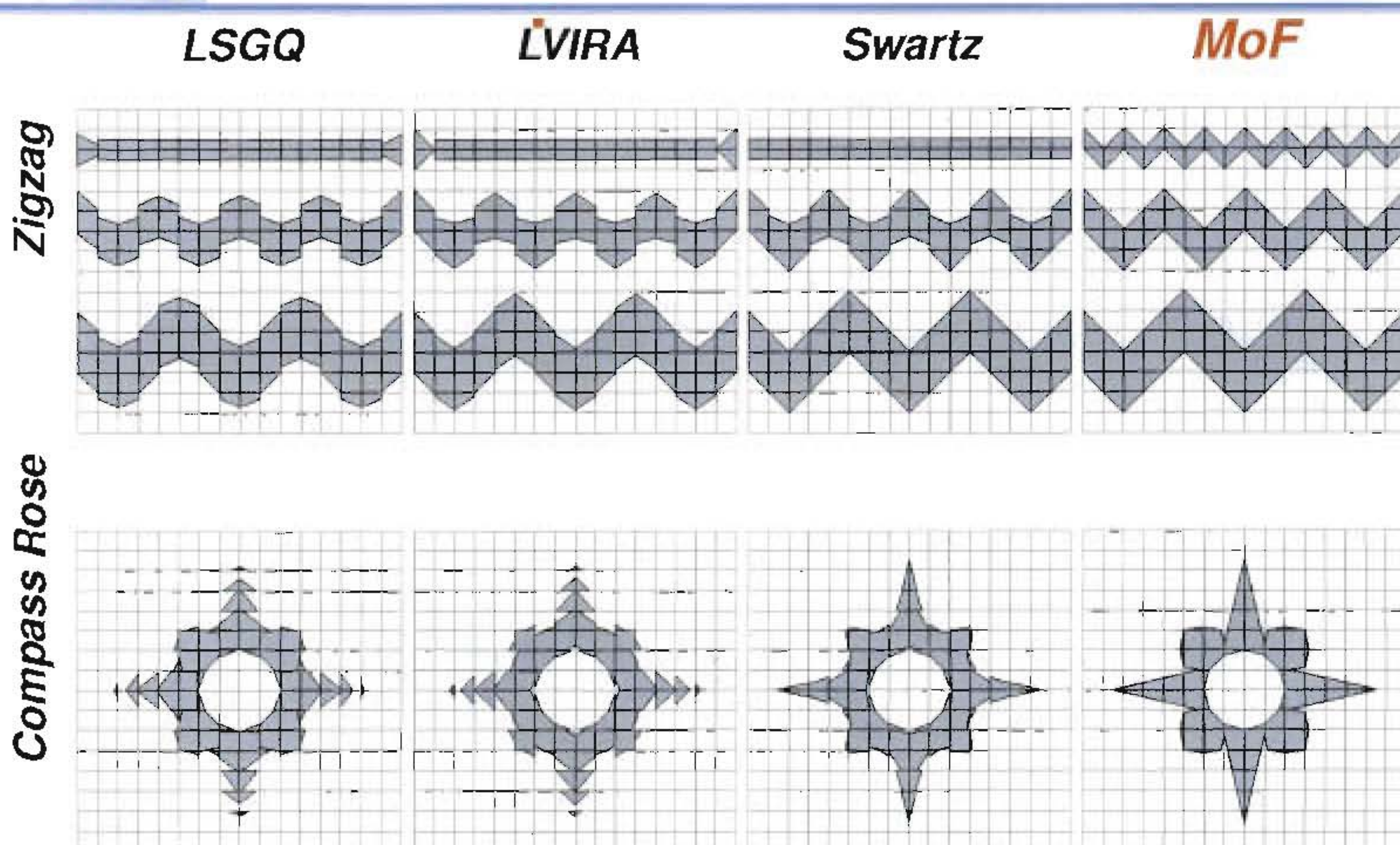
- If $|\Omega_Z^{cut}| = V^{ref}$ then cutout Ω_Z^{cut} can be uniquely determined from angle, φ, which determines the normal to corresponding straight line
- Centroid of cutout with given volume fraction is function of the angle φ
- $\mathcal{F}_{V^{ref}}(\varphi) = |\mathbf{x}_c\left(\Omega_Z^{cut}(\varphi)\right) - \mathbf{x}_c^{ref}|^2$ — function of one variable φ
- Cutout in MoF interface reconstruction is obtained by solving following optimization problem:

$$\min_{\varphi} \mathcal{F}_{V^{ref}}(\varphi)$$

- Function evaluation: given V^{ref} and angle φ cut appropriate piece of zone Z and then compute its centroid (explicit formula)
- Initial guess: $\mathrm{n}^0 = \frac{\mathbf{x}_c(Z) - \mathbf{x}_c^{ref}}{|\mathbf{x}_c(Z) - \mathbf{x}_c^{ref}|}$

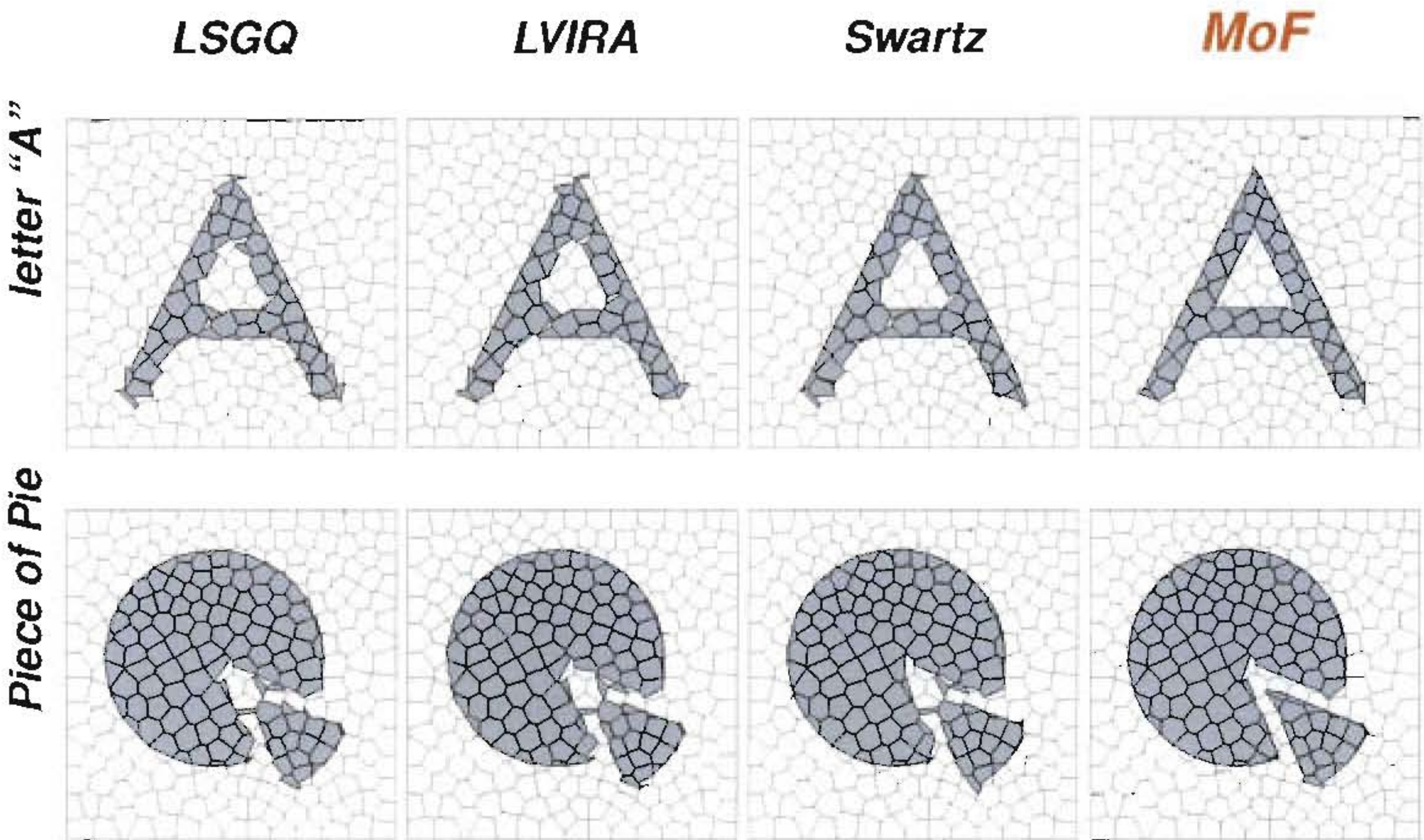


Examples - Resolution



LSGQ - Least Squares Gradient (Barth)
LVIRA - Least Squares VOF Interface Reconstruction Algorithm (Puckett)

Examples - Interface



LSGQ - Least Squares Gradient (Barth); LVIRA - Least Squares VOF Interface Reconstruction Algorithm (Puckett)

Multiple Material (≥3) Interface Reconstruction Nested Dissection - ND

Process materials in specified local order - $M1, M2, M3, \ldots$

- Reconstruct interface between $M1$ and the rest -$(M2,\ M3\ \ldots)$
- Remove relevant part of cell once material has been processed
- Reconstruction of next material interface in remaining part of the cell - $M2$ and the rest -$(M3,\ M4\ \ldots)$
- Repeat

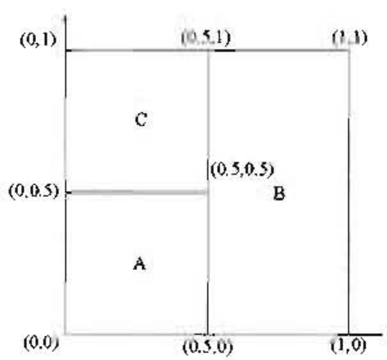
In MOF ordering defined automatically by choosing the order which minimizes overall error in centroids for all materials

---

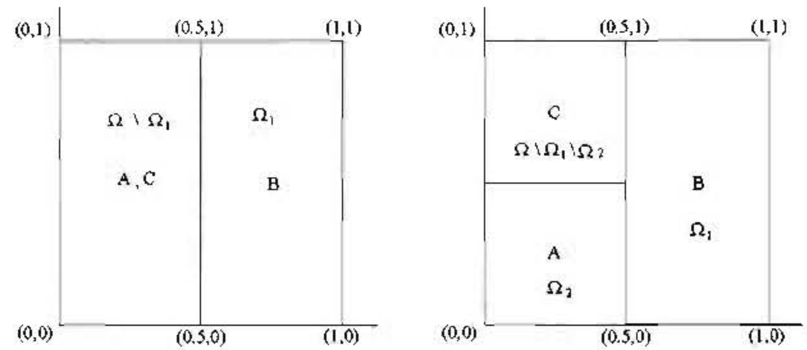
ND IS NOT an ONION-SKIN

$$M1 - (M2,\ M3,\ M4\ldots);$$
$$(M1,\ M2) - (M3,\ M4\ldots);$$
$$(M1,\ M2,\ M3) - (M4,\ M5,\ldots);\ldots$$

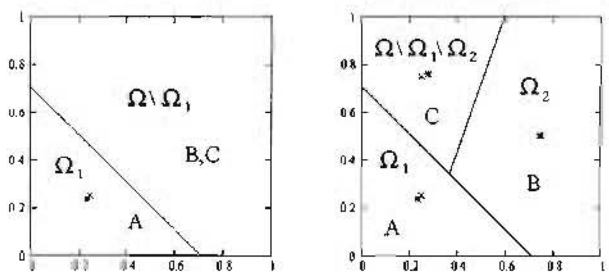
Example - T Junction



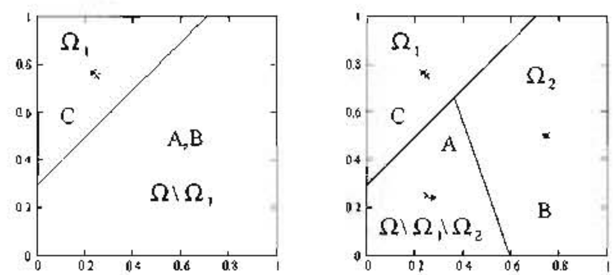
Original



(B, A, C) ordering.

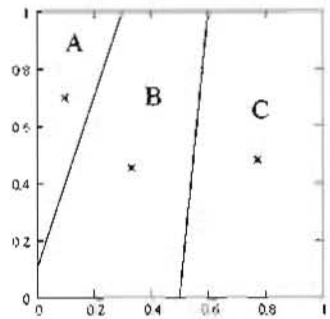


(A, B, C) ordering

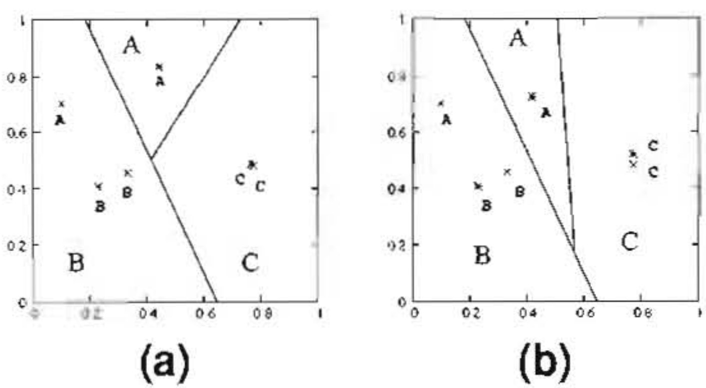


(C, B, A) ordering.

Example - Three material *layered configuration*

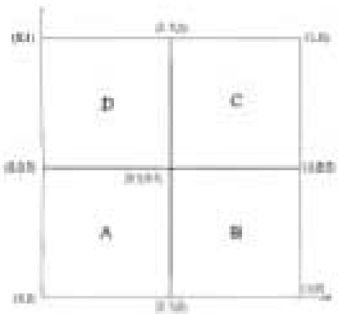


Original and (A, B, C), (A, C, B), (C, B, A), or (C, A, B) ordering

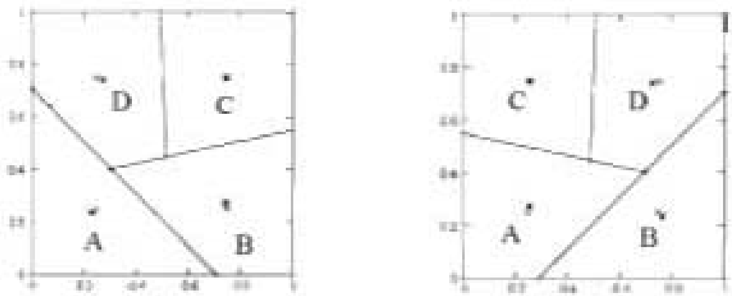


(a) Material ordering (B, C, A) (b) Material ordering (B, A, C).

Group Nested Dissection - GND



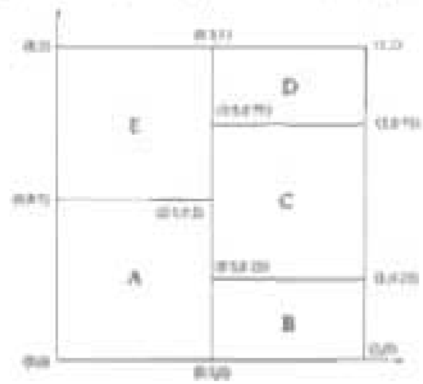
Four material - "four corner" configuration.



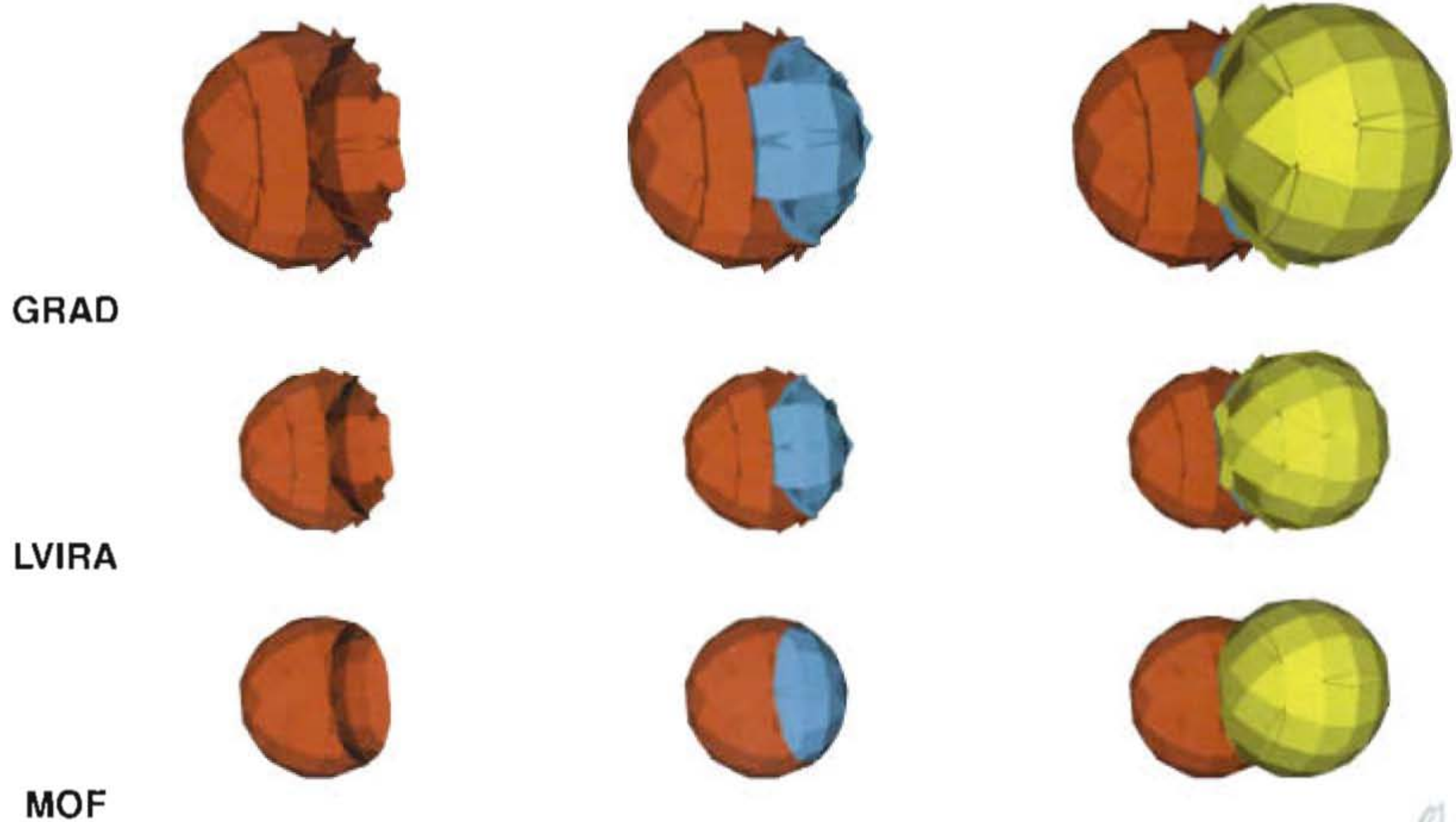
ND: left - (A, B, C, D) ordering, right - (B, A, C, D) ordering

Groups: $G_1 = (A, D)$; $G_2 = (C, B)$

Subgroups: $G_{1,1} = A$, $G_{1,2} = D$; $G_{2,1} = C$, $G_{2,2} = B$;

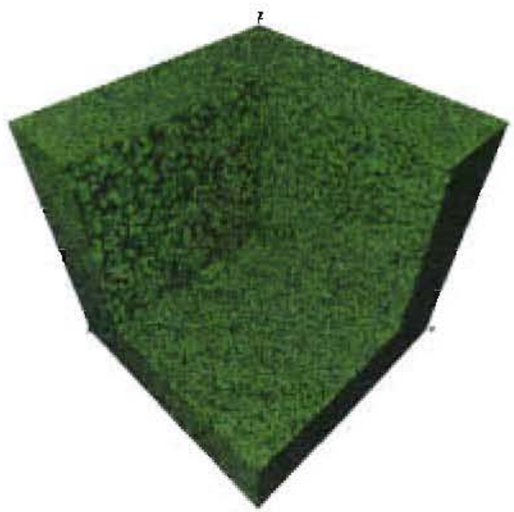


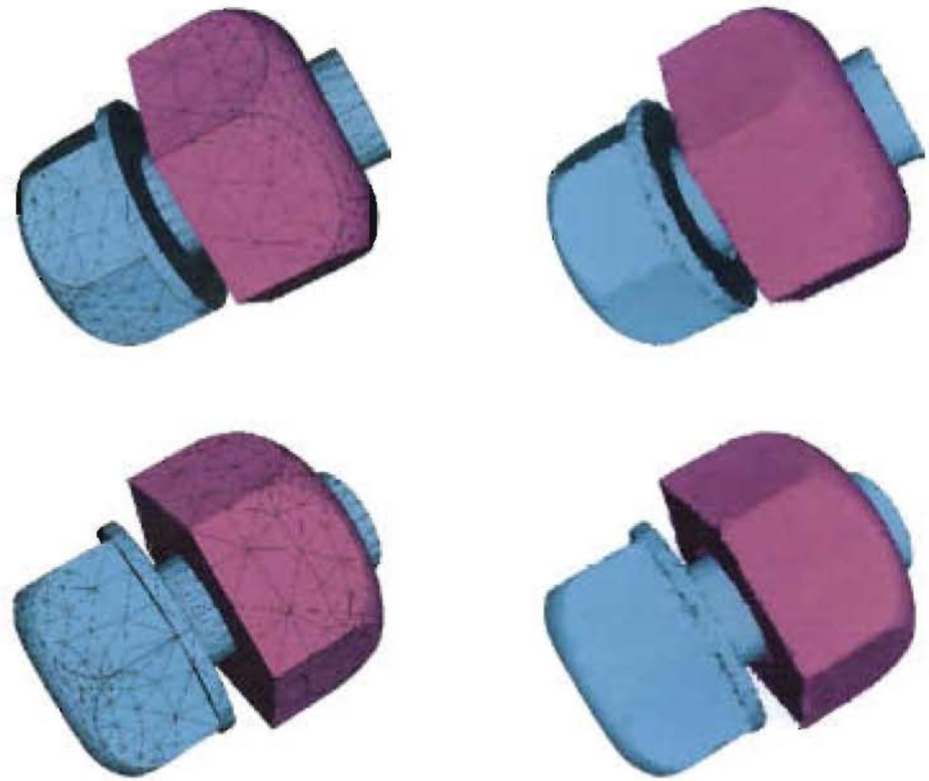
3D Multi-material Example Comparison of Methods



GRAD, LVIRA, and MoF of the two sphere example with a pre-determined local ordering given by MoF.

3D Multi-material Example Tet Mesh (Cubit Sandia)





Unstructured tetrahedral base mesh
$(n_{cells} = 555,468)$

References and Software

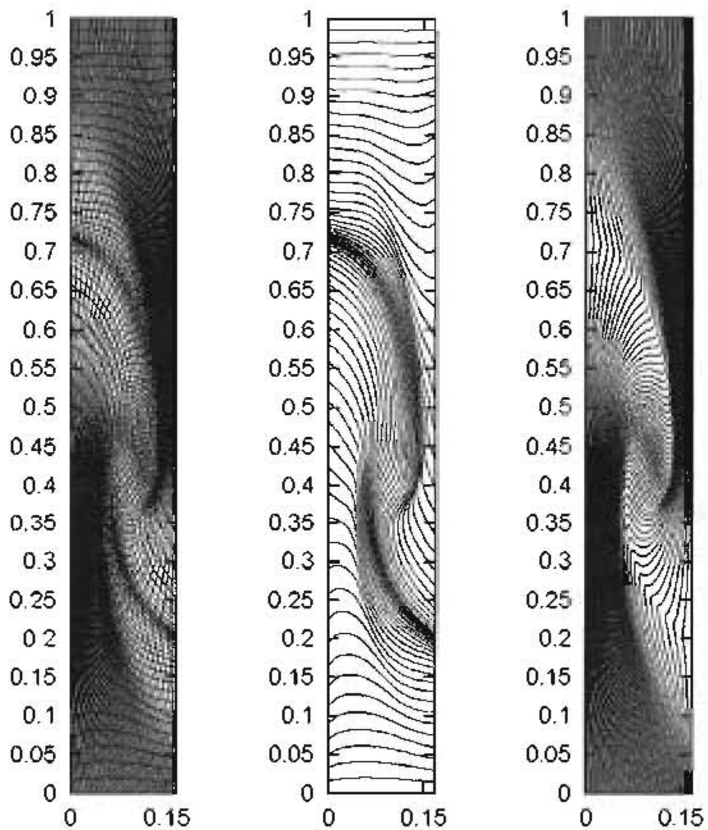
- Web page: cnls.lanl.gov/~shashkov
- V. Dyadechko and M. Shashkov, Moment-of-Fluid Interface Reconstruction, LAUR-05-7571, LANL Report.
- V. Dyadechko and M. Shashkov, Reconstruction of Multimaterial Interfaces from Moment Data, J. Comput. Phys., (2008) 227, pp.5361-5384.
- H.T. Ahn and M. Shashkov, Multimaterial interface reconstruction on generalized polyhedral meshes J. Comput. Phys., (2007) 226, pp 2096-2132.
- H.T. Ahn and M. Shashkov, Geometrical algorithms for 3D interface reconstruction, Proc. Of the 16th IMR; 2007; pp.405-422, Springer, 2008.
- M. Kucharik, R. Garimella, S. Schofield, M. Shashkov, A comparative study of interface reconstruction methods for multi-material ALE simulations, J. Comput. Phys.,(2010)229, pp.2432-2452.
- H.T. Ahn and M. Shashkov, Adaptive moment-of-fluid method J. Comput. Phys., (2009)228, pp.2792-2821.
- H.T. Ahn, M. Shashkov, M.A. Christon, The moment-of-fluid method in action, Commun. Num. Meth. Eng., (2008)25, pp 1009-1018.
- 2D code for one zone is available by request - LA-CC-07-078.
  LLNL, AWE and CEA are using this code.

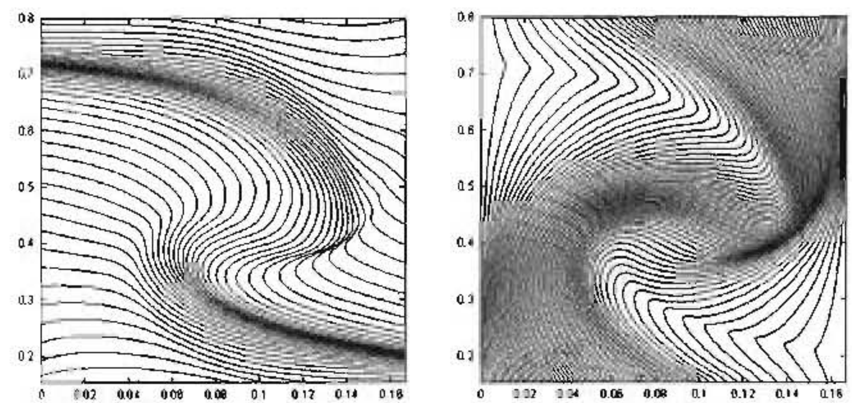
Conventional Arbitrary Langrangian-Eulerian (ALE) Methods

- Explicit Lagrangian (solving Lagrangian equations) phase - grid is moving with fluid –

  Lagrangian grid
- Rezone phase – changing the mesh (improving geometrical quality, smoothing, adaptation) – mesh movement – rezoned mesh
- Remap phase (conservative interpolation) – remapping flow parameters from Lagrangian grid to rezoned mesh

Rayleigh-Taylor Instability Limitation of Conventional ALE





Reference-Jacobian Rezone Strategy

(Knupp, Margolin, Shashkov)

Solution: ReALE - Reconnection-based ALE

Rezone phase—Mesh is allowed to change connectivity

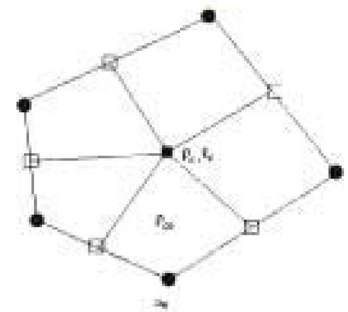
ReALE—Reconnection-based ALE

- Lagrangian phase—General polygonal meshes
- Rezone phase—Allows mesh reconnection
- Remap phase—Remapping from one polygonal mesh to another

The Devil is in the Details

R. Loubére, P.H. Maire, M. Shashkov, J.Breil, S.Galera
ReALE: A Reconnection-based Arbitrary-Lagrangian-Eulerian Method
J. Comput. Phys., 229(2010), pp.4724-4761

Lagrangian Hydrodynamics on General Polygonal Meshes



- **Staggered Discretization**
Density, internal energy, pressure - cells(zones), velocity - nodes (points); there is are also subzonal quantities

delete ?

- ALE.INC - Shashkov, Campbell, Loubere (2003)

Compatible discretization, internal energy equation, subzonal masses, edge and tensor artificial viscosity.

- **Cell-Centered Discretization**

All primary quantities are cell-centered, some algorithm for definition of nodal velocities

- CHIC - Bordeaux - Maire (2007)

Density, momentum, and total energy are defined by their mean values in the cells. The vertex velocities and the numerical fluxes through the cell interfaces are evaluated in a consistent manner due to an original Godunov-like solver located at the nodes (Geometric Conservation Law). There are four pressures on each edge, two for each node on each side of the edge. Conservation of momentum and total energy are ensured. Semi-discrete entropy inequality is provided.

Reconnection-based rezone strategy

- Initial mesh at $t=0$ is Voronoi mesh
- Voronoi mesh correspond to some generators - one generator per cell
- Location of generators control the mesh
- We use weighted – Voronoi meshes - accuracy, smoothness, adaptation
- On rezone stage we define new (rezoned) positions of generators which gives us new rezoned mesh-Voronoi mesh corresponding to new positions of generators.
- Rezone strategy is to how move generators
- Connectivity of the mesh corresponds to Voronoi mesh
- At each Lagrangian step we start with "almost" Voronoi mesh- "small" edges are removed

Voronoi Tessellation - Definition

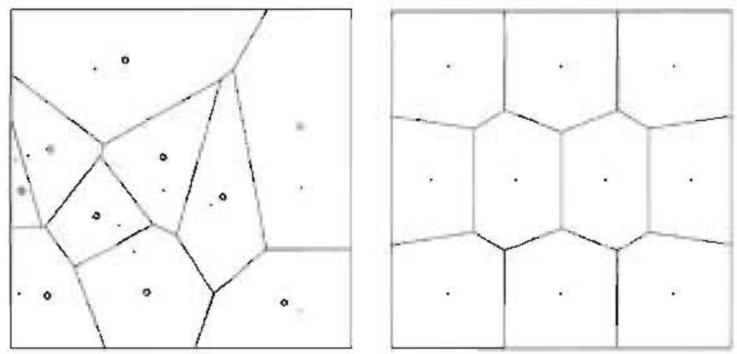
Set of generators: $g_i = (x_i, y_i)$

Voronoi cell: $V_i = \{r = (x, y) : |r - g_i| < |r - g_j|\,,\ \text{for all } j \neq i\}$

Mass centroid of the cell ($\rho(r) > 0$ - given function)

$$c_i^\rho = \int_{V_i} r\,\rho(r)\,dx\,dy / \int_{V_i} \rho(r)\,dx\,dy,$$

If $g_i = c_i^\rho$ - weighted-centroidal Voronoi tessellation

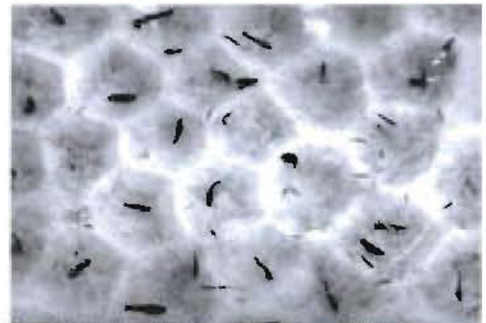


Left - generators, Voronoi cells, centroids; Right - centroidal Voronoi Tessellation ($\rho = 1$)

Centroidal Voronoi Tessellation - Lloyd's Algorithm

- Given $\rho(r) > 0$ and positive number n
- Set positions for n generators: g_i^0
- Construct Voronoi cells V_i^0 corresponding to g_i^0
- Define new positions of generators to be weighted-centroids of V_i^0: $g_i^1 = c^\rho(V_i^0)$

Voronoi Tessellation - Nature

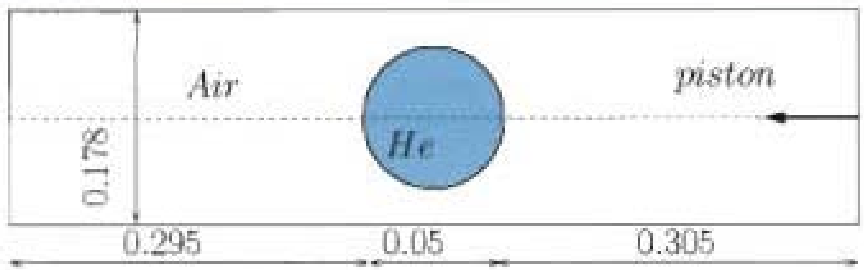


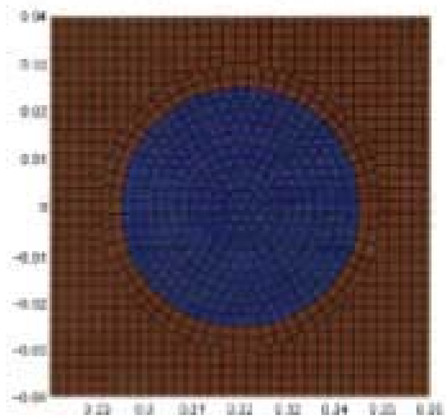
Left – from T. Ringler : Voronoi Tessellation for Ocean Modeling Methods Modes and Conservation;
Right – from G.W. Barlow, Hexagonal Territories, Animal Behavior, v.22, 1974
(The territories of the male Tilapia)

Somewhere in the Argentine Republic

Fruit - surface mesh - Maui

Initial Mesh
Shock-bubble Interaction





Generators at a similar distance perpendicular to material interface. Inside the bubble – uniform with respect to arc-length.

Reconnection-based Rezone Strategy

Requirements - Close to Lagrangian, Smooth Mesh, Adaptation capability

- **At the beginning of Lagrangian step mesh is Voronoi mesh, V_i^n corresponding to generators g_i^n**
- **At the end of Lagrangian step vertices of the cells are moved accordingly to Lagrangian method - Lagrangian cell at time t^{n+1} is $\tilde{V}_i^{n+1}$ - not a Voronoi mesh**
- **Lagrangian Phase - There is no equation for movement of the generators**

Algorithm for Movement of Generators

- Compute weighted-centroid $(c^\rho)_i^{n+1}$ of $\tilde{V}_i^{n+1}$ as follows
  $(c^\psi)_i^{n+1} = \int_{\tilde{V}_i^{n+1}} r\, \psi_i^{n+1}(r)\, dx\, dy / \int_{\tilde{V}_i^{n+1}} \psi_i^{n+1}(r)\, dx\, dy$
  $\psi_i^{n+1}(r)$ - piece-wise linear reconstruction based on mean values of some monitor function at t^{n+1}.
- "Lagrangian" Movement of Generators

$$g_i^{n+1,Lag} = g_i + \Delta t\, \bar{u}_i\,, \quad \bar{u}_i = \frac{1}{|\mathcal{P}(c_i^n)|} \sum_{p \in \mathcal{P}(c_i^n)} u_p$$

- Final position of generators

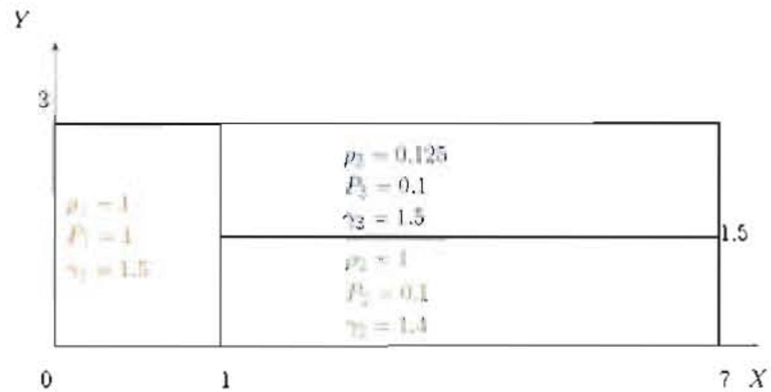
$$g_i^{n+1} = g_i^{n+1,Lag} + \omega_i \left[(c_i^\rho)^{n+1} - g_i^{n+1,Lag} \right] \quad \omega_i \in [0, 1]$$

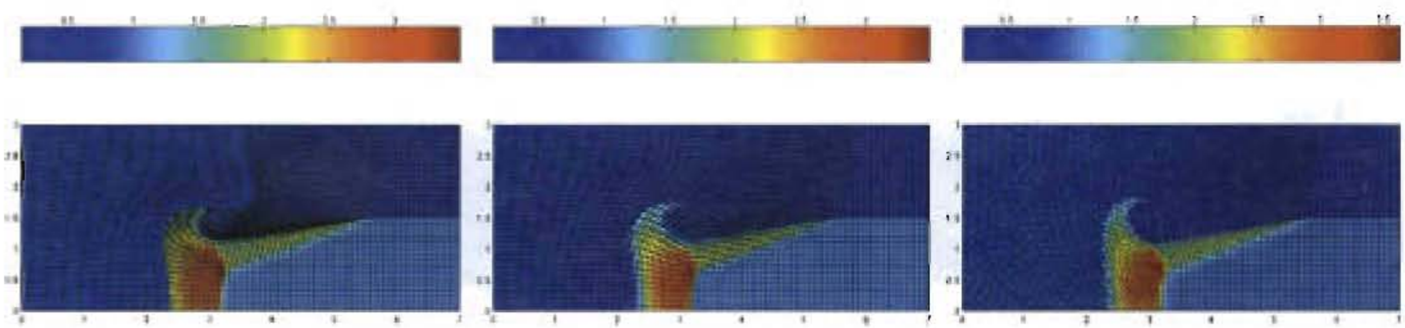
  - Computation of the ω_i
    The principle of material frame indifference: uniform translation or rotation $\omega_i = 0$
    Analysis of deformation gradient tensor F between two consecutive time steps.

Tests and Comparison of Methods

- Test Problems
  - Vortex formation
  - Interaction of shock with bubble
  - RT Instability
- Methods
  - Lagrangian
  - Standard ALE
    - Rezone – one iteration of Winslow (condition number)
    - Remap – swept region
- Eulerian = Lagrange + Remap
- ReALE

Vortex Formation

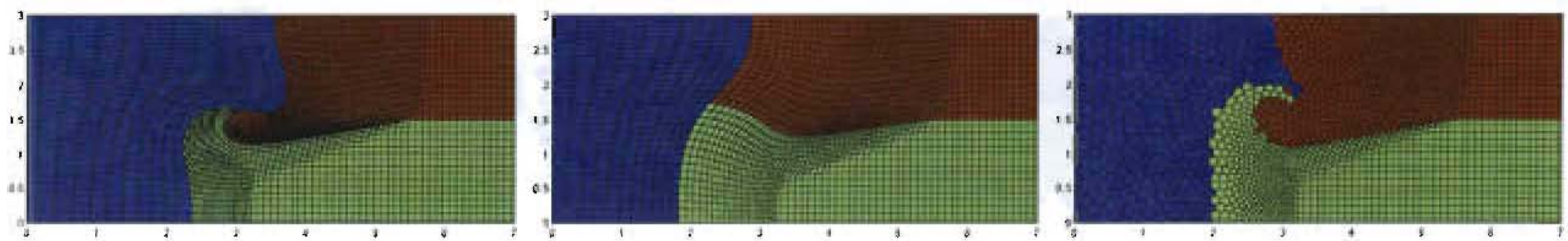




Time 2.7 - just before Lagrangian calculation stops because of mesh tangling - mesh and density.

Left - Lagrangian, Center - Standard ALE, Right - ReALE

Vortex Formation

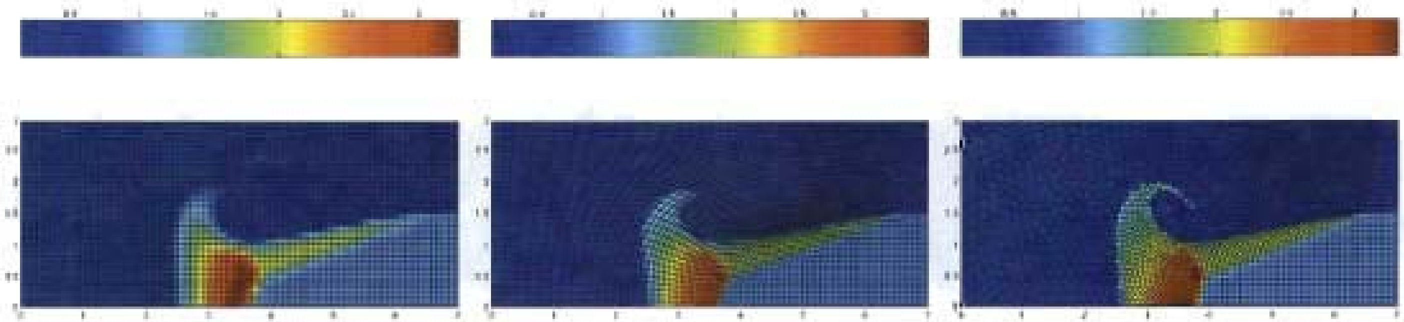


Time 2.72 - when Lagrangian calculation stops because of mesh tangling - coloring by initial region.

Left - Lagrangian, Center - Standard ALE, Right - ReALE

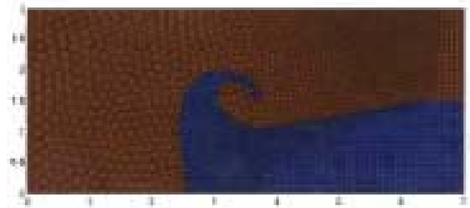
Shows how Lagrangian is movement of the mesh

Vortex Formation



Density

Left - Eulerian, Middle - Standard ALE, Right - ReALE

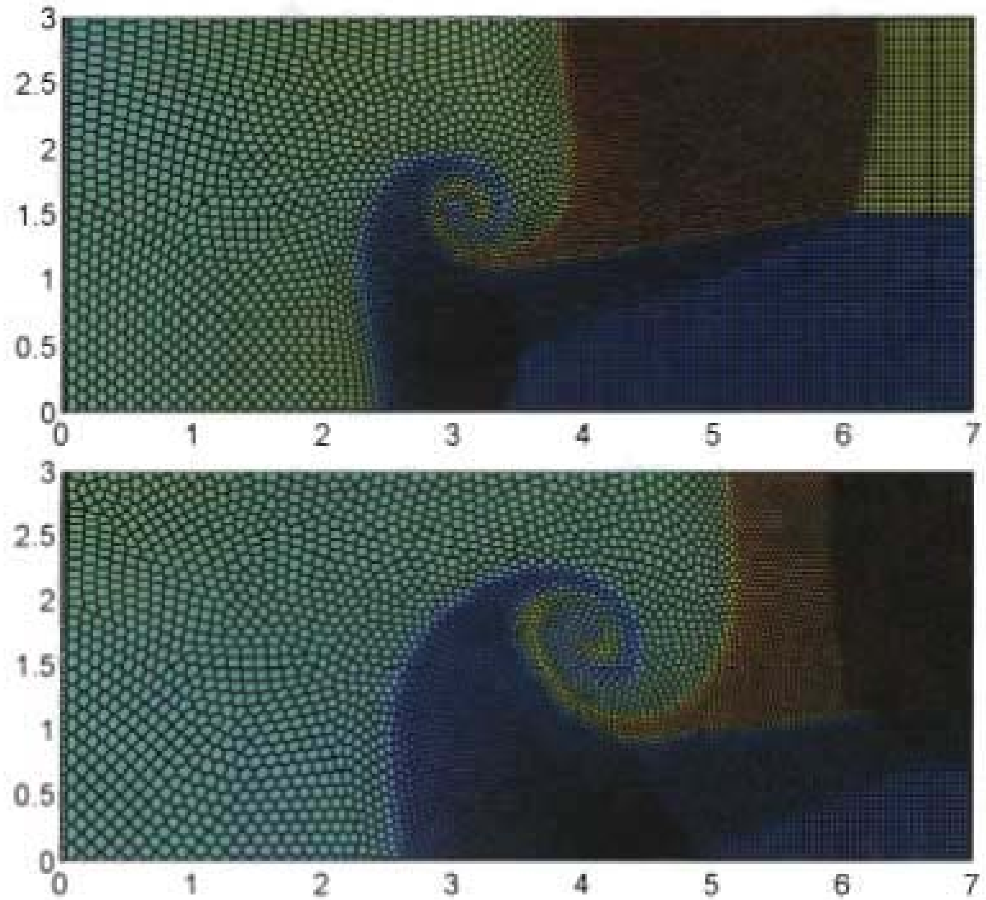


ReALE - Interface

Final time moment - 3.3

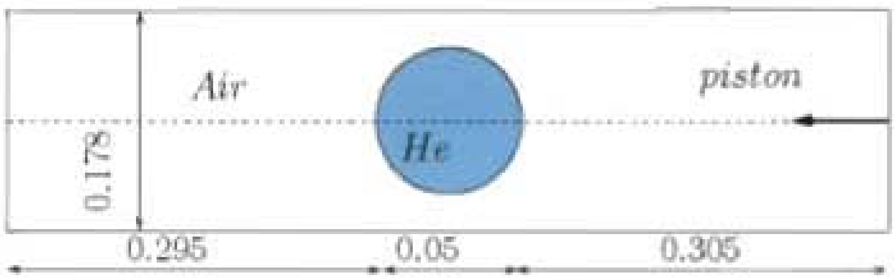
Vortex Formation

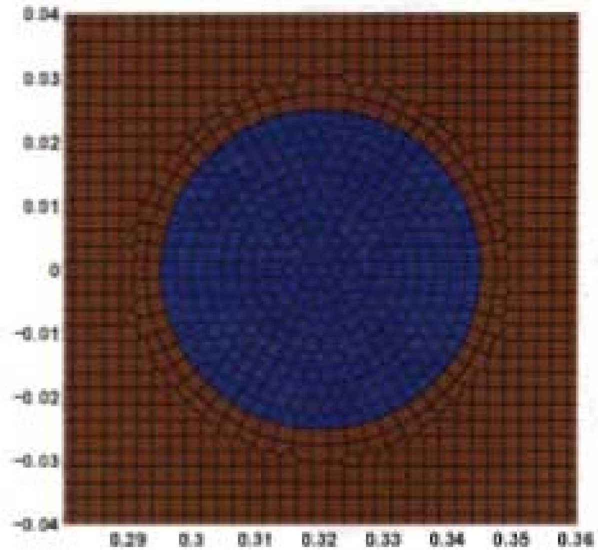
High Resolution Results - Wave Structure



Shock-bubble (cylindrical) Interaction
Statement of the problem and initial mesh

Air - $(\rho, P, \gamma) = (1, 10^5, 1.4)$
Helium - $(\rho, P, \gamma) = (0.182, 10^5, 1.648)$

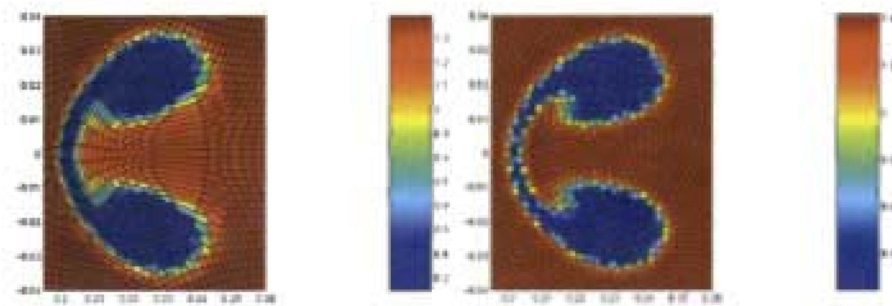




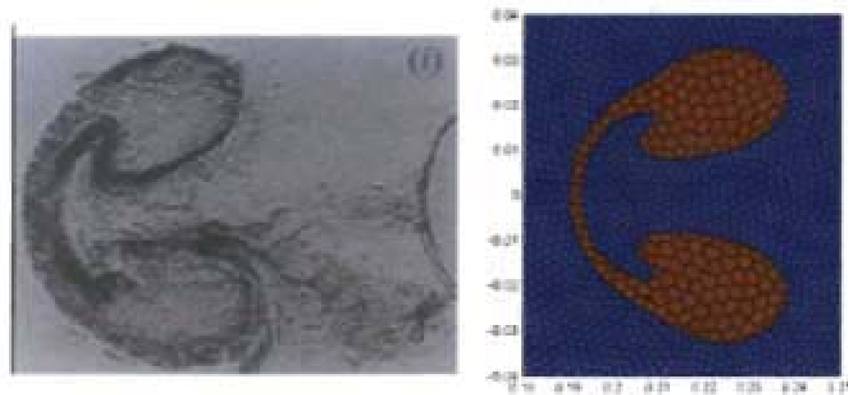
- J.F. Haas and B. Sturtevant, Interaction of Weak Shock Waves with Cylindrical and Spherical Gas Inhomogeneities, J. Fluid Mech. 181 (1987) 41-76.
- J. Quirk, S. Karni, On the Dynamics of a Shock-bubble Interaction, J. Fluid Mech. 318 (1996) 129-163.

Shock-bubble (cylindrical) Interaction

Comparison with conventional ALE and Experiment

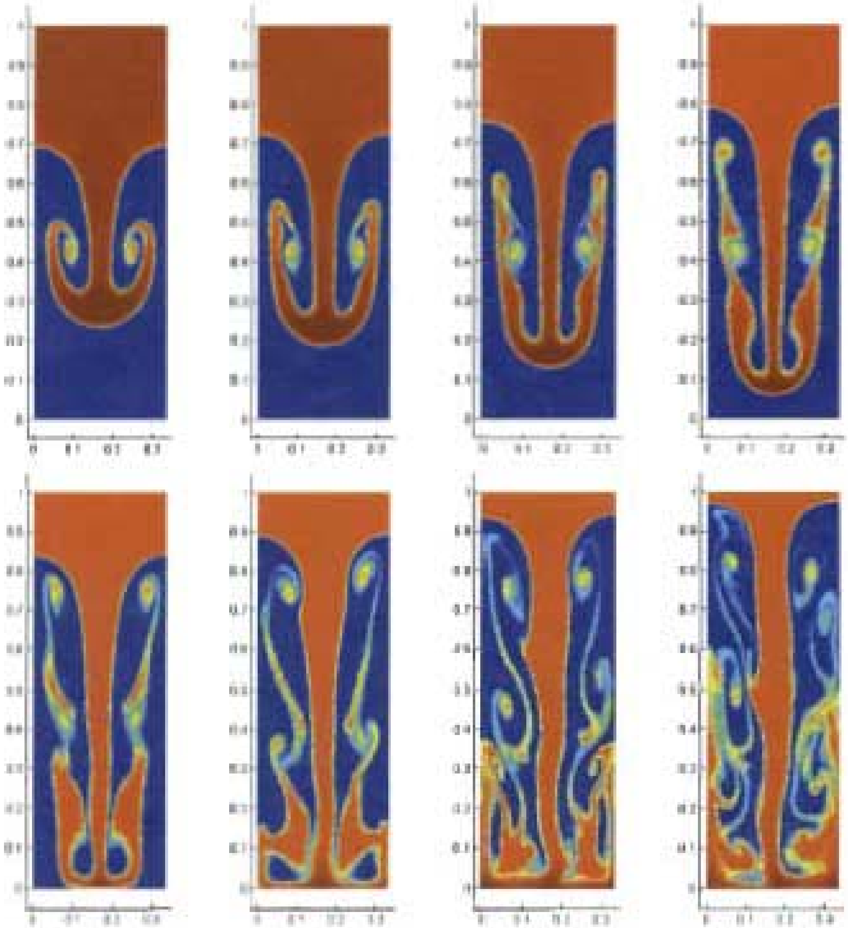


Left - Standard ALE - Density; Right - ReALE - Density



Left - Experiment from J. Quirk, S. Karni; Right - ReALE - Materials

Rayleigh-Taylor Instability
Late Stages
ReALE does not require user intervention



Reconnection-based ALE
Conclusion and Future Work

- Summary
  - New Reconnection-based ALE – ReALE Method
  - Robustness
  - Demonstrated performance on Test Problems
  - On Test Examples performs better than Standard ALE
- Future Work
  - Explore different options for "density" in weighted-centroidal Voronoi – error indicator – adaptation
  - Combination with explicit node movement
  - Adding and deleting generators
  - Combination with Lagrangian and standard ALE methods in subregions
  - More advanced closure models for mixed cells – sub-scale dynamics
  - Material strength
  - More Test Problems – quantitative comparison
  - Efficiency

Comparison with Peers

LANL is leader in method development for high-speed multi-material compressible hydrodynamics

- Our peers: US NNSA Labs –LLNL and SNL; The Predictive Science Academic Alliance Program (PSAAP) centers at the Universities; AWE (UK), CEA (France) and Russian Labs.
- We have very good knowledge of what numerical methods are used in these organizations because of participation in US meetings, with AWE participation like NECDC and JOWOG as well as international conferences like MULTIMAT.
- We are absolutely sure that we are leaders in method development for high-speed multi-material compressible hydrodynamics
- All Labs are using methods developed at LANL
  - Discretizations
  - Artificial viscosity
  - Interface reconstruction methods
  - Mesh improvement techniques
  - Remap algorithms

Status of Capability

We have developed solid mathematical foundation for high-speed mutlimaterial compressible computational hydrodynamics. It allows robust and predictive modeling of complex 3D multimaterial flows.

- Examples of Current Research:
  - Development of sub-scale modeling for mixed cells, which includes material strength and takes into account material configuration inside the mixed cell (ASCR Office of Science Project on Mimetic Methods)
  - Modeling of voids in mixed cells (ASC)
  - Developing reconnection-based methods, where connectivity of the mesh can change at rezone stage (ASC, ASCR)
  - Development of cell-centered discretizations (LDRD-DR) as opposed to staggered discretizations, which are used in almost all current codes

Livescu

Direct Numerical Simulations of Fluid Turbulence

Daniel Livescu / CCS-2

Applied Mathematics and Computational Physics
Capability Review June 8-10, 2010

Direct Numerical Simulations of fluid turbulence

- **Using high-resolution, controlled studies, DNS can provide a wealth of information, which complements the experiments and guides turbulence model development. The talk highlights recent results using large scale turbulence simulations, including** *turbulence control, new physics, turbulence model improvements*, **as well as** *next generation numerical algorithms for advanced architectures.*
- ***Funding:*** LDRD, Science Campaigns, ASC, DOE Office of Science
- **Present generation of DOE supercomputers has enabled accurate calculations of several flows of interest which can be used as "*numerical experiments*" to:**
  - complement and help design physical experiments,
  - develop and validate turbulence models,
  - discover new physics,
  - verify the large physics codes
- ***DNS of fluid turbulence*** supports several of the Laboratory's Grand Challenges (e.g. weapons physics evaluation needs, multiscale modeling, etc.) and programs (Campaigns 1 and 4, ASC) with accurate hydrodynamics simulations on advanced architectures, but also future missions and capabilities associated with the national security mission of the Laboratory.
- ***DNS efforts at LANL: CCS-2 Fluid Dynamics Team***, other efforts (e.g. Susan Kurien, T-5).
- ***Competitors:*** other DOE Labs, top tier universities (Stanford, Caltech, Princeton, etc.)

Large–scale accurate turbulence simulations are a powerful tool for: designing turbulence control techniques, develop and validate models, discover new physics, verify large physics codes.

- **Turbulence design using DNS and complementary physical experiments:**
  - LDRD 2009058DR, "Turbulence by Design," **PI:** Malcolm Andrews (CCS-2), **co-PIs:** Daniel Livescu (CCS-2), Kathy Prestridge (P-25), Ray Ristorcelli and Fernando Grinstein (XCP-4).
- **Turbulence model development and validation using DNS data; verification of RAGE:**
  - LANL-LLNL collaboration.
- **New important physics discovered using large-scale accurate turbulence simulations:**
  - Example: Two-fluid mixing is asymmetrical for different density fluids.
- **Next generation Direct Numerical Simulations of fluid turbulence:**
  - First implementation of a large fluid dynamics code on the Cell architecture (Roadrunner) with excellent performance.

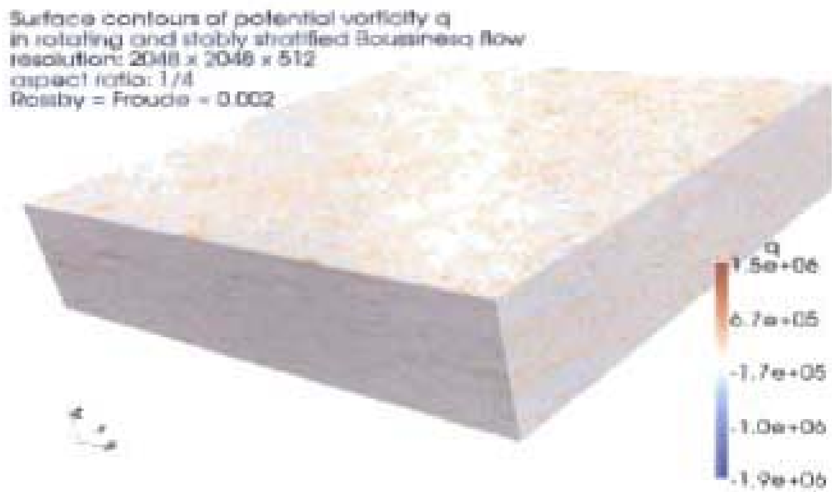
CCS-2 Fluid Dynamics team and collaborators

- <u>Rayleigh-Taylor Instability (Cartesian and convergent geometries):</u> Tie Wei, Mark Petersen, John Grove, Malcolm Andrews (CCS-2), Susan Kurien (T-5), Huidan Yu (Johns Hopkins), Arindam Banerjee (U Missouri), <u>Wavelet-based adaptive mesh:</u> Scott Reckinger, Oleg Vasilyev (U Colorado)
- <u>Shock-turbulence interaction:</u> Mark Petersen, Sumner Dean (CCS-2), Aaron Haley (U Missouri)
- <u>Supernovae, X-Ray Bursts:</u> Sanjay Reddy (T-4), Stan Woosley (UC Santa Cruz), Alex Heger (U Minnesota)
- <u>Turbulent Mixing:</u> Ray Ristorcelli, Fernando Grinstein, Len Margolin (XCP-4)
- <u>Turbulence analysis:</u> Ray Ristorcelli (XCP-4), Rob Gore, John Schwarzkopf (XTD-6), Krista Stalsberg-Zarling (XTD-2), Will Cabot, Andy Cook , Ye Zhou (LLNL), Robert Rubinstein (NASA Langley)
- <u>Advanced architectures:</u> Jamaludin Mohd-Yusof, Tim Kelley, Marcus Daniels (CCS-7)
- <u>Visualization:</u> <u>Advanced architectures:</u> Pat McCormick (CCS-7), Steve Martin (Ohio State U) ; <u>Paraview:</u> Jim Ahrens, John Patchet (CCS-1).

- <u>Computational resources:</u> Allocations on ORNL(Jaguar), LLNL (Purple and Dawn), and LANL (Roadrunner) and through Institutional Computing and ASC.

Other Direct Numerical Simulations of fluid turbulence efforts at the Lab

- **Very large simulations of stratified rotating turbulence, on ORNL Jaguar using an INCITE proposal, to study changes in the turbulence properties due to stratification and rotation. Results useful for parameterization of small-scale physics in ocean models (PI: Susan Kurien T-5).**



DNS requirements

- **Fully resolve all the relevant time and length scales.**

- **No numerical stabilizing algorithms, artificial dissipation, or subgrid models** (e.g. codes intended for coarse mesh calculations intentionally add numerical errors in the form of limiters, artificial dissipation, etc., to stabilize the calculations which are inherently unstable on coarse meshes).

- **Highly accurate numerical methods (spectral methods, high order central or compact finite differences) to minimize numerical errors** (low order schemes require orders of magnitude more points for accurate solutions).

- **Goal: "exact" solutions to the governing equations.**

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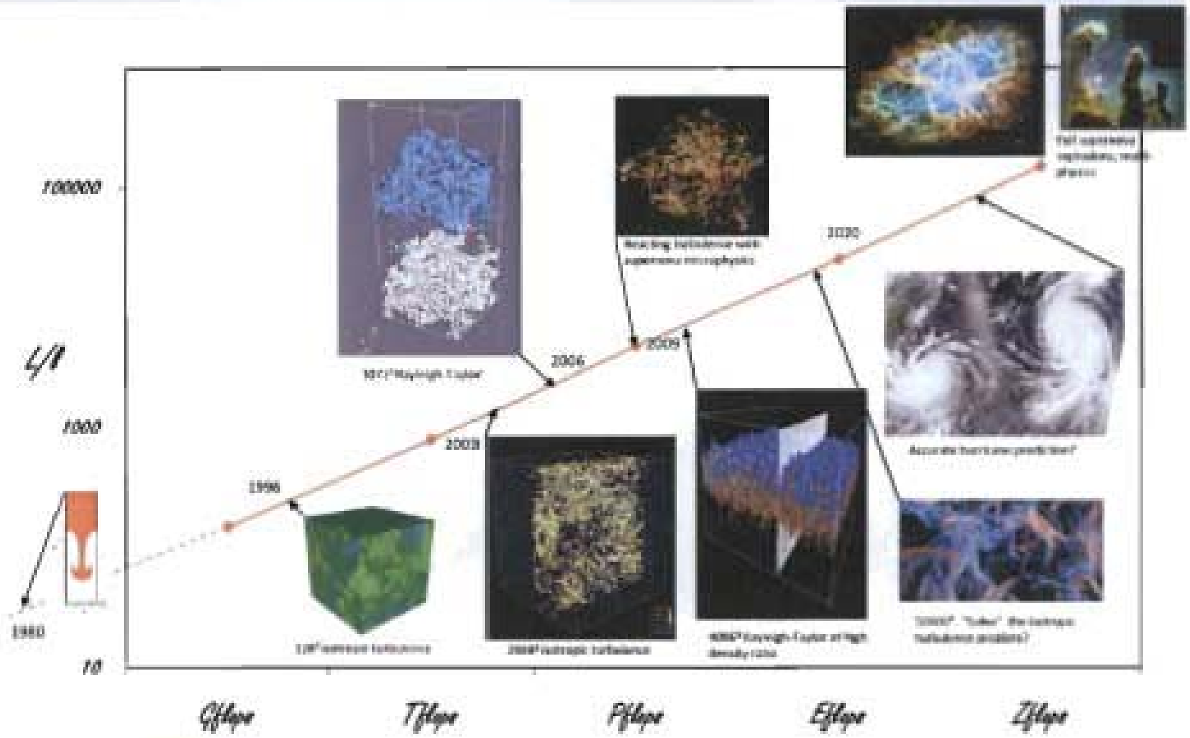
Evolution of accurate turbulence prediction: range of scales vs. computer speed.



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CFDNS code description

Developed within the CCS-2 group over the last 7 years.

Code Overview

- Structured grid finite differences and/or FFTs code suitable for direct numerical simulation (DNS) turbulence simulations.
- Compressible and incompressible Navier-Stokes equations in 3 dimensions.
- Allows multiple species, real material properties, exothermic reactions.
- A subset of the code has been ported to the Cell architecture with excellent performance
- Code scales well to ≈150,000 compute cores (BG/P Dawn, LLNL).

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Turbulence design using DNS and complementary physical experiments

- **LDRD 2009058DR, "Turbulence by Design"**

<u>PI:</u> Malcolm Andrews (CCS-2)
<u>co-PIs:</u> Daniel Livescu (CCS-2) – DNS
Kathy Prestridge (P-25) – RM experiments
Ray Ristorcelli (XCP-4) – Turbulence modeling
Fernando Grinstein (XCP-4) – ILES
<u>Collaborating University:</u> Texas A&M – RT experiments
<u>Post-doc's:</u> B. Rollin, S. Gowardan, S. Balasubramanian
<u>GRA's:</u> A. J. Wachtor, N. Hjelm, S. Reckinger

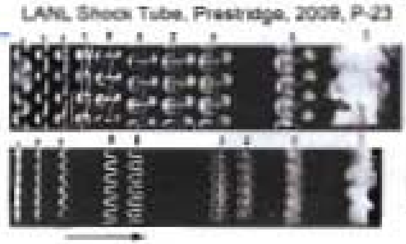
Applied Mathematics and Computational Physics
Capability Review, June 8-10, 2010

LDRD-Directed Research "Turbulence By Design"

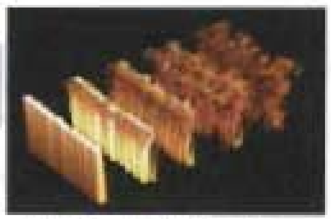
Carefully chosen initial perturbations can be used to control turbulent transport and mixing effectiveness

- Liquid disintegration.
- Degradation of ICF capsules. Geophysical flows.
- Formation of oil trapping salt domes.
- Super-Nova Remnants (SN1987A).
- Boundary layer separation (catastrophic loss of lift).
- The Eagle Nebula

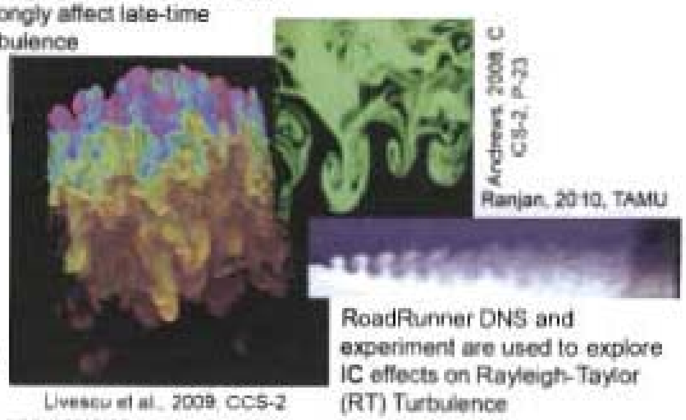
LANL Shock Tube, Prestridge, 2009, P-23



Changing initial conditions can strongly affect late-time turbulence



ILES Shock Tube, Grinstein, 2010, XCP-4



Ranjan, 2010, TAMU

Livescu et al., 2009, CCS-2

RoadRunner DNS and experiment are used to explore IC effects on Rayleigh-Taylor (RT) Turbulence

Two-Mode "Leaning" RT Experiments Using the New Computer Controlled Flapper (TAMU + LANL)

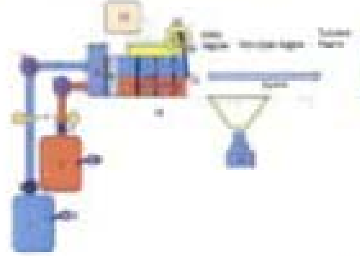
$$A(x) = A_1 \sin\left(\frac{2\pi x}{\lambda_1}\right) + A_2 \sin\left(\frac{2\pi x}{\lambda_2} + \delta\right)$$

$A_1 = 4mm$	$A_2 = 2mm$
$\lambda_1 = 4cm$	$\lambda_2 = 2cm$
$\rho_1 = 997.7kg/m^3$	$\rho_2 = 996.57kg/m^3$

Phase shift : δ=0, π/2

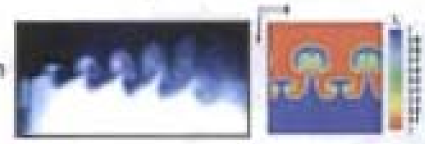
The flapper motion imposes an initial vertical velocity given by:

$$v = \frac{dA}{dt} = \frac{dx}{dt}\frac{dA}{dx} = U_0\left(A_1 k_1 \cos(k_1 x) + A_2 k_2 \cos(k_2 x + \delta)\right)$$

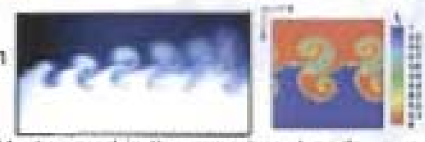


Computer controlled flapper system – up to 16 modes

Binary initial perturbation with δ ~ 0

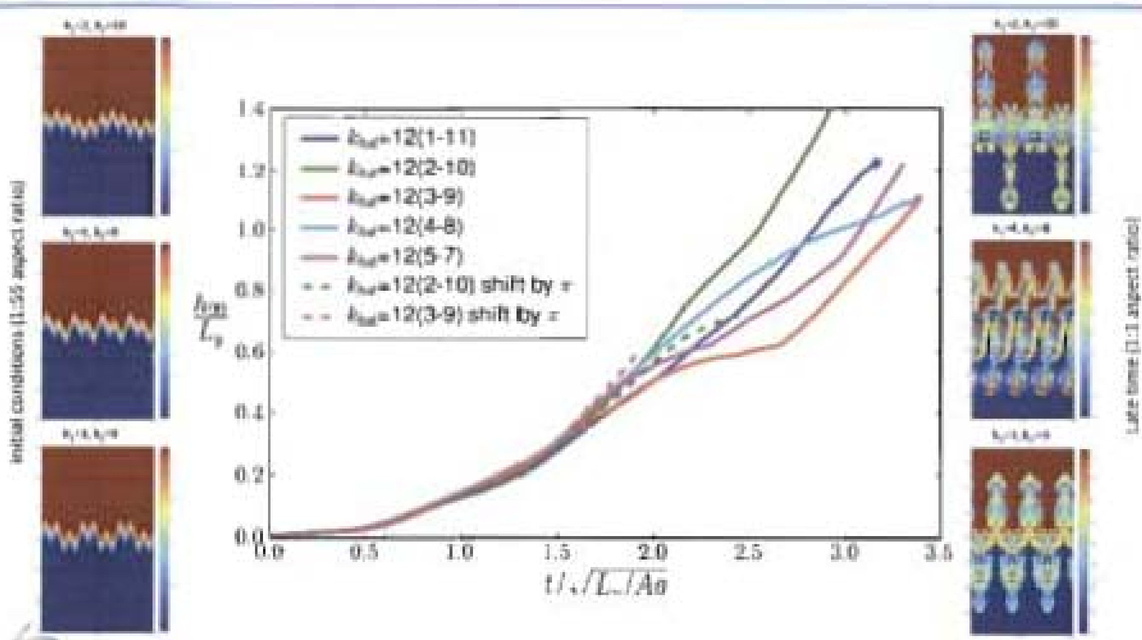


Binary initial perturbation with δ ~ π/2

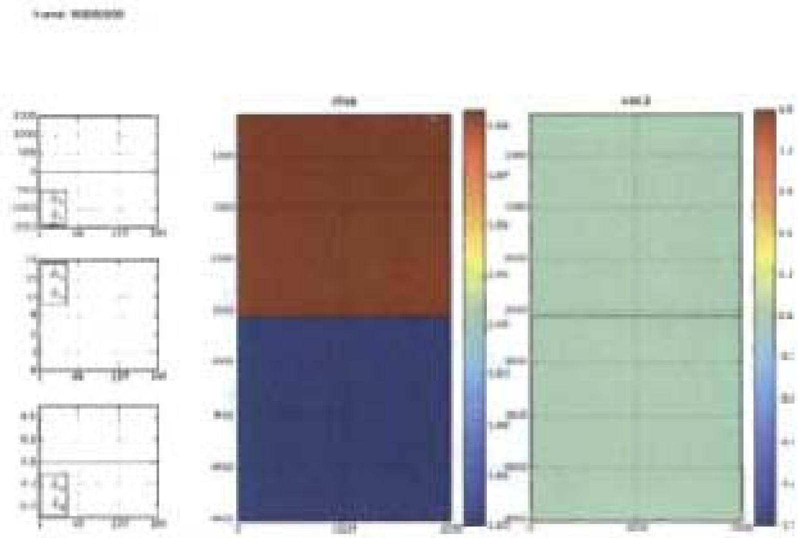


The "leaning" of the growing perturbation with an angle of π/4 observed in the experiment and the simulation due to mode dynamics, and not mode coupling.

DNS of two-mode Rayleigh-Taylor instability: role of mode number combination

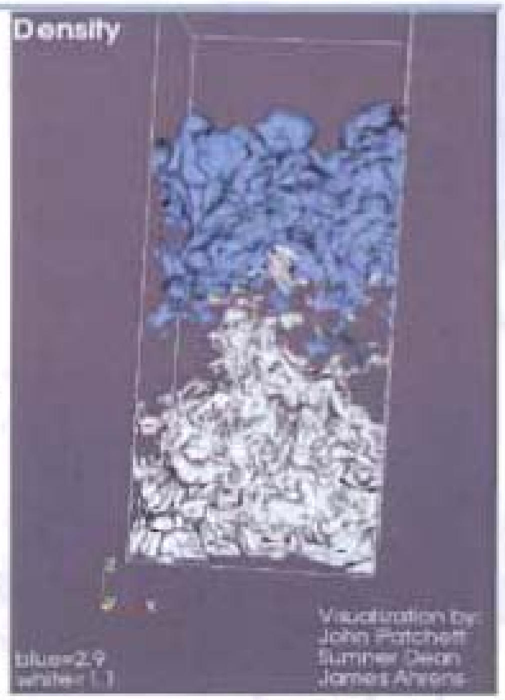


Two-mode density and vorticity evolutions: k = 2; 10.



Turbulence model development and validation using DNS data; verification of large physics codes (RAGE)

- Analysis of a 3072^3 DNS of Rayleigh-Taylor turbulence, the largest simulation to date of inhomogeneous turbulence.
- LANL – LLNL collaboration
- References
  - Cabot and Cook, *Nature Phys.*, 2006.
  - Livescu, Ristorcelli, Gore, Dean, Cabot and Cook, *J. Turbul.*, 2009.
  - Livescu, Ristorcelli, Petersen, and Gore, *Phys. Scr.*, 2010
- Related to
  - Campaign 4



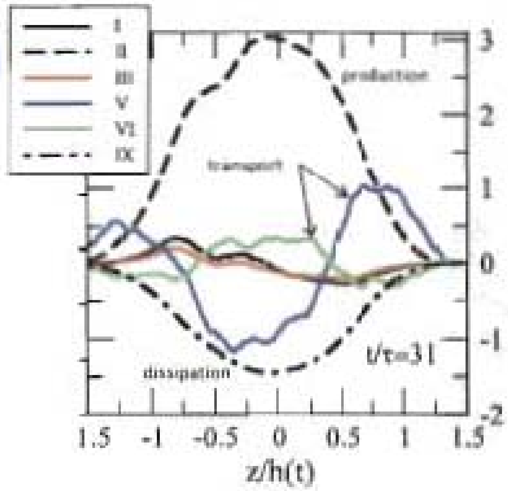
Turbulent kinetic energy transport equation budget

- **Dominant terms, RT layer interior:**

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{k} = \underbrace{+a_3 P_{,3}}_{II\ (\approx 3)}^{\text{production}} \underbrace{-\langle \tau_{ij} u_{i,j}\rangle}_{IX\ (\approx -1.5)}^{\text{dissipation}} \underbrace{-\frac{1}{2}R_{ii3,3}}_{V\ (\approx -1)}^{\text{transport}} \underbrace{-\langle u_3 p\rangle_{,3}}_{VI\ (\approx 0.5)}^{\text{transport}} + \cdots$$

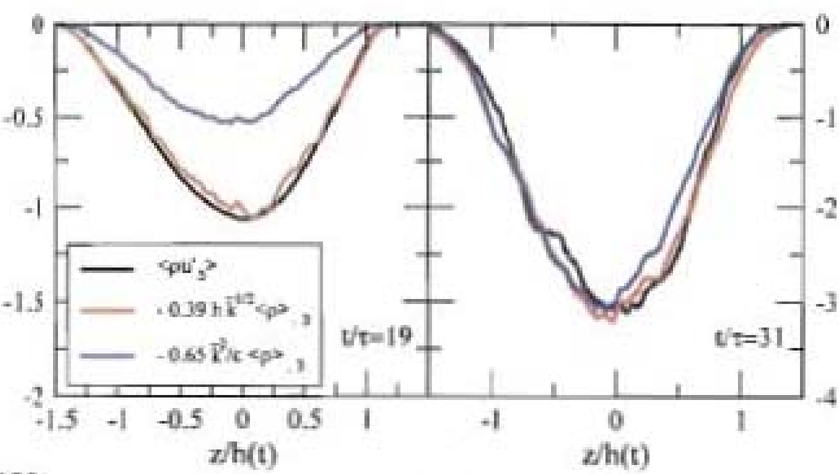
- **Dominant term, RT layer edges:**

$$\frac{\partial}{\partial t}\bar{\rho}\tilde{k} = \underbrace{-\frac{1}{2}R_{ii3,3}}_{V\ (\approx 1)}^{\text{transport}} + \cdots$$



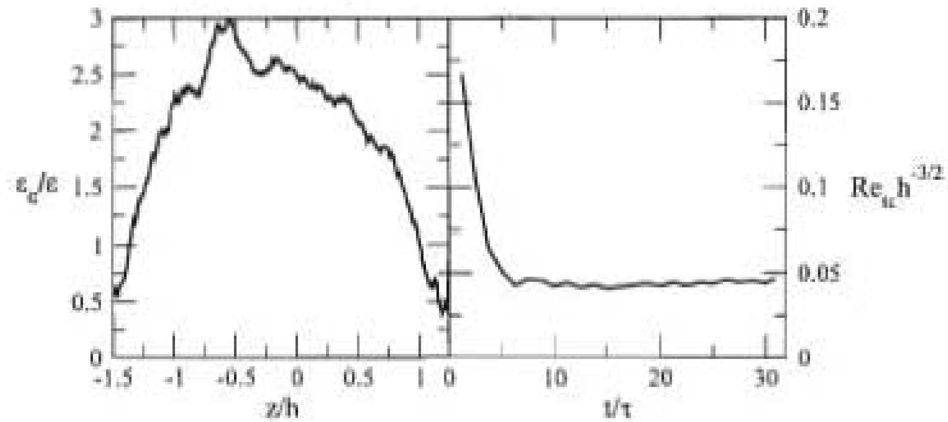
Gradient diffusion hypothesis

- Very popular in applications for simplicity; the turbulent diffusion is modeled using the available turbulence scales.
- E.g. the mass flux in RT turbulence modeled as: $\langle \rho u_3' \rangle = -\nu_t \langle \rho \rangle_{,3}$



Gradient diffusion hypothesis: DNS view

- The energy cascade rate, $\varepsilon_c = \tilde{k}^{3/2}/L$, and the dissipation rate, $\varepsilon = \langle \tau_{ij} u'_{i,j} \rangle$, are not the same (non-equilibrium flow) even after the layer width becomes self-similar.
- The usual turbulence Reynolds number, which is proportional to the eddy diffusivity, never reaches self-similarity; however a Reynolds number defined based on the cascade rate, $Re_{tc} = \tilde{k}^2/(\nu \varepsilon_c)$, has the large scale scaling.



Applied Mathematics and Computational Physics
Capability Review, June 8-10, 2010

Gradient diffusion hypothesis: conclusion

- Due to the lack of self-similarity of the turbulent Reynolds number, the usual closures for the moment equations using the turbulence length-scale, *l*, and gradient diffusion hypothesis for the turbulence transport or similarity arguments for the dissipation fail in Rayleigh-Taylor turbulence (at least until asymptotic self-similarity is reached).

- Solution: **In a single point modeling strategy for R-T turbulence, need two length-scale equations.**

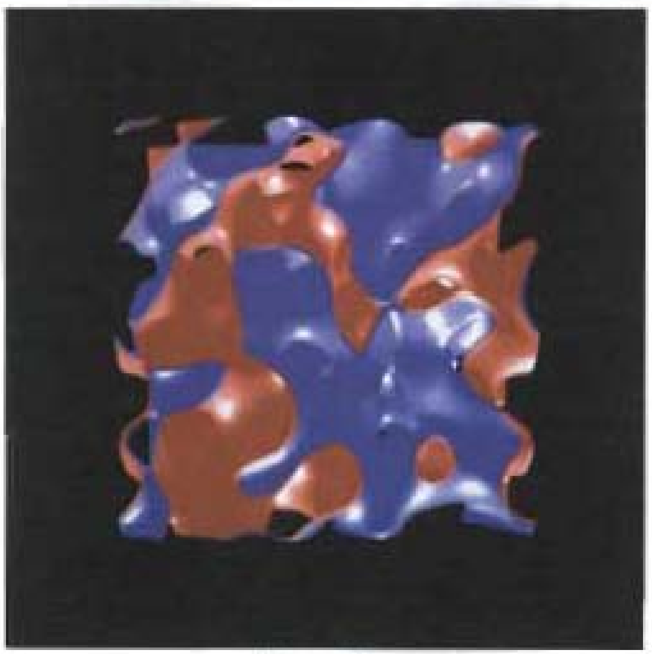
New important physics discovered using large-scale accurate turbulence simulations

- **Mixing asymmetry in two-fluid turbulent mixing**

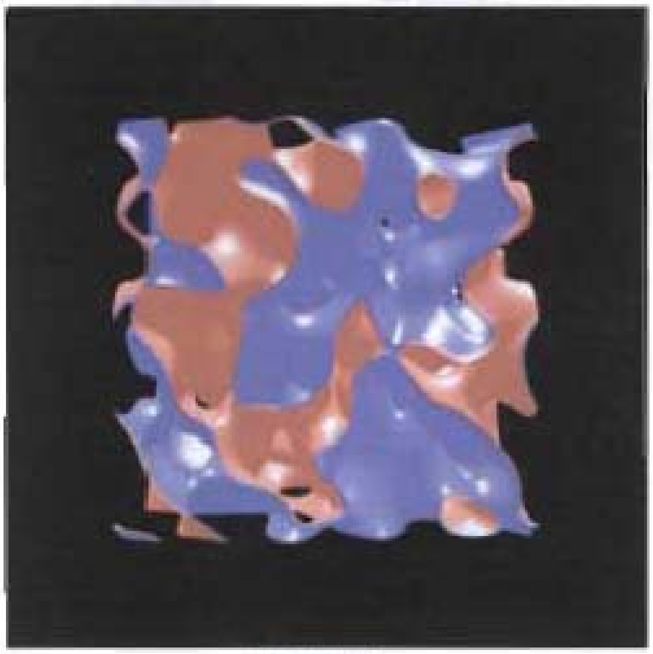
- References
  - Livescu and Ristorcelli, *J. Fluid Mech.* 2008.
  - Livescu, Ristorcelli, Gore, Dean, Cabot and Cook, *J. Turbul.* 2009.
  - Livescu and Ristorcelli, *Adv. In Turbul. XII*, 2010.
  - Livescu, Ristorcelli, Petersen, and Gore, *Phys. Scr.*, 2010.

- Related to
  - Campaign 4, ASC, LDRD

Mixing in homogeneous Rayleigh-Taylor turbulence

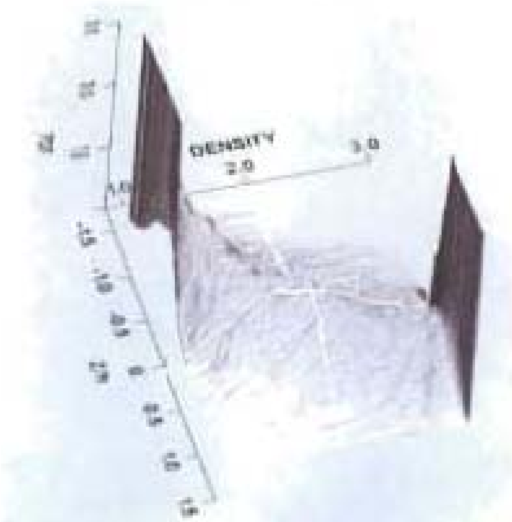


Mixing asymmetry in homogeneous Rayleigh-Taylor turbulence: evolution of pure fluids



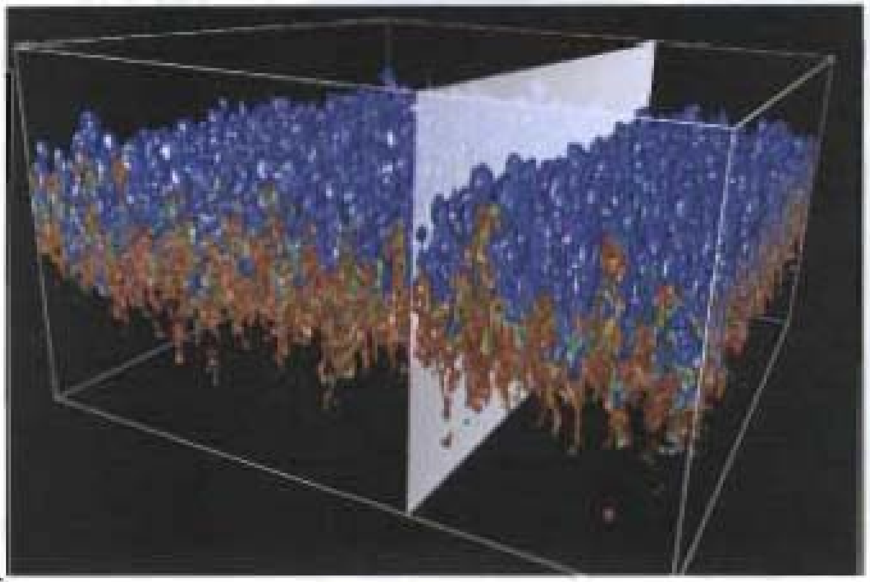
Mixing asymmetry in Rayleigh-Taylor turbulence

- **Density PDF across the Rayleigh-Taylor layer:**



Rayleigh-Taylor Instability at high density ratio

- Visualization of density from the largest turbulence simulation to date (at the time of completion): 4096^2x 4608 Rayleigh-Taylor instability at 7 to 1 density ratio



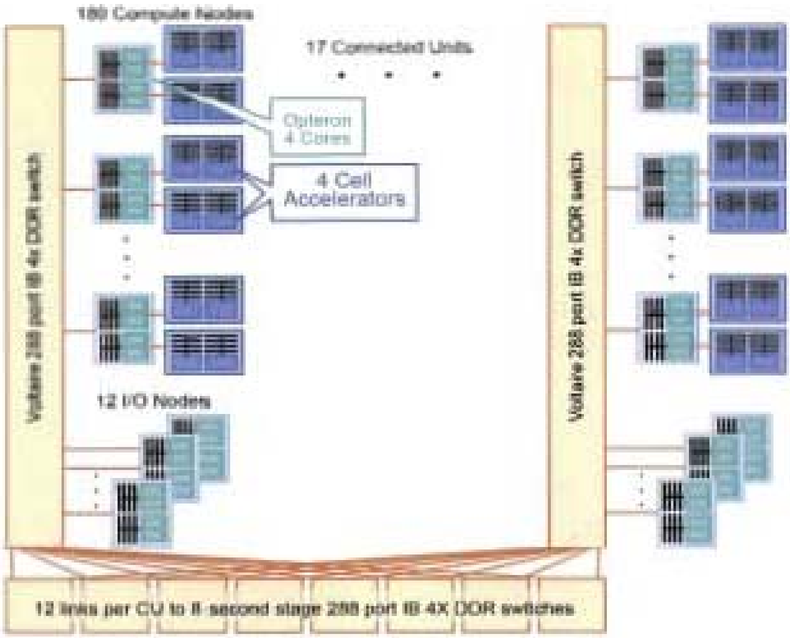
Next generation Direct Numerical Simulations of fluid turbulence

- **First implementation of a large fluid dynamics code on the Cell architecture (Roadrunner) with excellent performance**

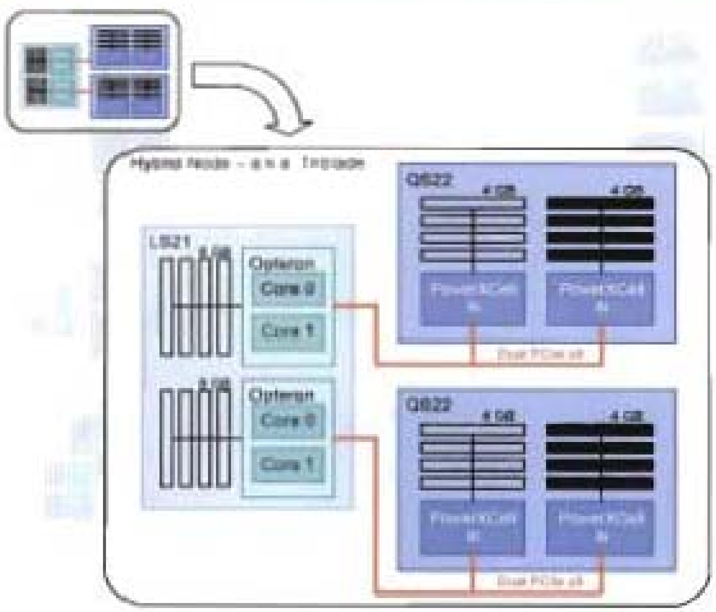
- References
  - Livescu, Mohd-Yusof and Kelley, *SIAM PP10*, 2010.
  - Mohd-Yusof, Livescu and Kelley, *ParCFD09*, 2009.
  - Mohd-Yusof, Livescu, Kelley, Petersen and Desai, *SIAM CSE09*, 2009.
  - Mohd-Yusof, Livescu, Kelley, Petersen and Desai, *Supercomputing*, 2008.

- Related to
  - ASC, LDRD

Roadrunner is a cluster of cluster with accelerators

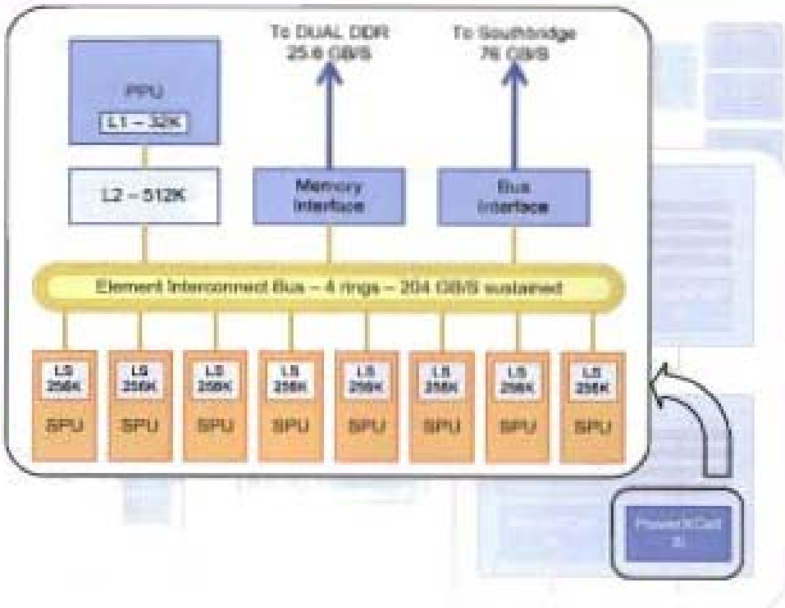


Roadrunner hybrid compute node



IBM PowerXcell 8i Processor

- 3.2 GHz
- 8 SPUs
- 4 way SIMD (SP)
- 102.4 GFlop/S DP
- 25.6 GB/S BW to memory
- C/C++, Fortran supported on PPU and SPU
- A variety of Cell and hybrid programming models are enabled by DaCS, ALF and libSPE



Roadrunner implementation challenges

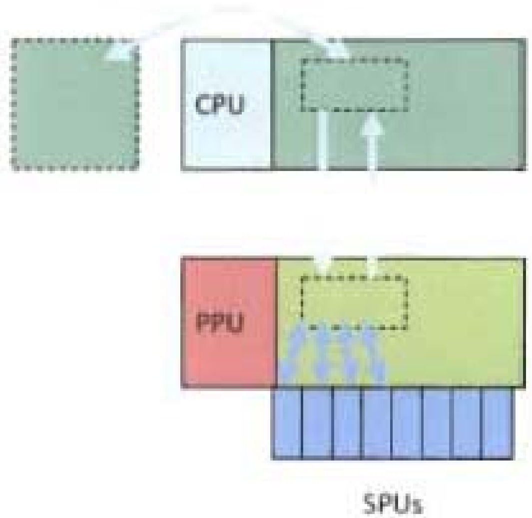
- **3-way node heterogeneity**
  - *Need to program each separately*
  - *Need to synchronize all 3 levels*
- **PPU is not particularly fast**
- **SPUs**
  - *Have 256KB local store for code and data*
  - *Explicit memory management*
  - *Asynchronous independent DMAs*
  - *Poor branching performance*

Roadrunner implementation of CFDNS (CFDNS-rr)

- **Data layout**
  - *C vs. Fortran, but also optimization for DMA operations*
- **Spatial derivative calculation**
  - *6th order compact finite differences:* $a_1 f'_{i-1} + a_2 f' + a f'_{i+1} = b_1 f_{i-2} + b_2 f_{i-1} + b_3 f_i + b_4 f_{i+1} + b_5 f_{i+2}$
  - *requires tridiagonal solver*
  - *parallel version requires communication, either*
    - data transpose (usual solver)
    - ghost cells, intermediate values (distributed solve)
- **Update calculation**
  - *point-wise, requires no communication*
  - *easily vectorized for SPU*
- **Table look-up and inversion**
  - binary search
  - interpolation or inversion

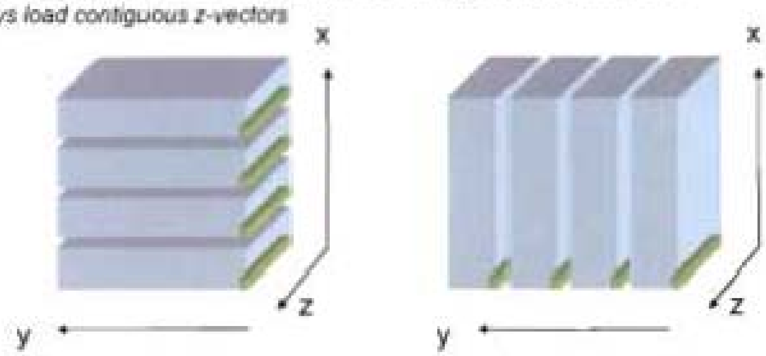
Division of work for the Roadrunner implementation

- **Opteron**
  - *Load correct Cell executable*
    - based on MPI rank
  - *Handle MPI calls*
  - *Handle disk access*
  - *DaCS put/get to Cell memory*
- **PPU**
  - *Share Cell memory with Opteron*
  - *Pass messages between SPUs and CPU*
- **SPUs**
  - *DMA in/out of Cell memory*
  - *Crunch*



Data access in Cell memory

- Each SPU accesses memory independently
  - *only 4 shown for clarity*
- Different offsets, strides, starting addresses for y and z derivatives
  - *always load contiguous z-vectors*



- Data in cell memory never re-ordered
- Either access pattern is fine for update equation

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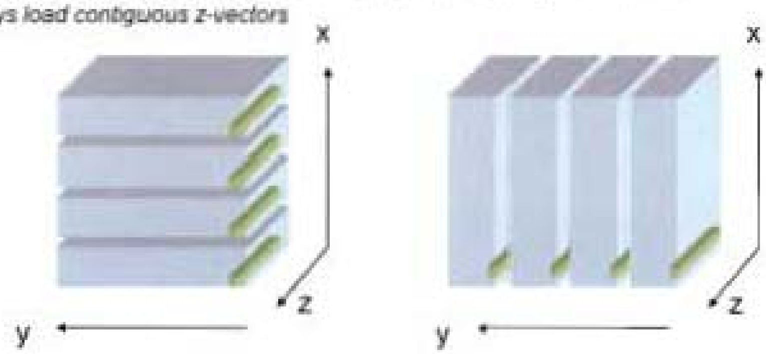

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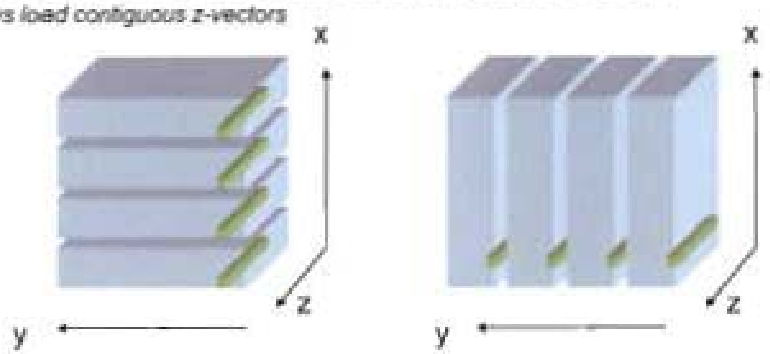


- Data in cell memory never re-ordered
- Either access pattern is fine for update equation

Other changes for the Roadrunner implementation

- **Consolidation of derivative calls**
  - *6 grouped derivative calls per RHS evaluation*
  - *Reduce number of sync points between processors*
- **Overlapping of compute and communication**
  - *First x-pass while y-derivative ghost cells are formed, etc.*
    - Uses different processor and memory spaces
- **Control of local store usage**
  - *20 local store arrays (size NZ) used*
  - *Extra LS arrays needed for*
    - RK45 RHS arrays
    - Ghost cells

Table look-up and inversion

- **Look-up**
  - *Straightforward: calculate offsets, load local data and interpolate*
- **Inversion**
  - *Binary search*
    - Loading full lines of data saturates the Cell's Element Interconnect Bus
    - Use a two stage approach which improves the memory access pattern and vectorizes the local computations, albeit at increased local number of operations
      - load data corresponding to the first 7 points the binary search could visit and perform the search
      - repeat, until the data reaches manageable size
      - complete the search in the reduced region
      - find the inverted values, using the corner data of the corresponding table cell
    - Pre-compute terms in the interpolation formulas which are re-used
    - Compute separate polynomials concurrently, based on data locality

Summary: excellent performance of the Roadrunner implementation

- **For this problem**
  - **Serial tests show speedup of > 30x, double precision**
  - ***Parallel speedup is ~20x at scale***
  - Significant restructuring of the code was needed
    - latency vs data volume tradeoff
    - more complicated scheduling and synchronization
- **In general**
  - *For large structured data sets, the Cell acceleration potential is very good*
    - changes compute/communication ratio significantly
    - excellent memory performance is largely responsible
    - overall speedup will depend on communication overhead for parallel codes

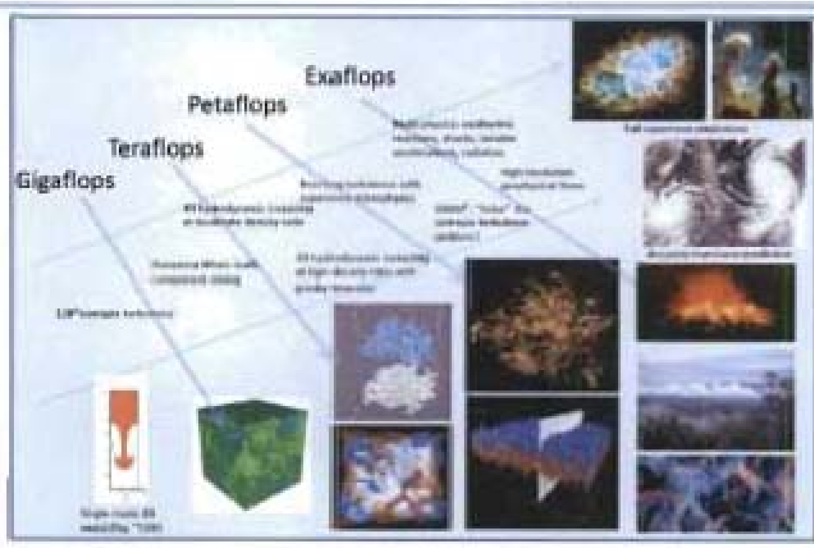
Large–scale accurate turbulence simulations are a powerful tool for: designing turbulence control techniques, develop and validate models, discover new physics, verify large physics codes.

- **Turbulence design using DNS and complementary physical experiments:**
  - LDRD 2009058DR, "Turbulence by Design," **PI:** Malcolm Andrews (CCS-2), **co-PIs:** Daniel Livescu (CCS-2), Kathy Prestridge (P-25), Ray Ristorcelli and Fernando Grinstein (XCP-4).
- **Turbulence model development and validation using DNS data; verification of RAGE:**
  - LANL-LLNL collaboration.
- **New important physics discovered using large-scale accurate turbulence simulations:**
  - Example: Two-fluid mixing is asymmetrical for different density fluids.
- **Next generation Direct Numerical Simulations of fluid turbulence:**
  - First implementation of a large fluid dynamics code on the Cell architecture (Roadrunner) with excellent performance.

Direct Numerical Simulations of fluid turbulence: Roadmap to Exascale

After decades of research, turbulence and turbulent mixing still remain unsolved problems in physics; this due in part to the very large range of spatio-temporal, dynamically relevant scales.

Large scale computing is expected to bring a number of breakthroughs in science. One of the areas most likely to benefit is fluid turbulence, where very large scale computations can bring the insight and indicate the appropriate modeling approaches for the routine coarse mesh calculations needed in applications.



The road to Exascale will enable accurate turbulence simulations which will dramatically increase the predictability of complex practical flow and, thus, will directly impact the US competiveness, economy, and policy landscape.

Knoll

Overview of PDE Theme

Dana Knoll / T-3

Computational Physics and Applied Mathematics Capability Review June 8-10, 2010

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Definition of "PDE Theme"

- For Purposes of Organization, NOT:
  - CFD, Monte-Carlo, Integrated Codes, Discrete Event Simulation
- PDE Theme IS:
  - Applied Math
  - Deterministic Transport
  - Solvers
  - Computational Plasma Physics
  - Computational Mechanics
  - Meshing

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Brief Overview of PDE Theme

- Funded by NNSA, Office of Science, LDRD, and other sources as well.
- Supports the mission by developing fundamental capabilities.
- These fundamental capabilities are typically intended to improve the performance and/or predictability of large scale integrated codes (IC).
- Members of LANL PDE community can be found primarily in CCS, T, XCP, EES, ISR.

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Outline of Talk

- Overview of PDE Self-Assessment, Including:
  - Level of effort estimate
  - Overview of sub-topical areas
  - Quick pointers to other talks and posters
- Thoughts on two important LANL directions
  - Thought Topic 1: Multiphysics methods and time integration errors: the relationship to aspects of Uncertainty Quantification.
  - Thought Topic 2: Scale-bridging algorithms on exascale platforms: a test bed for computational co-design.

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Level of Effort in PDE Theme: ESTIMATES for a few groups

- T-5, *Applied Mathematics and Plasma Physics*, 38 FTE
- CCS-2, *Computational Physics and Methods*, 15 FTE
- T-3, *Fluid Dynamics and Solid Mechanics*, 6 FTE
- XCP-4, *Methods and Algorithms*, 6 FTE

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Applied Math Overview

- An historic core strength of LANL
- Large concentration of activity in T and CCS
- Traditional funding sources have been NNSA, Office of Science, and LDRD
- Topics include numerical analysis, computational mathematics, complex far-from-equilibrium systems, multiscale analysis, stochastic PDE analysis ...

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Two High Profile Activities in Applied Math

- Center for Nonlinear Studies (CNLS)
  - Focus on nonlinear, complex, far-from-equilibrium systems
  - A gateway between LANL and the academic community
- DoE/ASCR Applied Math Research Program
  - Fundamental pursuits with successful connection to programs
  - Activities in computational math, stochastic PDEs, theory of nonlinear evolution equations, networks, ...

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Two Presentations Supporting Applied Math

- Talk by B. Wingate: *On the Slow Dynamics in the Arctic Ocean*
  - Fundamental multiscale analysis applied to climate
  - Physical insights have been gained. Could impact solvers for multi-scale problems (synergistic connection)
- Poster by K. Lipnikov: *Mimetic Finite Difference Methods: Theory and Application*
  - Development of advanced discretization methods
  - Impact on core LANL simulation mission, ASC

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Result from K. Lipnikov's Poster

- The MFD method uses one degree of freedom on a moderately curved face to approximate velocity u^h.

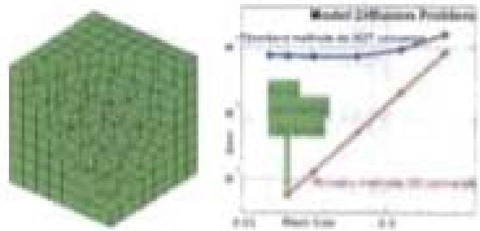

Figure 2: *A part of a logically cubic mesh with randomly perturbed interior nodes. The graphs show optimal convergence rates for the MFD method (red), and lack of convergence for the lowest-order mixed FE (blue) method.*

An Overview of Deterministic Transport

- Long LANL history of foundational research in simulation of Boltzmann equation for photon and neutron transport
- Primary concentration of effort in CCS-2
- Primary funding source is NNSA / ASC
- Research topics include:
  - Spatial discretization and analysis
  - Parallel solver issues
  - Eigenvalue methods
  - Issues related to multiphysics coupling

Presentation Representing Deterministic Transport

- Talk by J. Warsa: *Netwon's Method for S_N Transport Applications*
  - Impact of nonlinear solvers on linear transport
    - Spatial discretization
    - Eigenvalue problem is a nonlinear problem
  - Advanced discretization on polygon meshes
  - Synergistic connection with nonlinear solvers research
  - Synergistic connections to new directions in advanced scale-bridging algorithms

Overview of Solvers

- Research in linear and nonlinear solvers
- LANL community exists in T and CCS
- Funding sources: NNSA / ASC, Office of Science, Advanced Simulation Capability for Environmental Management (ASCEM), LDRD, ...
- Deterministic transport and implicit CFD methods have been big drivers
- Multiphysics methods and analysis of operator splitting approaches

Current Status of Solvers

- Available software includes BoxMG and LAMG
- ASC solvers project cancelled in 2007 as a result of reduced funding and reprioritization
- Evolving / Growing opportunities
  - ASCEM and Climate
  - Re-engage ASC

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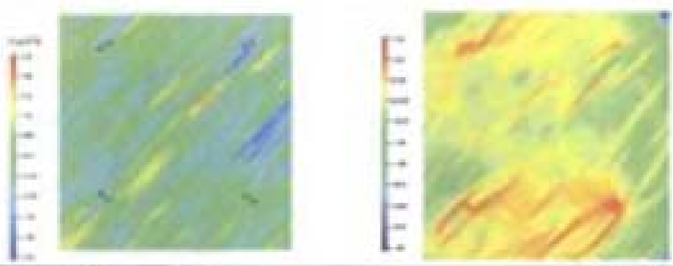
Presentation Representing Solvers

- Poster by D. Moulton: *Solvers Development for Subsurface Applications:*
  - Subsurface applications span a wide variety of complex nonlinear, multiscale, multi-process models and offer a rich set of challenges for robust and scalable solvers.



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Overview of Computational Plasma Physics

- History of mission and program support (ICF and MFE)
- LANL community exists in T , XCP and ISR
- Funding sponsors have included NNSA, Office of Science, NASA, DoD, and LDRD
- Application areas have included magnetic confinement fusion, inertial confinement fusion, high energy density physics, space plasma physics ...

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Highlights and Presentation in Computational Plasma Physics

- Rich history of foundational, high visibility, algorithm development at LANL
- Talk by B. Albright: *VPIC: Kinetic Plasma Modeling at the Petascale and Beyond*
  - Highly efficient mapping of explicit EM PIC code onto advanced supercomputers such as Roadrunner
  - First-of-a-kind physics simulations in Laser-Plasma-Interaction, Magnetic Reconnection, Fast Ion generation
  - Synergistic connection to scale-bridging direction

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Overview of Computational Mechanics

- Strong mission and program need
- Model development and algorithm development are tightly coupled here.
- LANL model and algorithms community exists in T-3, T-1, XCP-5, XCP-4, CCS-2, and MST-8.
- Limited support for methods and code development at LANL (NNSA and DoD).
- Model development has enjoyed stronger support

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Computational Mechanics: A Challenge and a Presentation

- Standard spatial discretizations and solution methods can be challenged on LANL problems.
- Poster by D. Zhang: *Advances in the Material Point Method for Nonlinear Mechanics.* (picture)
  - Multimaterial interaction theory with in Material Point Method . An advanced particle method for ALE.
  - Connection to advanced nonlinear solvers started.
  - Synergistic connection to scale-bridging direction

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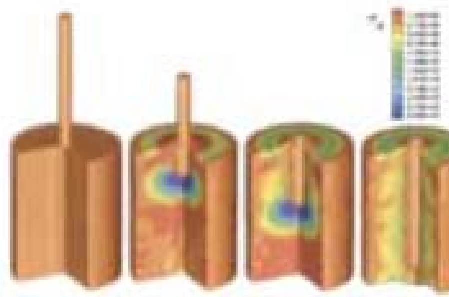
Computational Mechanics: A Results from D. Zhang's Poster

- High strain-rate, large deformation, multimaterial application is rather unique to a few NNSA labs.



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Overview of Meshing

- Strong mission and program need
- Has some support from ASC / NNSA and some support from LDRD. Support has been decreasing.
- LANL community includes T-5, XCP and EES-6.
- LANL meshing needs are fairly non-standard.
- Focuses heavily on capturing very complex physics precisely.

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Presentation on Meshing

- Poster by R. Garimella . *Overview of LANL Meshing Research.*
  - Covering ASC setup project (XCP and T), LaGriT (EES-6), ALE research (T-5), Monge-Kantorovich research (T-5)

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Thought Topic 1: Multiphysics Time Integration Errors and UQ

- Some Requirements for Predictive Simulation
  - Proper Physics Model / Equation Set
  - Accurate spatial discretization / adequate grid refinement (3-D)
  - High end computing platforms and parallel, scalable, algorithms.
  - Accurate time integration for multiphysics equation systems. We must understand this area when we are taking $10^5 - 10^7$ time steps.
- Relationship between time integration error and aspects of "UQ" ?

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Main Points / History

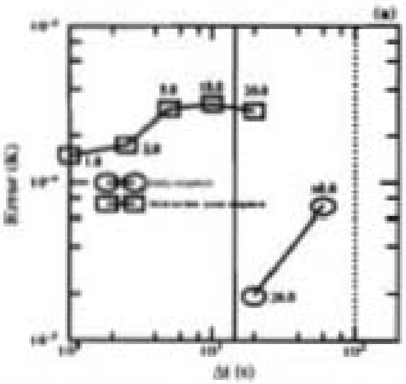
- Operator splitting and linearized time integration was driven by computers and solvers of the 60's and 70's.
- This is the algorithmic "weak link".
- May lead to significant accumulation of long time integration errors.
  - Solution can appear physical and conserve energy, but be wrong !
  - Historic goal has been numerical stability

Concern in the Era of "Predictive Simulation"

- Numerical Stability does not equate to Numerical Accuracy (as will be shown)
- Examples in thermal radiation diffusion, MHD physical instabilities, hurricane intensification, multiphysics nuclear reactor systems ...
- Who is impacted: Weapons simulation, climate change predictions, ...
- Impact on / interaction with "UQ" approaches and activities ?

Hurricane Intensification Example: Time Step Convergence Study

- 3-D compressible flow with phase-change (7 eqs). 150x150X51 grid (Reisner et, al. Mon. Wea. Rev. (2005)). Fixed grid, small time step for "base solution", simulate to fixed point in time.
- Nonlinearly converged solution has increased accuracy at same time step (efficient when equivalent accuracy is the measure!)



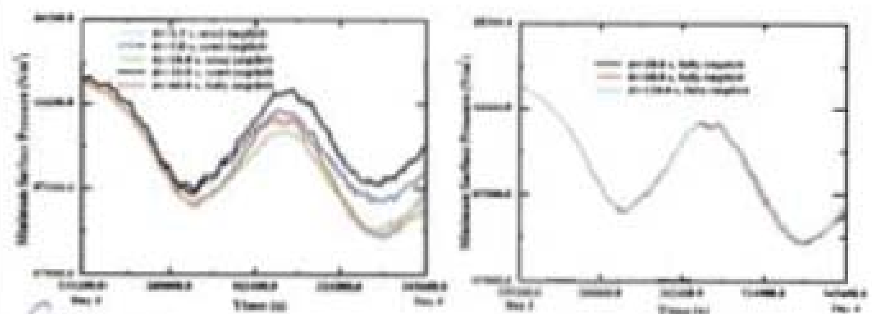
Hurricane Intensification Example: Stable solution, but with "drift"

Linearized and Split:

(Significant variation in transient solution)

Nonlinearly Converged:

(transient solution is "converged")



Poster Presentation by J. Reisner on Hurricane Simulation

- Poster by J. Reisner: *Utilization of a Multi-phase Particle Model to Develop Self-Consistent Bulk Microphysical Paramaterizations of Hurricane Models*
  - Advanced physical model with some UQ efforts
  - Advanced multiphysics time integration of LCCF
  - Historic connection to multiphysics methods
  - Synergistic connection to scale-bridging direction

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Questions Regarding Multiphysics Time Integration Error + UQ

- What do we want from multiphysics simulation + UQ ? Need to ask up front.
  - Answers to important / measurable quantities (often integral) with some defined uncertainty ?
  - Is this the same as clearly quantified long time integration error ?
- Opportunity to bring together "Optimal UQ" (next slide) and the long standing problem of accumulation of time integration error.

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Optimal Uncertainty Quantification (OUQ) for Long-time Prediction

- Premise: UQ ill-posed; (Presently that is: how do you compare different UQ results?)
- Resolution: OUQ problem formulation – A New Approach from LANL/CALTECH
  - Inputs: Objectives, expert knowledge, simulation results, experimental data, assumptions
  - Output: OUQ optimization problem
- Solution to OUQ optimization problem: Optimal Uncertainty Quantification
  - Optimal means that it is the best given the Inputs!

Tasks for Evolving Multiphysics Time Integration Error + OUQ

- Develop theory for long time integration error accumulation in a multiphysics setting.
  - We MUST respect the possibility that: 10^{-6} error per time step times 10^{6} time steps results in order one error
- Incorporate into "OUQ". Co-design including UQ.
  - Domain experts, code experts, statistics and applied math experts, optimization experts, computer science experts working together to obtain rigorous, quantified, optimal, guarantees of uncertainty for high-impact objectives.

Thought Topic 2: Scale-bridging Algorithms on Exascale Platforms

- Multi-time scale, multi-space scale phenomena ubiquitous. Scale-bridging algorithms are rare.
- Prototype fine-scale (kinetic) problem:
  - time, configuration space, and phase space as independent variables.
- Desire a scale-bridging algorithm which accelerates an accurate solution of the fine-scale equations such that coarse (engineering) time and length scale simulations are achievable.

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Scale-bridging algorithms on Exascale platforms: The Scales

- High Order (HO) problem (Fine scale).
  - Discretized version of the fine-scale equation
  - Solved by either a deterministic or Monte-Carlo approach.
- Low Order (LO) problem (Engineering scale).
  - small number of phase space moments of the HO problem.
  - Can solve on a "coarser" configuration space mesh.
- Both the LO problem and the HO problem are solved over the entire geometry

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Scale-bridging algorithms on Exascale platforms: The Algorithm

- LO problem solution provides accelerating information to the HO problem solver (collision sources, EM fields, ..)
- Closures required to solve LO problem come from the HO problem solution (Eddington tensor, stress tensor, heat flux, …)
- Multigrid-like:
  - LO problem solver relaxes the "long wave length" aspects of the solution
  - HO problem solver relaxes ONLY the "short wavelength" aspects of the solution

Broad Application and Advanced Architectures: The Big Win

- Fundamental algorithm can provide consistent scale-bridging to a number of important physical systems (we will highlight a few).
- JFNK is used to ensure tight coupling between HO and LO problems
- Algorithm appears to map to evolving heterogeneous parallel architectures.
- Test bed for computational co-design on exascale platforms

Mapping to heterogeneous parallel architectures: Related Example

- Poster by S. Habib: *The Roadrunner Universe Project*
  - Particle-in-Cell simulation of Vlasov-Poisson system
  - Poission solve (similar to LO problem) executed on *Opteron layer*
  - Particle pushing for Vlasov solve (similar to HO problem) done on *Cells*
  - Over-simplified picture, need to visit poster
- Not the proposed sale-bridging algorithm, but a successful mapping of the required components.

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Algorithm Application, The Roots: Neutron Transport

- LO problem solves for scalar flux with "closure" coming from angular flux.
- HO problem is solved for angular flux (deterministic or MC) given fission and scattering source from LO problem solution.
- Long history, working algorithms in industry, algorithm research continues.
- LANL staff have made contributions and many issues have been worked.

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Algorithm Application, New: Thermal Radiation Transport

- LO problem:
  - PDE system involving material temperature, radiation energy and radiation flux.
  - Eddington tensor closure from HO problem solution.
- HO problem:
  - Solve Boltzmann eq. for angular intensity (deterministic or MC)
  - material temperature source provided from LO problem solution.
- Avoids artificial Fleck-factor scattering term from IMC, and converges nonlinear source coupling.

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New Algorithm Application: Implicit Plasma Simulation

- Collisionless, electrostatic example:
  - HO problem: ion and electron Vlasov equations (solved on a grid or with PIC). Electric field (E) is provided by LO problem solution.
  - LO problem: first two moments of ion and electron Valsov system. Electron "momentum" equation is solved for E. Stress tensors are closed from solution of HO problem.
- Large, stable, and accurate time steps demonstrated. Research continues. Many possible applications (implicit VPIC ?).

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Conclusions and Future Directions

- Conclusions:
  - Provided definition of PDE Theme
  - Overview of PDE Self-Assessment, including:
    - Overview of sub-topical areas
    - Quick pointers to other talks and posters
  - Thoughts on two new LANL directions
- Two Possible Future Directions:
  - Multiphysics methods and time integration errors: the relationship to aspects of Uncertainty Quantification.
  - Scale-bridging algorithms on Exascale platforms: a test bed for computational co-design.

Albright

VPIC: Kinetic plasma modeling at the petascale and beyond

Brian J. Albright/XCP-6

Computational Physics and Applied Mathematics
Capability Review June 8-10, 2010

VPIC is a "best-in-class" explicit kinetic plasma modeling code

- VPIC (Vector Particle-In-Cell) is the fastest and most scalable PIC code extant – several innovations in VPIC* have become industry standard
- Support for VPIC development: DSW, ASC, Science Campaigns, LDRD, DOE (OFES), DoD, DNDO, DTRA, NASA
- Kinetic plasma physics modeling is critical to the Laboratory and guides several experiments
  - DAHRT, Trident, MaRIE, NTS experiments, NIF, Omega
- People:
  - Code Development: Brian Albright, Kevin Bowers (XCP-6); Ben Bergen (CCS-7); Lin Yin, Bill Daughton, Tom Kwan (XCP-6); Charlie Snell (XCP-2); Cornell Wright (IBM)
  - Visualization: Jeremy Margulies (XCP-2), Pat Fasel (CCS-3), Jim Ahrens (CCS-7)
  - Customers: ~20 users across the Laboratory in XCP, T, P, ISR, CCS
- Competing codes exist at universities, other labs, private companies, but VPIC is widely regarded as best in many areas

* Bowers et al. Phys. Plasmas 2008 (APS DPP Invited Talk); Bowers et al. Proc. 2008 ACM/IEEE Conf. Supercomput. (Gordon Bell Prize Finalist); Bowers et al. J. Phys. Conf. Series 2009 (SciDAC Invited Talk)

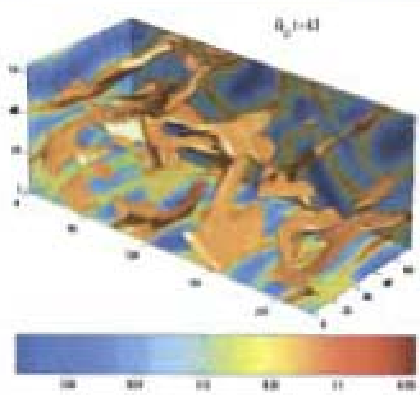
VPIC is a "best in class" capability enabling scientific discovery

- VPIC is a 3D explicit relativistic particle-in-cell kinetic plasma code with wide applicability
- With VPIC, discoveries have been made in a wide range of problems
  - laser-plasma interaction, magnetic reconnection, ultraintense laser-matter interaction, x-ray sources, active interrogation, magnetic fusion, space, and astrophysics, thermonuclear burn
- VPIC has been deliberately designed for future computer platforms starting in 2002 - we are well poised to take advantage of next-generation multicore, hybrid supercomputers (Roadrunner, GPU, path to Exascale) – Co-Design
- This unique capability gives LANL substantial competitive advantage in plasma and high energy density science


Self-focusing from laser-plasma interaction in ICF hohlraum plasma [Yin et al. PRL 2009]

Outline

- The VPIC algorithm
- Data flow and high performance supercomputing in the multicore era
- VPIC Application areas
  - Laser plasma interaction for inertial fusion expts.
  - Magnetic reconnection
- Future Directions


Current density iso-surfaces in MHD turbulence show current sheet and filament formation during magnetic reconection in astrophysical plasma [Bowers and Li, PRL 2007]

What does VPIC do?

$$\partial_t f_s + c\gamma^{-1}\vec{u}\cdot\nabla f_s + \frac{q_s}{m_s c}\left(\vec{E} + c\gamma^{-1}\vec{u}\times\vec{B}\right)\cdot\nabla_u f_s = \left(\partial_t f_s\right)_{coll}$$

$$\partial_t \vec{E} = \varepsilon^{-1}\left(\nabla\times\mu^{-1}\vec{B} - \vec{J} - \sigma\vec{E}\right)$$

$$\partial_t \vec{B} = -\nabla\times\vec{E}$$

$$d_t \vec{r}_{s,n} = c\gamma_{s,n}^{-1}\vec{u}_{s,n}$$

$$d_t \vec{u}_{s,n} = \frac{q_s}{m_s c}\left(\vec{E}\big|_{\vec{r}_{s,n}} + c\gamma_{s,n}^{-1}\vec{u}_{s,n}\times\vec{B}\big|_{\vec{r}_{s,n}}\right)$$

- VPIC integrates the relativistic Maxwell-Boltzmann system in a linear background medium for multiple particle species
- An explicit-implicit mixture of velocity Verlet, leapfrog, and exponential differencing is employed based on a reversible phase-space-volume conserving 2nd order Trotter factorization (see attachments)
- Direct discretization of f_s is prohibitive; sample with particles that obey the same Boltzmann equation (outside of collisions)
- Smooth J extrapolated from particles; E, B, J sampled on a mesh and interpolated to/from particles

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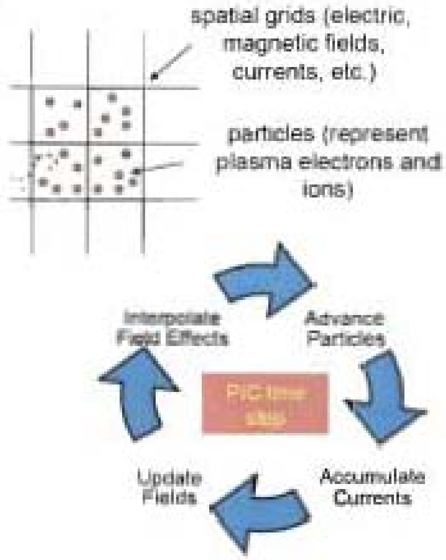
VPIC is a Particle-In-Cell (PIC) kinetic plasma simulation code

- Plasmas are ionized gases with complex, collective behavior (long range forces are important)
- The particle-in-cell (PIC) technique provides a fundamental computational description of plasma
- VPIC is state-of-the-art:
  - Designed for high efficiency on memory-bandwidth-limited platforms
  - Makes heavy use of SIMD vector intrinsics
  - Employs MPI + multithreading



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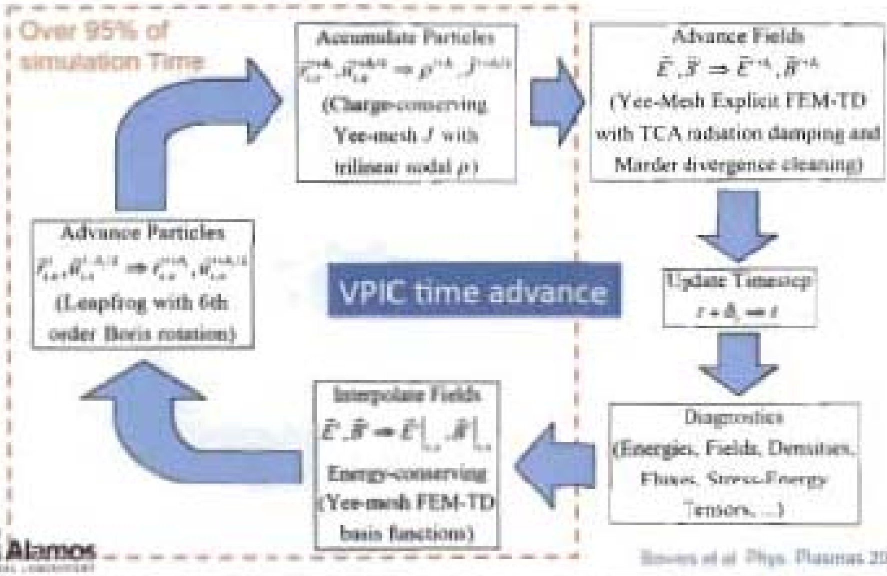
In a time step, typically >95% of the time is spent advancing particles



Bowers et al. Phys. Plasmas 2008

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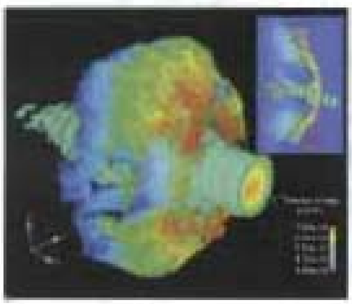
VPIC algorithm: good and bad features for modern architectures



VPIC simulation of novel "Break-Out Afterburner" ion acceleration mechanism – discovered first in simulations [Yin et al. Laser Part. Beam 2006, Yin et al. PRL (submitted)] and realized in Trident experiments [Hegelich et al. Nature (submitted)]

- The good:
  - Computation dominated by a single "hot spot" (particle scatter/gather > 95% of flops)
  - Particle advance is intrinsically local
  - Small amount of data needed to represent and advance particle
  - Electromagnetic field advance is also local (speed of light is finite)
  - Relatively straightforward algorithm
  - With care, single precision is sufficient
- The bad:
  - Few operations to do a particle advance (common case: 246 operations for 232 bytes moved)
  - Memory bandwidth limited
- The bad++:
  - Random access to memory in inner loop - particularly tricky for hybrid, e.g., Cell or GPU

Roadrunner focused how to get high performance on multicore

- Data motion
  - Single pass through particle list, single precision where possible
  - Locate VPIC kernel closer to the "leaves", not the "trunk"
  - MPI relay abstracts communication layer
  - LRU software caches used on SPE to reduce memory fetches
  - Frequent particle sorting to improve data locality
- Throughput
  - Simple interface in C++ to for SIMD vector intrinsics
  - Static scheduling makes performance analysis/prediction more reliable
- Concurrency
  - Data-parallel programming model
  - Triple-buffered I/O to/from Cell SPE to overlap communication and computation
  - Major operations in particle push, field solve, etc. have been turned into independent threads of computation that are dispatched

VPIC employs single pass processing to reduce data motion

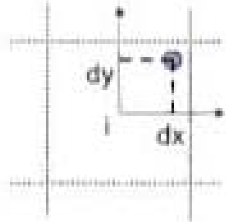
```
for each particle,
  interpolate E and B
  update u and compute movement
  update r and accumulate J
  if an exceptional boundary hit,
    save particle index and
      remaining movement
  end if
end for
```

- Performance is limited by moving particle data to and from memory
- We limit the times a particle is accessed to once per time step
- Particle data is stored contiguously, memory aligned and organized for 4-vector SIMD
- The inner loop streams through particle data once using large, aligned transfers under the hood—the ideal access pattern

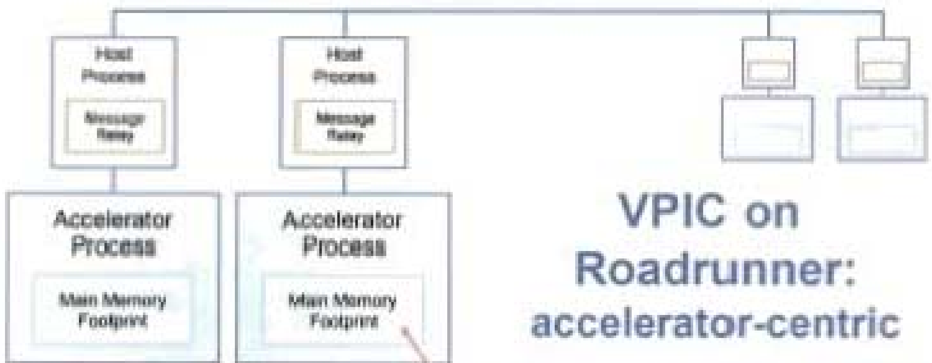
```
typedef struct {
  float dx, dy, dz; int i; // Cell offset (on [-1,1]) and index
  float ux, uy, uz, q;     // Normalized momentum and charge
} particle_t;
```

VPIC was designed so that single precision would suffice

- Positions given by the cell index and offset from the cell center, normalized to cell dimensions
- Numerical algorithm and "hygiene" techniques used
  - Divergence cleaning of E and B divergence errors
  - Radiation damping (control num. heating)
  - Mathematical properties of operator split (see supplemental material)
- Sensitivity to roundoff – truncate gives about 10x the numerical heating as IEEE standard



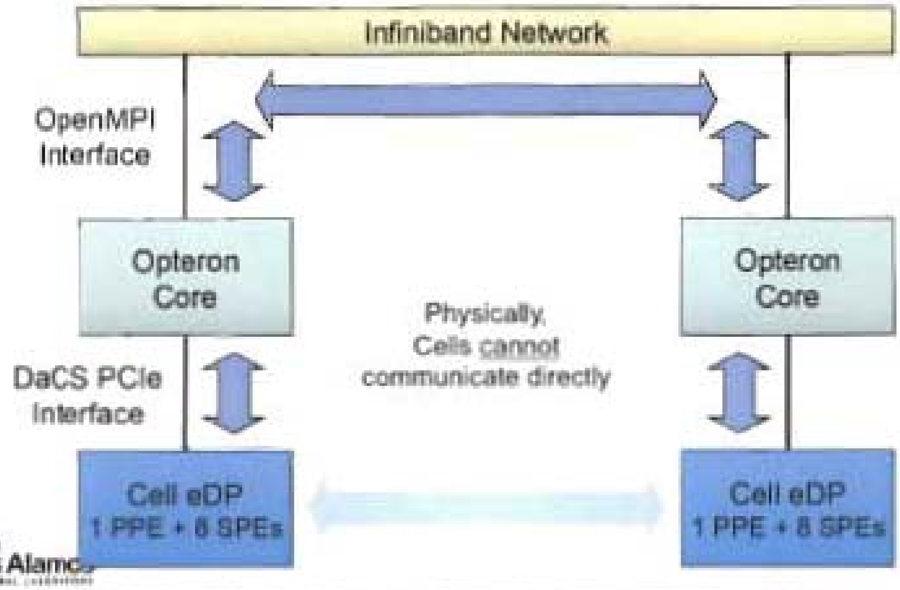
Data motion issues: accelerator-centric programming model



VPIC on Roadrunner: accelerator-centric

VPIC has such a low compute/data ratio (common case: 246 ops/232 bytes), we locate the main memory as close to the SPE as possible

On Roadrunner, communications among cells is tricky



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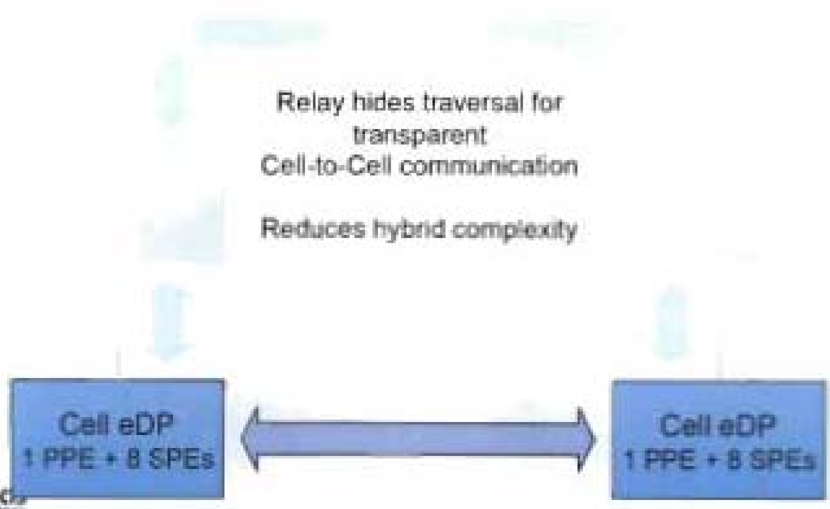
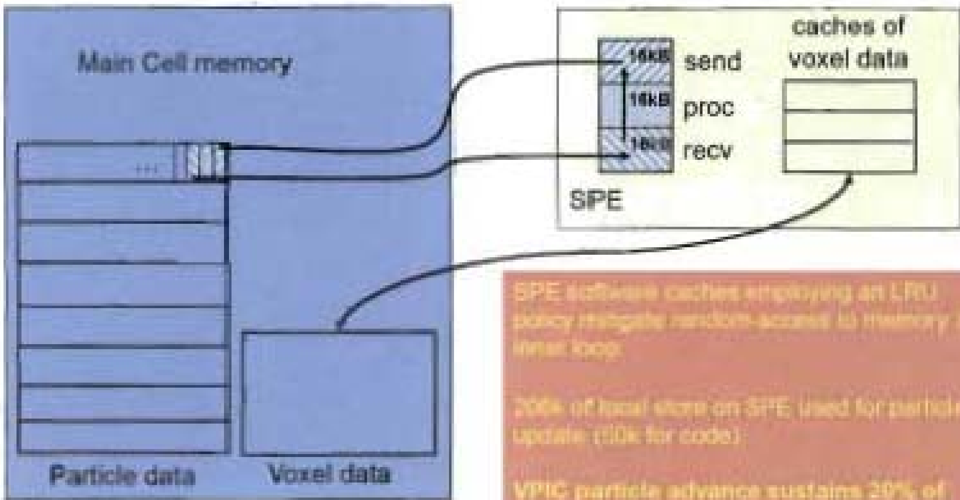
We implemented an MPI relay to hides this complexity



Caches and multi-buffering hide memory latency & improve locality

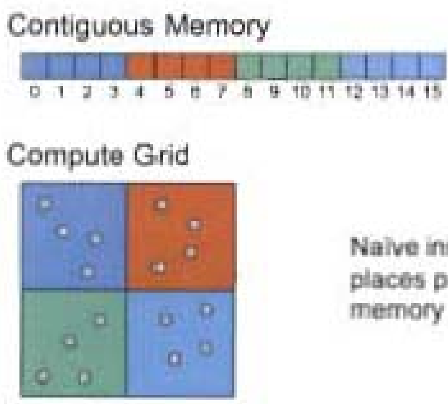


SPE software caches employing an LRU policy mitigate random-access to memory in inner loop

200k of local store on SPE used for particle update (<50k for code)

VPIC particle advance sustains 20% of theoretical single precision floating point performance on SPE

Frequent sorting helps maintain nearly ordered particle data

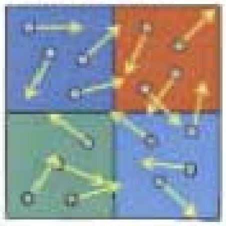


Naive initial particle distribution by voxel places particle data spatially "close" in memory

Frequent sorting helps maintain nearly ordered particle data

Contiguous Memory

Compute Grid



Advancing particles potentially moves them into new voxels

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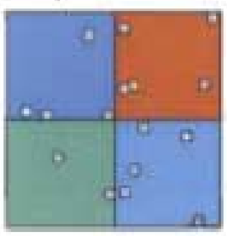
Frequent sorting helps maintain nearly ordered particle data

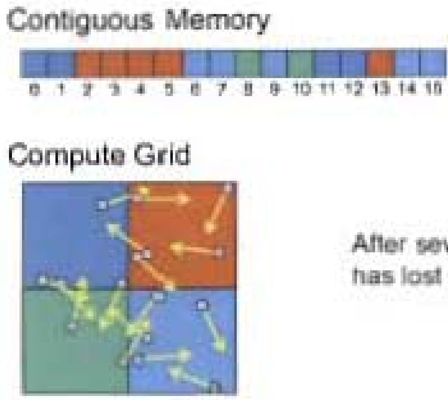
Contiguous Memory

Compute Grid



New particle positions interleave memory access with respect to voxels

Frequent sorting helps maintain nearly ordered particle data



After several time iterations, particle data has lost spatial locality

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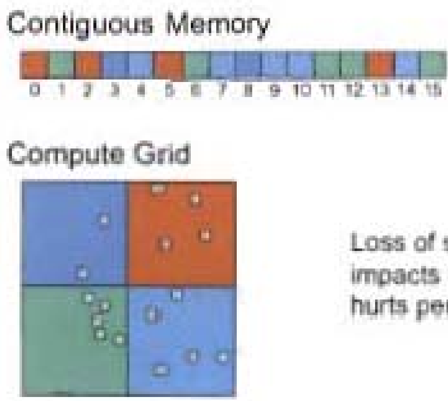
Frequent sorting helps maintain nearly ordered particle data



Loss of spatial locality in data access impacts temporal access of field data and hurts performance

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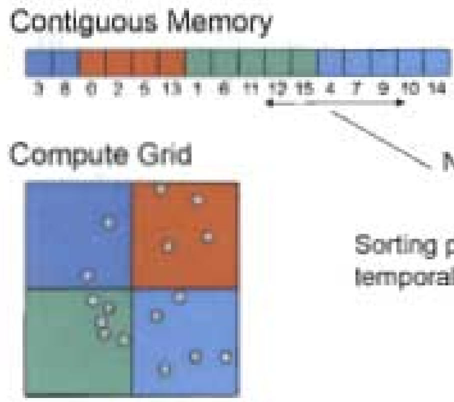
Frequent sorting helps maintain nearly ordered particle data



Numbering indicates original indices

Sorting particle data by voxel restores spatial/ temporal locality

On Roadrunner, VPIC employs a very efficient, thread-parallel, out-of-place sort

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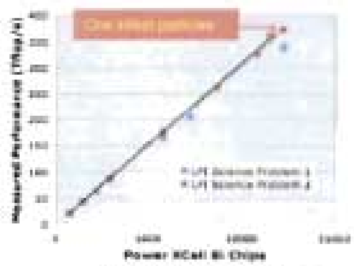
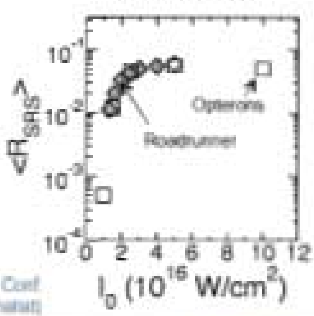
VPIC performance on Roadrunner is outstanding

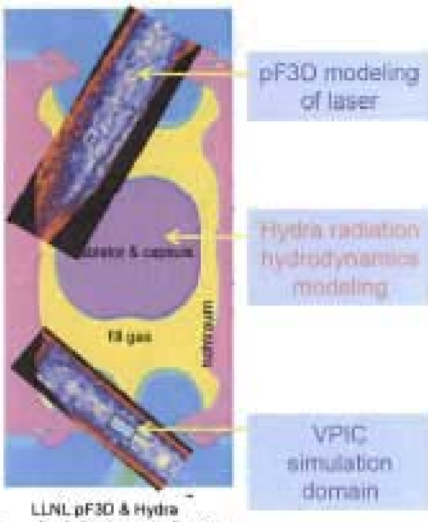
- Laser-plasma interaction (LPI) modeled on up to 12240 Cell chips and obtained linear weak scaling
  - 1T particles: then the world's largest plasma PIC calculation
  - Sustained >0.374 Pflop/s
- Success on Roadrunner led to high performance on other multicore supercomputers
  - 0.25 Pflop/s on 1.2T particle simulation 100k cores of ORNL's Kraken





Bowers et al. Proc. 2008 ACM/IEEE Conf. Supercomput. (Gordon Bell Prize Finalist)

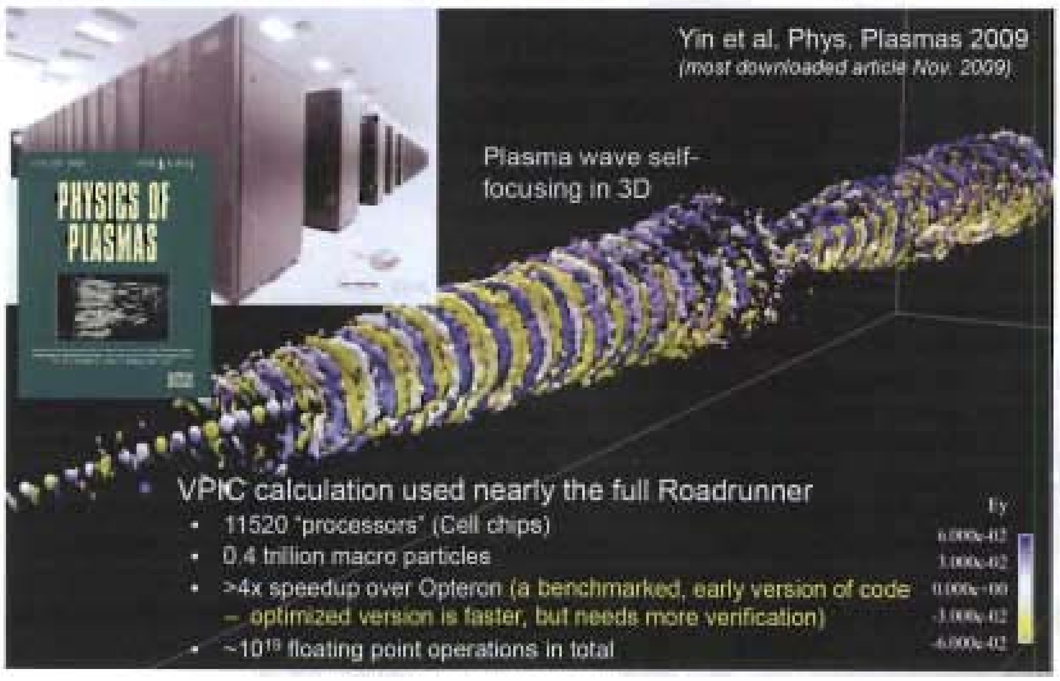
With these simulations, we simulate entire inertial fusion laser speckles



LLNL pF3D & Hydra simulations – compliments of D. Hinkel et al.

- In inertial confinement fusion experiments (ICF) at the National Ignition Facility, the laser beams are broken into "speckles" to smooth the intensity profile across the beam
- In intense speckles, nonlinear LPI can scatter the laser and risk fusion ignition
- With VPIC on Roadrunner, we model entire laser speckles (even multiple speckles) in 3D at all relevant scales
- This is a major step toward predictive capability for ICF

VPIC on Roadrunner enables "at scale" simulations of NIF speckles



At the Pflop scale, VPIC enables exploration of new LPI physics

pF3D modeling of laser

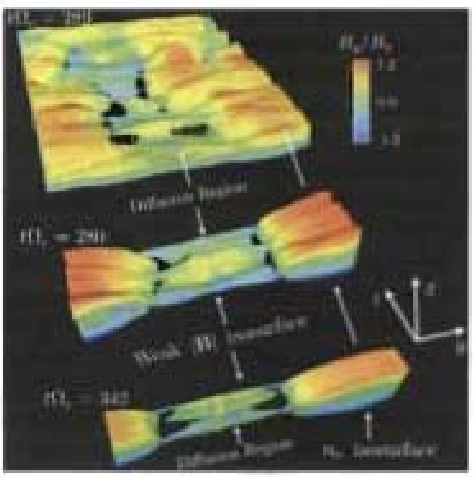
Hydra Radiation hydrodynamics modeling

pF3D & Hydra simulations courtesy of LLNL

First-ever kinetic simulation of multiple laser speckles in 3D

- Laser speckles exhibit nonlinear laser-plasma interaction, greatly enhanced back-scatter
- In the multi-speckle environment (relevant for NIF beams), strong backscatter in one speckle can lead to much higher backscatter in neighboring speckles – new physics!

Also at the petascale – new physics in 3D magnetic reconnection



- Multiple, small reconnection sites self-organize in the current direction to form a large diffusion region
- The diffusion region expands in the outflow direction
- The resulting thin diffusion region is unstable to secondary processes (kinking and tearing)
- Only in the largest simulations:
  - Secondary king modes do not evolve to longest wavelength available
  - Diffusion region has finite extent in the current direction

Electron-positron plasma
1024 X1024X1024 cells
172 billion particles

Yin et al. PRL 2008; Daughton et al. PRL 2009; Roytershteyn et al. Phys. Plasmas 2009 (APS Invited Talk)

VPIC is a "best in class" capability enabling scientific discovery

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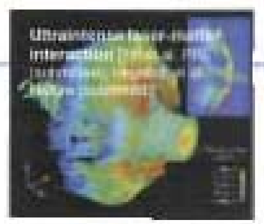
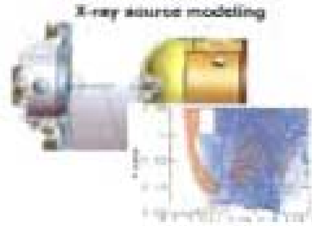
- With VPIC, discoveries have been made in a wide range of problems
  - laser-plasma interaction, magnetic reconnection, ultraintense laser-matter interaction, x-ray sources, active interrogation, magnetic fusion, space, and astrophysics, thermonuclear burn
- VPIC has been deliberately designed for future computer platforms starting in 2002 - we are well poised to take advantage of next-generation multicore, hybrid supercomputers (Roadrunner, GPU, path to Exascale) – Co-Design
- This unique capability gives LANL substantial competitive advantage in plasma and high energy density science

Where do we go from here?

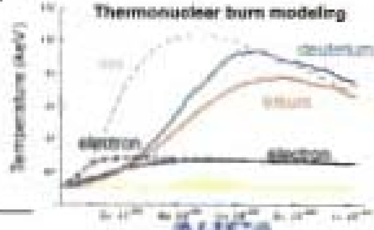


- Future directions
  - Expand solvers – electrostatic, implicit, hybrid, gyrokinetic
  - Physics models
    - laser-plasma modeling beyond I = 10^{22} W/cm^2
    - Kinetic thermonuclear burn
    - Monte Carlo electron transport in materials
  - 2D r-z geometry (replace a legacy code)
  - Exploit hierarchical computation on hybrid architectures to "pre-digest" diagnostics, etc.

X-ray source modeling



Thermonuclear burn modeling



Supplemental: VPIC operator splitting

- For a well-behaved operator, the operator equation:

  $$d_t X = \hat{L} X$$

  has the formal solution:

  $$X(t+\delta_t) = e^{\delta_t \hat{L}} X(t)$$

- If L can be split into the sum of N well-behaved operators:

  $$\hat{L} = \sum_{i=1}^{N} \hat{L}_i$$

  a 2nd order approximation of the operator exponential is:

  $$e^{\delta_t \hat{L}} \sim e^{\delta_t \hat{L}_1/2} \ldots e^{\delta_t \hat{L}_{N-1}/2} e^{\delta_t \hat{L}_N} e^{\delta_t \hat{L}_{N-1}/2} \ldots e^{\delta_t \hat{L}_1/2}$$

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Supplemental: VPIC Time Discretization

- A 2nd order Trotter factorization of the relativistic Maxwell-Boltzmann equations is:

  $$e^{\delta_t \hat{L}} \sim e^{\delta_t \hat{L}_{uB}/2} e^{\delta_t \hat{L}_{uE}/2} e^{\delta_t \hat{L}_x/2}$$
  $$e^{\delta_t \hat{L}_B/2} e^{\delta_t \hat{L}_E} e^{\delta_t \hat{L}_B/2}$$
  $$e^{\delta_t \hat{L}_x/2} e^{\delta_t \hat{L}_{uE}/2} e^{\delta_t \hat{L}_{uB}/2}$$

  where:

  $$\hat{L}_E : \partial_t \vec{E} = \varepsilon^{-1} \nabla \times \mu^{-1} \vec{B} - \varepsilon^{-1} \vec{J} - \varepsilon^{-1} \sigma \vec{E}$$
  $$\hat{L}_B : \partial_t \vec{B} = -\nabla \times \vec{E}$$
  $$\hat{L}_x : d_t \vec{r}_{s,n} = c \gamma_{s,n}^{-1} \vec{u}_{s,n}$$
  $$\hat{L}_{uE} : d_t \vec{u}_{s,n} = \tfrac{q_s}{m_s c} \vec{E}\Big|_{\vec{r}_{s,n}}$$
  $$\hat{L}_{uB} : d_t \vec{u}_{s,n} = \vec{u}_{s,n} \times \tfrac{q_s}{m_s \gamma_{s,n}} \vec{B}\Big|_{\vec{r}_{s,n}}$$

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Supplemental: VPIC Time Discretization (cont)

- Repeatedly applying this splitting and grouping particle and field operators separately yields VPIC's field advance:

  $$e^{\delta_t \hat{L}_B/2} e^{\delta_t \hat{L}_E} e^{\delta_t \hat{L}_B/2}$$

  and VPIC's particle advance:

  $$e^{\delta_t \hat{L}_r/2} I_J e^{\delta_t \hat{L}_r/2} e^{\delta_t \hat{L}_{ue}/2} e^{\delta_t \hat{L}_{ub}} e^{\delta_t \hat{L}_{ue}/2}$$

  (I_J means J for the field advance is computed but the state is unchanged)

- Thus, a mixed implicit-explicit method consisting of velocity Verlet, exponential differencing and leapfrog is used to advance *E*, *B* and *r* from *t* to $t+\delta_t$ and *u* from $t-\delta_t/2$ to $t+\delta_t/2$

- This underlying time discretization has robust theoretical properties, reversible, phase space volume conserving, ...

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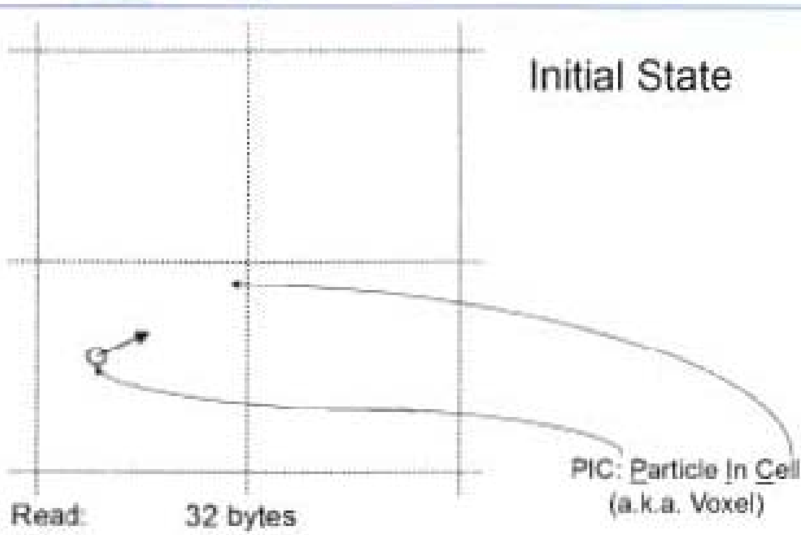
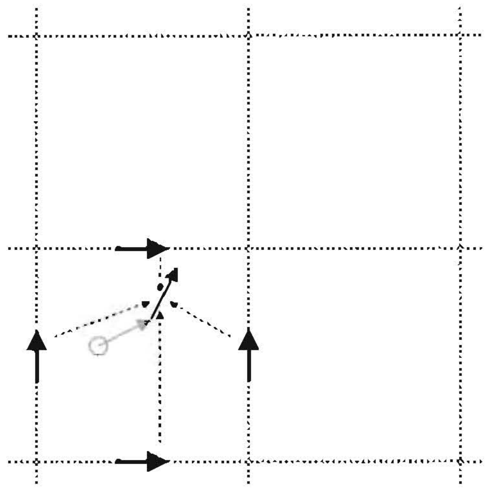
Supplemental: What is involved in this particle advance?



Read: 32 bytes
Write: 0 bytes
Compute: 0 flop

Supplemental: What is involved in this particle advance?



Initial State

Interpolate *E* and *B*

Read: 72 bytes
Write: 0 bytes
Compute: 27 flop

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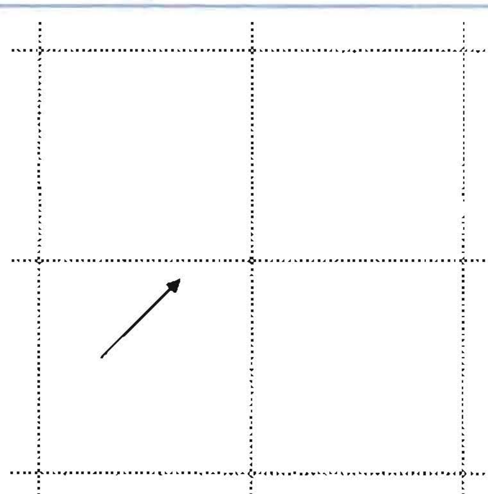
Supplemental: What is involved in this particle advance?

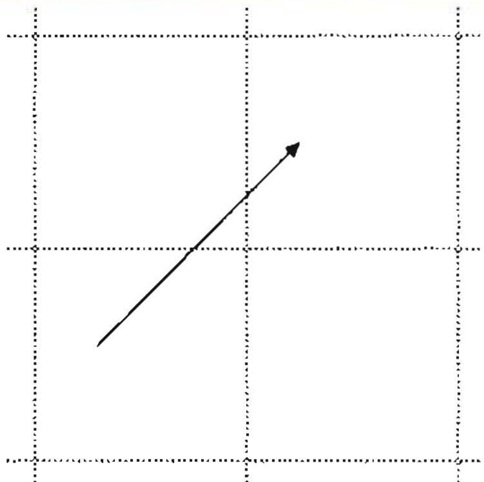


Interpolate *E* and *B*

Update *u*

Read: 0 bytes
Write: 0 bytes
Compute: 107 flop

Supplemental: What is involved in this particle advance?



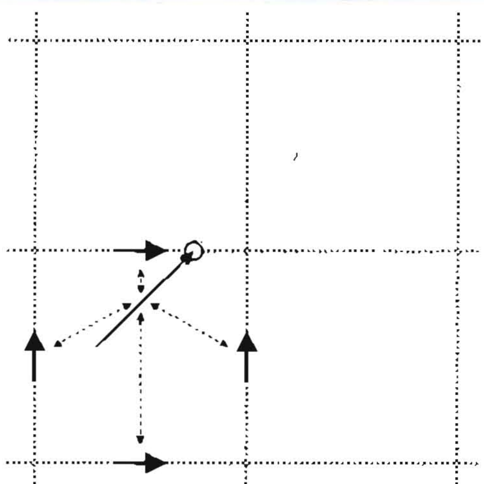
[illegible] E and B

Update u

Compute Motion

Read: 0+48 bytes
Write: 0+48 bytes
Compute: 42+70 flop

Supplemental: What is involved in this particle advance?



Compute Motion

Update r and J

Read: 56 bytes
Write: 48 bytes
Compute: 168 flop

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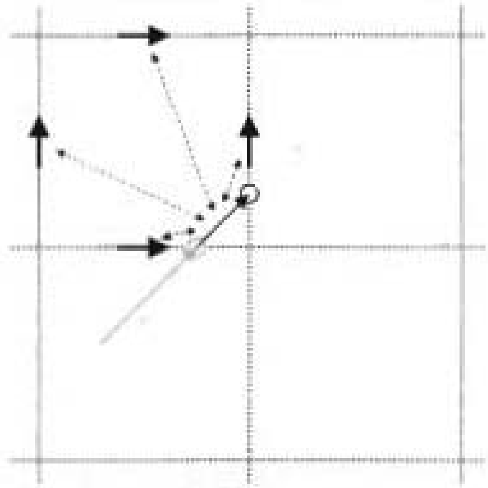
Supplemental: What is involved in this particle advance?



Update *r* and *J*
Update *r* and *J*

Read: 56 bytes
Write: 48 bytes
Compute: 168 flop

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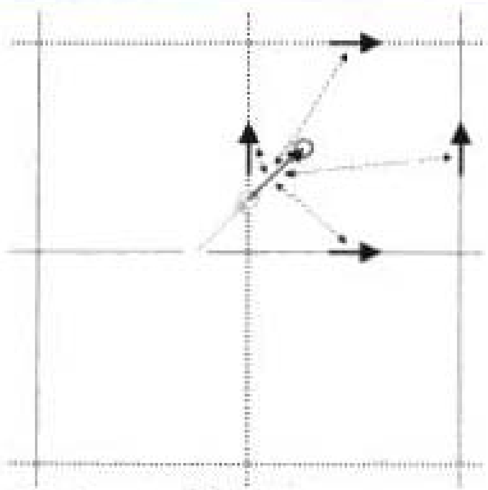
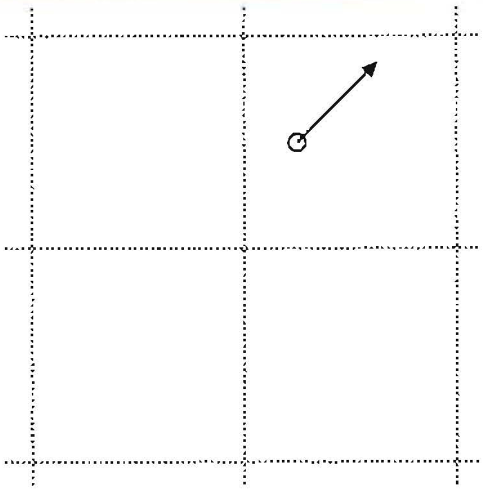
Supplemental: What is involved in this particle advance?



Update *r* and *J*
Update *r* and *J*

Read: 56 bytes
Write: 48 bytes
Compute: 168 flop

Supplemental: What is involved in this particle advance?



Update r and J

Final State

Read:	0 bytes	Net Read:	152+ 56 n_c bytes
Write:	32 bytes	Net Write:	80+ 48 n_c bytes
Compute:	0 flop	Net Compute:	246+168 n_c flop

Supplemental: VPIC designed for effective use of short-vector SIMD

```
// Interpolate ex for the next 4 particles
load_4x4_tr( interp_coeff[ i(0) ].QUAD( ex, dexdy, dexdz, d2exdydz ),
             interp_coeff[ i(1) ].QUAD( ex, dexdy, dexdz, d2exdydz ),
             interp_coeff[ i(2) ].QUAD( ex, dexdy, dexdz, d2exdydz ),
             interp_coeff[ i(3) ].QUAD( ex, dexdy, dexdz, d2exdydz ),
             ex, dexdy, dexdz, d2exdydz );
ex = (ex + dy*dexdy) + dz*(dexdz + dy*d2exdydz);
```

- Programming languages (e.g. C, FORTRAN) are not expressive enough (e.g. data alignment restrictions) to allow compilers to use 4-vector SIMD in operations as complex as those in VPIC
- To compensate, VPIC has a language extension that allows C-style portable 4-vector SIMD code to be written and converted automatically to high performance 4-vector SIMD instructions on a wide variety of platforms. A similar approach was used in Bowers *et al* 2006

Warsa

Deterministic Transport Methods

James S. Warsa, CCS-2
Erin D. Fichtl, Jeffery D. Densmore, Jae H. Chang, Randal S. Baker

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Overview

- Overview of Research Activity
- Newton's Method for *k*-Eigenvalues
- Newton's Method applied to S_N Transport with Negative-flux Fixup
- CFEM-Based DFEM Spatial Discretization
- Final Remarks
- Supplemental Items
  - Manufactured Solutions in the Thick Diffusion Limit

- Overview of Research Activity

Deterministic Transport Methods

- Deterministic transport methods research, and the organizational thread it follows, has a 60 year history at Los Alamos
- Numerical methods are developed that provide the capability to efficiently model the interactions of neutrons ("neutronics") and photons ("radiative transfer")
- These computations are an important part of multi-physics computational simulations that are part of the Laboratory mission
- Research has kept pace with changing requirements due to changing mission activities or scientific or technological concerns
- Increasing fidelity and complexity of the applications to which transport solutions are coupled has require increasingly more accurate and efficient solution methods
- Hence, there is strong connection of the basic research to applications, through both funding and technical concerns

General Research Areas

- Parallel and Heterogeneous Computing Architectures
  - Development of new algorithms and techniques
  - Previously discarded algorithms reconsidered
- Multi-physics Applications
  - Coupling to high energy density applications requires robust methods
  - Additional terms in the transport equation increase complexity
  - Efficient and accurate discretizations and algorithms are needed
  - Operator splitting versus fully-coupled, nonlinear solution methods
- Theoretical Analysis
  - Methods developed for numerical solutions must have certain characteristics for particular applications
  - Analysis is conducted to determine the numerical properties of discretizations and algorithms

Recent Specific Research Activities

- Iterative solution methods implemented on Roadrunner
- Parallel angular SN sweeps implemented on Roadrunner
- Neutron transport in moving materials
- Efficient iterative solution methods for radiative transfer
- Apply Newton's method to eigenvalue problems (essentially Nonlinear)
  - Criticality eigenvalue (*k* -eigenvalue) problems
  - Negative-flux fixup in S_N transport
  - Time eigenvalue (α-eigenvalue) problems
- Two-dimensional spatial discretization on unstructured polygon meshes
- Numerical verification of SN transport discretizations in the thick-diffusion limit

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Introduction

- Space, angle, energy and time dependent transport equation
  - Angular flux particle distribution $\psi(r, \hat{\Omega}, E, t)$ at point r, direction $\hat{\Omega}$, energy E, time t
  - Material interaction probabilities $\sigma_{t,g}(\mathbf{r})$, $\sigma_{s,g' \to g}(\mathbf{r})$, $\sigma_{f,g'}(\mathbf{r})$
  - S_N multigroup approximation, angle $m = 1, \ldots, N$ and energy group $g = 1, \ldots, G$

$$\left[\frac{1}{v_g}\frac{\partial}{\partial t} + \hat{\Omega}_m \cdot \nabla + \sigma_{t,g}(\mathbf{r})\right]\psi_{g,m}(\mathbf{r}, t) = \frac{1}{4\pi}\sum_{g'=1}^{G} \sigma_{s,g' \to g}(\mathbf{r})\,\phi_{g'}(\mathbf{r}, t) + \frac{1}{k}\frac{\chi_g(\mathbf{r})}{4\pi}\sum_{g'=1}^{G} \nu\sigma_{f,g'}(\mathbf{r})\,\phi_{g'}(\mathbf{r}, t)$$

  - Scalar flux for group g

$$\phi_g(\mathbf{r}, t) = \sum_{m=1}^{N} w_m \psi_{g,m}(\mathbf{r}, t).$$

Introduction (cont.)

- Steady-state operator notation
  - ψ vector of length NG, ϕ vector of length G

$$\mathbf{L}\psi = \left(\mathbf{S} + \frac{1}{k}\mathbf{F}\right)\phi, \quad \phi = \mathbf{D}\psi$$

  - $\mathbf{L}$ is $(NG \times NG)$, $\mathbf{S}$ and $\mathbf{F}$ are $(NG \times G)$, $\mathbf{D}$ is $(G \times NG)$
- Maximum eigenvalue k is the "critical" eigenvalue of interest
  - Generalized eigenproblem

$$\mathbf{A}\phi = \frac{1}{k}\mathbf{B}\phi$$

  - Standard eigenproblem

$$k\phi = \mathbf{A}^{-1}\mathbf{B}\phi$$

$$\mathbf{A} = \left(\mathbf{I} - \mathbf{D}\mathbf{L}^{-1}\mathbf{S}\right), \quad \mathbf{B} = \mathbf{D}\mathbf{L}^{-1}\mathbf{F}$$

Newton's Method

- Anselone and Rall (1967): Eigenvalue problems are in general nonlinear
- Newton's method applied to *k*-eigenvalue problems
  - Mahadevana and Ragusa (2008): diffusion and transport
  - Gill and Azmy (2009): intermediate levels of iteration
  - Knoll, Park and Smith (2009): diffusion and preconditioning for efficiency
- Very efficient compared to traditional methods (nonlinear fixed-point iteration)
- No proof of convergence to fundamental mode (the same is true for fixed-point iteration)
- Gill, Azmy, Densmore and Warsa (2010)
  - Investigate splittings to minimize the number of SN sweeps
  - Investigate a number of constraints, or update, equations

Newton's Method (cont.)

- Nonlinear fixed-point iteration

$$\phi^{\ell+1} = \mathbf{P}(k^{\ell})\phi^{\ell}$$
$$k^{\ell+1} = \kappa(\phi^{\ell}, k^{\ell})$$

- Newton's Method
  - For $k = 0, 1, \ldots,$ until $\| F(u_{k+1}) \| < \epsilon$

$$\mathbf{J}(u^k)\delta u^k = -F(u^k)$$
$$u^{k+1} = u^k + \delta u^k$$

  - Nonlinear residual $F(u) = 0$ (Jacobian $\mathbf{J}(u) \equiv F'(u)$)

$$F(\mathbf{u}) = \begin{bmatrix} \phi - \mathbf{P}(k)\phi \\ \kappa(\phi, k) \end{bmatrix}$$

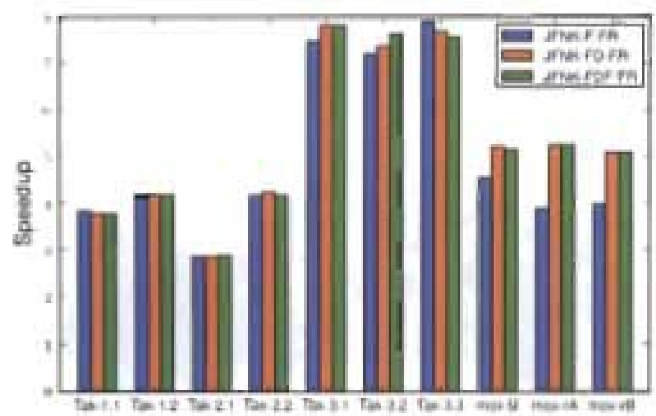
Newton's Method (cont.)

- Formulations and constraints based on splittings of **A** and **B**

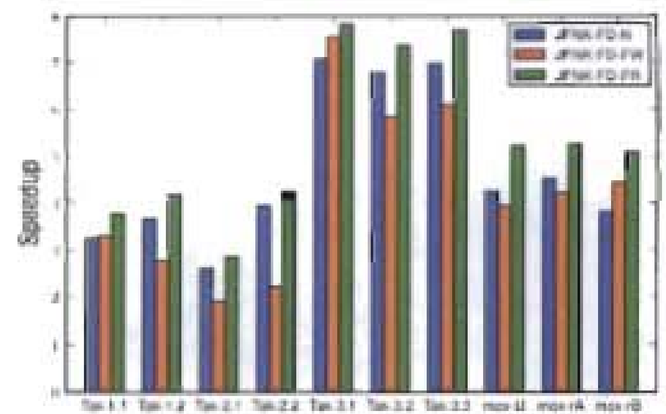
Formulation $\mathbf{P}(k)$		Constraint	
$\frac{1}{k}\mathbf{A}^{-1}\mathbf{B}$	PI		
$\mathbf{A}_{LD}^{-1}\left(\frac{1}{k}\mathbf{B}-\mathbf{A}_U\right)$	FPI	$(\phi^T\phi)-1$	N
$\mathbf{D}\mathbf{L}^{-1}\mathbf{M}\left(\mathbf{S}+\frac{1}{k}\mathbf{F}\right)$	F	$k-k\left(\frac{\mathbf{E}^T\mathbf{F}\mathbf{P}(k)\phi}{\mathbf{E}^T\mathbf{F}\phi}\right)$	FR
$\mathbf{A}_L^{-1}\left(\frac{1}{k}\mathbf{B}-\mathbf{A}_{DU}\right)$	FD	$k-k\frac{(\phi^T\mathbf{P}(k)\phi)}{(\phi^T\phi)}$	FW
$\left(\mathbf{A}_L-\frac{1}{k}\mathbf{B}_L\right)^{-1}\left(\frac{1}{k}\mathbf{B}_{DU}-\mathbf{A}_{DU}\right)$	FDF		

Results

- 3D benchmarks
  - Takeda 1: 1/8 core LWR, 2-group, S_8, 15,625 cells
  - Takeda 2: 1/4 core FBR, 4-group, S_8, 5,880 cells
  - Takeda 3: axially heterogeneous 1/4 core FBR, 4-group, S_8, 18,432 cells
  - C5G7-MOX: 1/8 core, 4 17 x 17 LWR assemblies, 327,726 cells
- Speedup compared to traditional fixed-point iteration



(a) Formulations



(b) Constraints

Conclusions

- NK and JFNK can be successfully applied to the multigroup, S_N *k*-eigenvalue problem
- The Jacobian-Free approximation in JFNK does not adversely affect NK convergence
- Speedups in large-scale problems are significant
- JFNK is currently being deployed in mission-related *k*-eigenvalue applications

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Introduction

- Fluxes ψ and ϕ represent distributions that *physically* must be non-negative
- Both unrefined meshes (spatial discretization) and inadequate scattering cross section (angular discretization) may lead to negative solutions
- *Mathematically* correct solutions may be negative but are undesirable
  - Slow iterative convergence (never proven to converge)
  - Degradation or failure of iterative acceleration schemes
  - Reduced accuracy in coupled multi-physics simulations
- Negative-flux fixup
  - Set negative fluxes in a mesh cell to zero
  - Re-scale positive cell fluxes to maintain particle balance
  - Nonlinear

Introduction

- Nonlinearity precludes the direct use of Krylov iterative methods
- Hamilton, Warsa, and Benzi (2007) developed a "hybrid method"
  - Alternate between source iteration with fixup and Krylov iteration with "fixed fixups"
  - Superior convergence rate compared to fixed-point iteration
  - Inner and outer iteration parameters required for efficiency
- Apply JFNK as a means by which to exploit the rapid convergence of Krylov iterative methods observed in linear transport (integral equations)
- Any other nonlinearities (eigenvalues, for example) may be addressed simultaneously

Transport Equation with Negative-flux Fixup

- Source (Richardson) iteration

$$\phi^{k+1} = \mathbf{DL}^{-1}\left(\mathbf{S}\phi^{k} + q\right)$$

- $\mathbf{L}^{-1}$ represents a "transport sweep"
  - For each direction *n* and cell *i* a sweep ordering is determined
  - Calculate the flux vector for all spatial degrees of freedom on a cell

$$\Psi_{i,n} = \mathbf{L}_{i,n}^{-1}\left(v_{i,n} - \sum_{i'} \mathbf{L}_{i' \to i,n}\Psi_{i',n}\right)$$

$$vv_{i,n} = \mathbf{S}_i\phi_i^k + Q_{i,n}$$

  - $\Psi_{i',n}$ are angular fluxes that are incoming with respect to cell *i* in direction *n*

Transport Equation with Negative-flux Fixup (cont.)

- Negative-flux fixup
  - p spatial degrees of freedom for every cell i
  - Any $\psi_{j,i,n} < 0$ for $j = 1, \ldots, p$ are first set to zero

$$\Psi^F_{i,n} = 0.5\left(|\Psi_{i,n}| + \Psi_{i,n}\right) = H(\Psi_{i,n})\Psi_{i,n}$$

  - $\Psi^F_{i,n}$ is "re-balanced" to preserve particle balance

$$\Psi^R_{i,n} = \Psi^F_{i,n} \frac{\left(E^T\left[v_{i,n} - \sum_{i'} \mathbf{L}_{i'\to i,n}\Psi^R_{i',n}\right]\right)}{\left(E^T \mathbf{L}_{i,n}\Psi^F_{i,n}\right)} = r_{i,n}\Psi^F_{i,n}$$

  - E^T is a vector of ones of length p

JFNK Applied to Negative-flux Fixup

- Let $\tilde{\mathbf{L}}^{-1}$ denote the nonlinear transport sweep operator with negative-flux fixup
- The nonlinear residual is

$$F(\mathbf{u}) = \mathbf{u} - \mathbf{D}\tilde{\mathbf{L}}^{-1}(\mathbf{S}\mathbf{u} + q) = 0$$

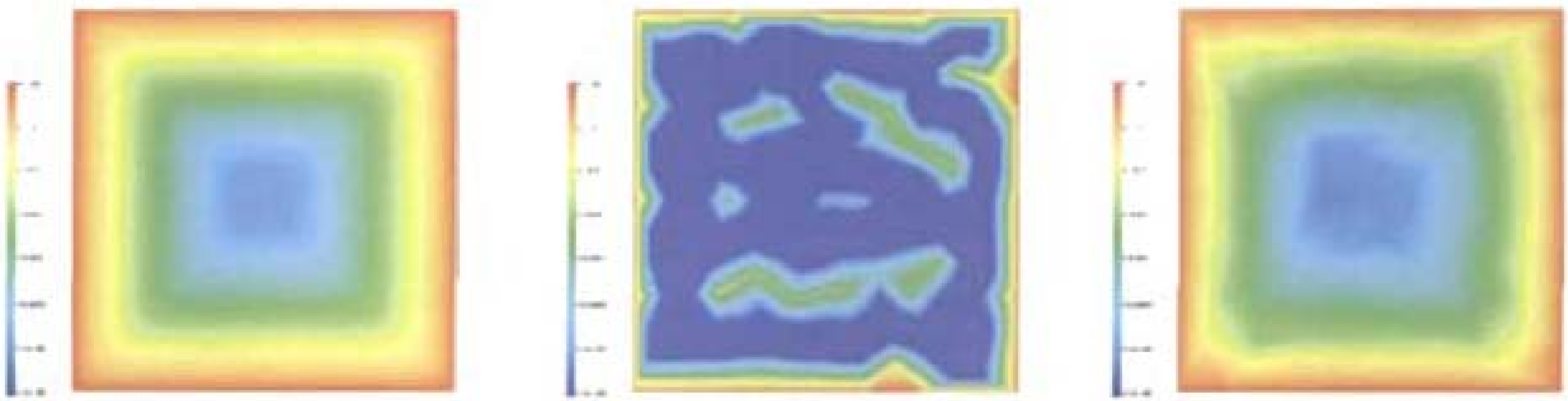
- Defining $v = (\mathbf{S}\mathbf{u} + q)$, the Jacobian is

$$\mathbf{J} = \mathbf{I} - \mathbf{D}\frac{\partial\left(\tilde{\mathbf{L}}^{-1}v\right)}{\partial v}\mathbf{M}\mathbf{S}$$

- The Jacobian is non-singular
- If $\tilde{\mathbf{L}}^{-1} = \mathbf{L}^{-1}$ the Jacobian is the transport operator $\mathbf{J} = \mathbf{I} - \mathbf{D}\mathbf{L}^{-1}\mathbf{S}$
- A sweep implementation has the mechanisms needed to apply the Jacobian

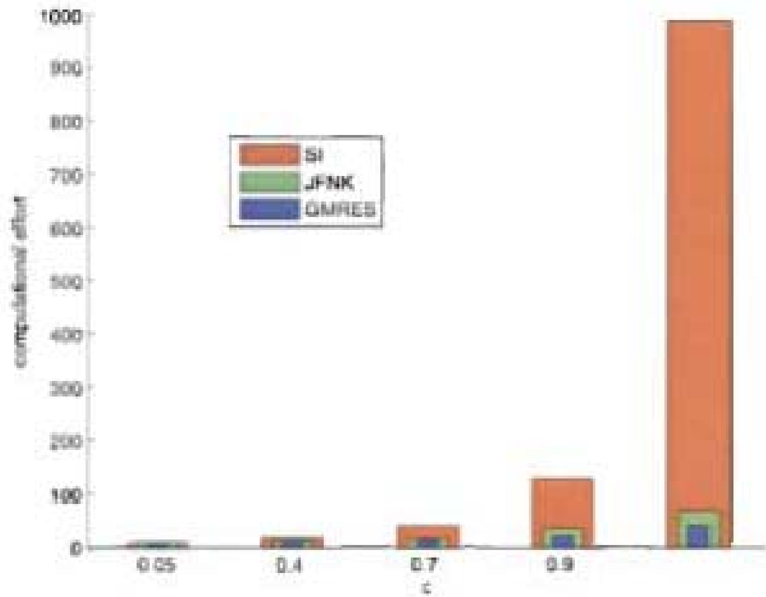
Results

- 1 cm × 1 cm square with σ_t = 40.0 cm^{-1}
- Small, distributed source, isotropic incident flux on all boundaries
- LDFEM on triangles
- Scalar flux solutions for c = 0.7

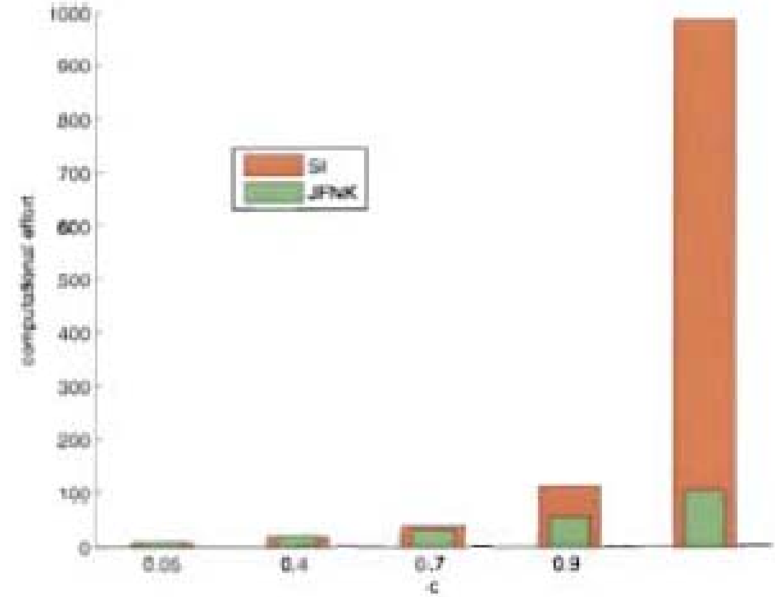


(c) 3137 Cells (d) 150 Cells (e) 150 Cells with Fixup

Results



(f) Without fixup



(g) With fixup

Computational effort for the 150 cell problem as c → 1

Conclusions

- Newton's method is a natural choice for nonlinear, negative-flux fixup algorithms
- The Jacobian is non-singular
- NK and JFNK can be viewed as a means to exploit the rapid convergence properties of Krylov iterative methods for integral equations
- Convergence is not adversely affected by the Jacobian-Free approximation in JFNK
- This capability has already been deployed in mission-related applications

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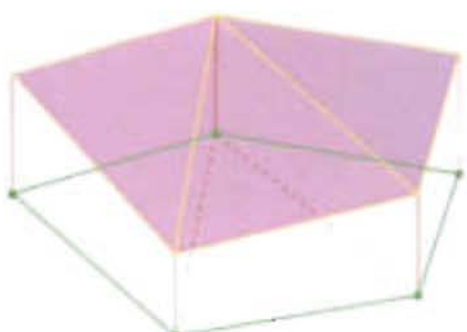
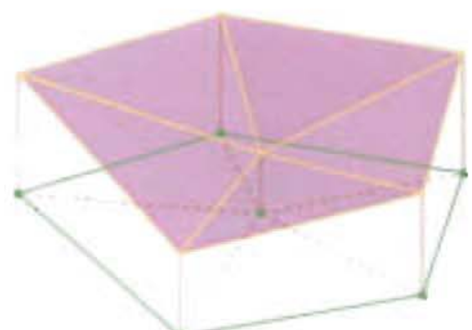
CFEM-Based DFEM

- CFEM: "Continuous Finite Element Method"
- DFEM: "Discontinuous Finite Element Method"
- A polygon is considered a "sub-problem" coupled discontinuously across faces of downwind neighbors
- A piecewise linear CFEM assembled over a triangular subdivision of the polygon
- Two possible solution representations within a convex polygon



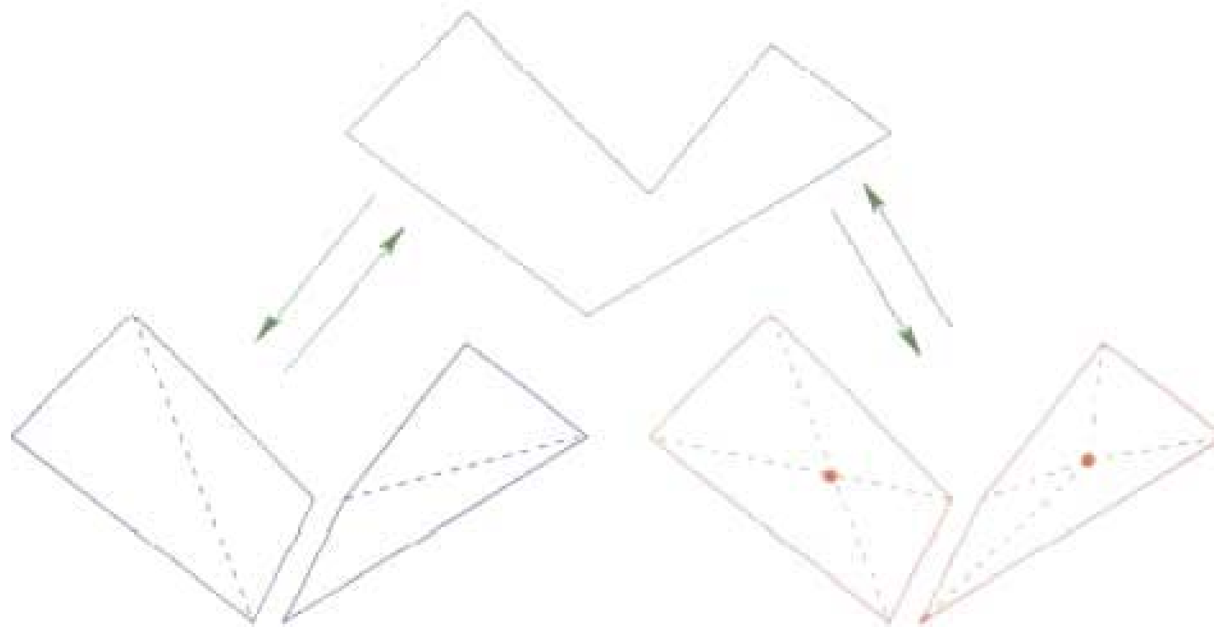
(h) No additional point



(i) Additional point

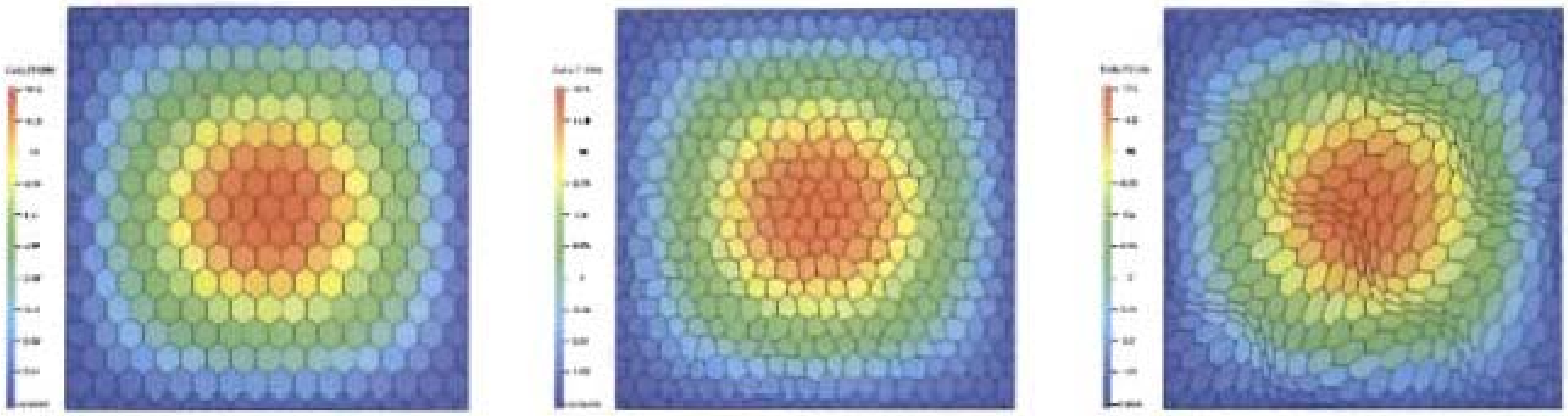
CFEM-Based DFEM

- Different from previous efforts using basis functions
- Not tied to a specific subdivision or type of discretization
- Extensible to higher-order finite elements
- Eliminate sweep cycles by subdividing nonconvex polygons into convex polygons and project/interpolate



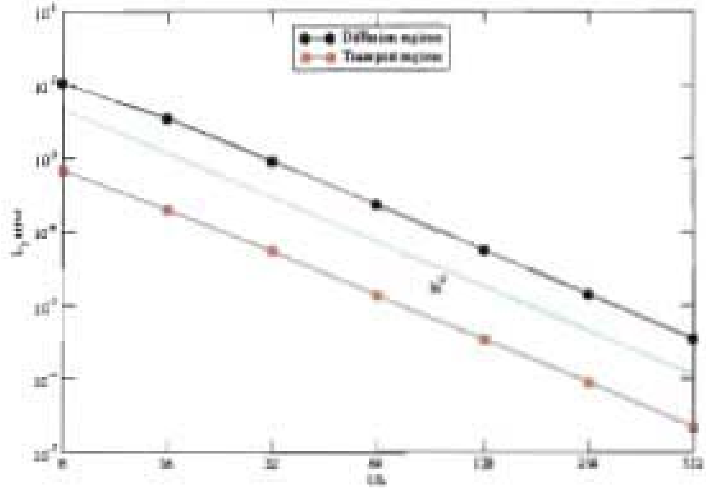
CFEM-Based DFEM (cont.)

- Scalar flux solutions on various polygonal meshes



(j) Regular (k) Randomized (l) Sinusoidal

Results



- Convergence in discrete L_2 norm to manufactured solution
  - $\psi_M(x, y, \hat{\Omega}) = x^2(1 - x^2)\, y^2(1 - y^2) \left(1 + \Omega_x^2 + \Omega_y^2\right)$
  - 1cm × 1cm square, n intervals in x and y dimensions
  - Characteristic mesh size $h \approx 1/n^2$
- Thin, highly-absorbing problem (transport regime) and thick, highly-scattering problem (diffusion regime)

Conclusions

- This capability developed specifically to handle 2D unstructured polygons and AMR-type grids in laboratory applications
- Has been extended easily to axisymmetric coordinates
- Extension to 3D by subdividing polyhedra into tetrahedra
- DFEM-compatible diffusion synthetic acceleration (DSA) can be used directly
- Issues raised in exploring the diffusion regime with a mesh convergence numerical experiment using a manufactured solution is discussed the Supplemental Items

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- Deterministic transport methods research and development impacts multiphysics simulations related to the laboratory mission
- Research and code development for applications capability go hand-in-hand
- New, often cutting-edge, capabilities are almost immediately leveraged for use in simulations
- The transport equation has a variety of application areas
  - Nuclear power
  - Astrophysics
  - Oil-well logging
  - Medical applications
- Publishing research in peer-reviewed journals enhances our reputation and influence on the scientific community

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Introduction

- Verification of spatial discretizations with manufactured solutions
  - Generate a source by applying the SN transport operator to a chosen flux
  - Solutions computed with the discretized source should match the chosen flux
  - Convergence in mesh-refinement numerical experiments indicates correctness and accuracy of a spatial discretization
  - Useful when analytic solutions are not be available
  - May be used with any coordinate system in any number of dimensions
- Thick diffusion limit
  - Under a certain scaling the transport equation goes over to the diffusion equation asymptotically
  - Spatial discretizations should preserve this limit when mesh cells are optically thick
  - Otherwise meshes would have to be over-refined in thick and diffusive problems

Introduction

- Morel and Warsa (2007) and Warsa (2008) presented newly-developed spatial discretizations
- Mesh-refinement numerical experiments were presented using manufactured solutions
- Can manufactured solutions be used to verify problems in the thick diffusion limit, even though computed solutions are independent of problem characteristics?
- Is there any conflict between asymptotic convergence and mesh-refinement convergence?
- Does mesh-refinement convergence in the thick diffusion limit prove anything about the discretization?

Asymptotic Diffusion Limit of the Transport Operator

- $\mathcal{L}_\epsilon$ is the transport operator scaled according to the standard diffusion limit scaling

$$\mathcal{L}_\epsilon \equiv \hat{\Omega} \cdot \nabla + \frac{\sigma_t}{\epsilon} - \frac{1}{4\pi}\left(\frac{\sigma_t}{\epsilon} - \epsilon\sigma_a\right)\int_{4\pi} d\hat{\Omega}',$$

$$\phi(r) = \int_{\mathcal{S}} d\hat{\Omega}'\psi(r, \hat{\Omega}')$$

- ϵ is a smallness parameter such that $\epsilon \ll 1$
- The problem becomes thick with respect to the total mean-free path and weakly absorbing (diffusive) as $\epsilon \longrightarrow 0$

Manufactured Solutions in the Diffusion Limit

- Assume that ψ_M is an $O(1)$ manufactured solution

$$S_\epsilon = \mathcal{L}_\epsilon \psi_M$$

- Asymptotic analysis on $\mathcal{L}_\epsilon \psi = S_\epsilon$ shows

$$\mathcal{D}\phi(r) = \mathcal{D}\phi_M(r), \quad \mathcal{D} = -\nabla \cdot D(r)\nabla + \sigma_a(r), \quad D(r) = 1/3\sigma_t(r)$$

- The same $\psi_M(r, \hat{\Omega})$ will be computed when solving the transport equation whether or not the problem is thick and diffusive
- Solving $\mathcal{L}_\epsilon \psi = S_D$

$$S_D = \frac{1}{4\pi}\mathcal{D}\phi_M(r)$$

yields a scalar flux solution $\phi(r) = \phi_M(r)$ with error $O(\epsilon)$

Mesh Refinement in the Thick Diffusion Limit

- ϕ_ϵ^T is the scalar flux solution to the transport equation
- ϕ^D is the solution to the diffusion equation
- The asymptotic diffusion limit can be stated as

$$\lim_{\epsilon \to 0} \left\| \phi_\epsilon^T - \phi^D \right\| = 0,$$

Mesh Refinement in the Thick Diffusion Limit (cont.)

- $\phi^{\mathrm{T}}_{\epsilon,h}$ and ϕ^{D}_{h} are the solutions evaluated on the grid *h*
- $\widetilde{\phi}^{\mathrm{T}}_{\epsilon,h}$ and $\widetilde{\phi}^{\mathrm{D}}_{h}$ are the *numerical* solutions to transport and diffusion equations with characteristic mesh size *h*
- Assume *h* that is small enough to resolve the length scale of the analytic solutions
- To preserve the diffusion limit . . .
  - . . . the discretized transport equation limits to a discretized diffusion equation
  $$\lim_{\epsilon \to 0} \left\| \widetilde{\phi}^{\mathrm{D}}_{h} - \widetilde{\phi}^{\mathrm{T}}_{\epsilon,h} \right\| = 0$$
  - . . . the discretized diffusion equation is valid (convergent and stable)
  $$\lim_{h \to 0} \left\| \phi^{\mathrm{D}}_{h} - \widetilde{\phi}^{\mathrm{D}}_{h} \right\| = 0$$

Mesh Refinement in the Thick Diffusion Limit (cont.)

- In addition to the requirement that h resolves the solution length scale, require that h remains large enough such that $\sigma_t h/\epsilon \gg 1$ as $\epsilon \longrightarrow 0$
- Let $(h \to 0, \sigma_t h \gg \epsilon \to 0)$ denote a conditional approach to zero

$$\lim_{(h\to 0,\, \sigma_t h \gg \epsilon \to 0)} \left\| \widetilde{\phi}_h^{D} - \widetilde{\phi}_{\epsilon,h}^{T} \right\| = 0$$

$$\lim_{(h\to 0,\, \sigma_t h \gg \epsilon \to 0)} \left\| \phi_h^{D} - \widetilde{\phi}_h^{D} \right\| = 0$$

$$\lim_{(h\to 0,\, \sigma_t h \gg \epsilon \to 0)} \left\| \phi_{\epsilon,h}^{T} - \phi_h^{D} \right\| = 0$$

Mesh Refinement in the Thick Diffusion Limit (cont.)

- Use the triangle inequality to find a necessary but not sufficient condition

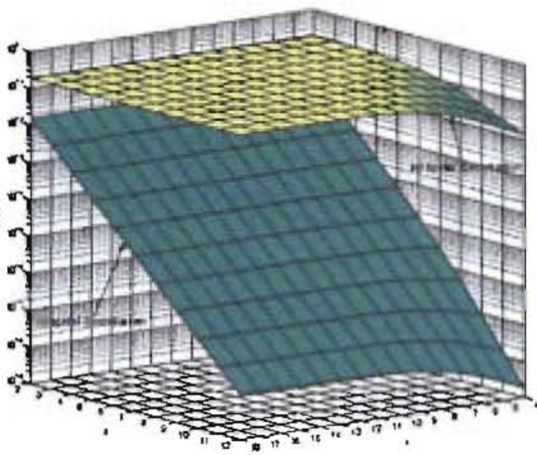
$$\lim_{(h\to 0,\, \sigma_t h \gg \epsilon \to 0)} \left\| \phi^{\mathsf{T}}_{\epsilon,h} - \widetilde{\varphi}^{\mathsf{T}}_{\epsilon,h} \right\| = 0$$

- A numerical mesh refinement experiment can be used to measure $\left\| \phi^{\mathsf{T}}_{\epsilon,h} - \widetilde{\varphi}^{\mathsf{T}}_{\epsilon,h} \right\|$ with decreasing mesh cell spacing h
  - Use S_ϵ or S_D for some ψ_M and let $\phi^{\mathsf{T}}_{\epsilon,h} = \phi_{M,h}$
  - ϵ small enough that the problem is thick and diffusive
  - h chosen so cells remain optically thick over all h
  - h chosen small enough to resolve spatial variation of the solution

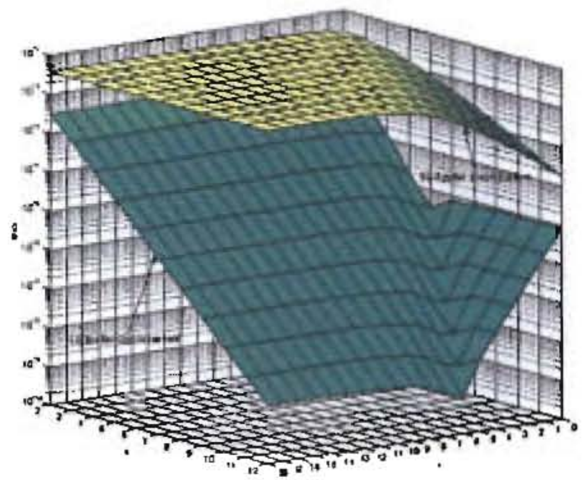
Numerical Experiments

- One-dimensional linear discontinuous (LD) discretization has the thick diffusion limit
- One-dimensional step-differencing (SD) discretization does not have the diffusion limit
- Show examples that confirm these properties and illustrate our approach
- Determine an appropriate range of ϵ for future use
- Issues
  - Ensure that S_ϵ and S_D discretized consistently
  - Use manufactured solutions for which $\phi_{M,h} > 0$
  - Angular quadrature must be used that adequately integrates ψ_M
  - Poor conditioning may cause issues for iterative solution methods
  - Used high numerical precision (in software) for calculations
  - Symmetrized LD in order to use conjugate gradients

Numerical Experiments



(m) Transport source S_ϵ



(n) Diffusion source S_D

- $\psi_M(x,\mu) = (x^2(1-x)^2)(1+3\mu^2)$
- S_4 quadrature, $x \in [0,1]$ cm, vacuum boundary conditions
- $h = 1/2^k$, for $k = 2,\ldots,12$
- $\epsilon = 1/2^n$, $n = 4,\ldots,18$, $\sigma_t = 128\text{cm}^{-1}$, $\sigma_a = 1/1024\,\sigma_t$

Conclusions

- Asymptotic and mesh-refinement convergence requires that
- $\varepsilon \rightarrow 0$ and $h \rightarrow 0$ in a certain way
- If this conditional approach to zero is maintained, a numerical
- mesh-refinement convergence study can be used to show that a
- spatial discretization may have the thick diffusion limit
- Sample mesh-refinement numerical experiments confirm this is a
- necessary, but not sufficient, condition
- This provides a means for researchers to rule out spatial
- discretizations that do not have thick diffusion limit
- May be viewed as an unusual type of code verification
- Especially useful when a spatial discretization (method, mesh,
- coordinate system) makes analysis difficult or intractable

Wingate

On the Slow Dynamics in the Arctic Ocean

Beth A. Wingate/CCS-2

Computational Physics and Applied Mathematics
Capability Review June 8-10, 2010

Overview

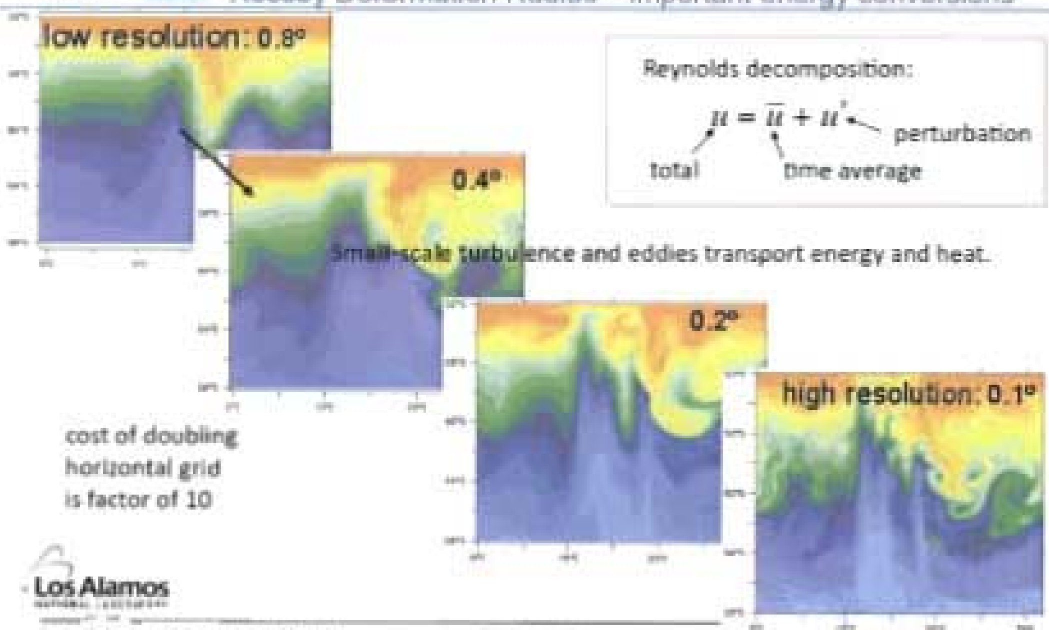
- Summary: Ocean model resolution is becoming fine enough that, especially at high latitudes, they will soon violate one of their foundational mathematical assumptions: the hydrostatic balance. In this work I present a multiscale-in-time approach that reveals a new kind of physics in the Arctic and suggests a new numerical strategy for efficiently computing nonhydrostatic ocean models.
- Funding: ASCR-Multiscale for the mathematical theory, BER-climate change for numerical algorithm development
- Programs the work supports: ASCR mission in multi-scale mathematics and the BER mission in climate model development and climate change science.
- Capabilities the work supports: LANL's interests in applied math and numerical capability as well as the COSIM project in ocean modeling and high latitude science
- Other LANL collaborators: Mat Maltrud (T-3), Matthew Hecht (CCS-2), Elizabeth Hunke (T-3) , and Rob Lowrie (CCS-2)
- Competitors: Ocean modelling teams (NOAA/NASA/International)

Take-home message: rethinking slow dynamics in the ocean

- Using multiscale-in-time mathematics I show that in the Arctic the *slow dynamics evolves independently of the fast and that it is nonhydrostatic*.
- I derive *new equations for the slow nonhydrostatic dynamics* in the Arctic that involves a projection operator.
- Numerical simulations and observations support the theory
- The projection operators, used in concert with the Newton Krylov framework, are a path forward to taking large time steps even with nonhydrostatic equations.
- Key Point: There are slow, nonhydrostatic dynamics in the Arctic. The projection operator, generalizable to all 3 limits found in the ocean, is the key to taking large time steps in nonhydrostatic ocean models.

The example of POP-α:

At IPCC resolutions most ocean models do not resolve the Rossby Deformation Radius – important energy conversions



Reynolds decomposition:

$$u = \overline{u} + u'$$

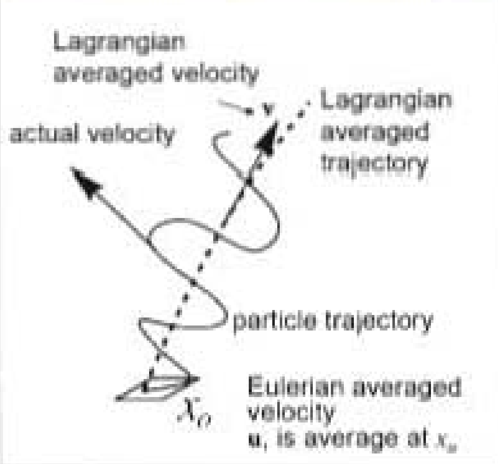
total — time average — perturbation

Small-scale turbulence and eddies transport energy and heat.

cost of doubling horizontal grid is factor of 10

Overview of the LANS-α model : Lagrangian versus Eulerian (GLM)

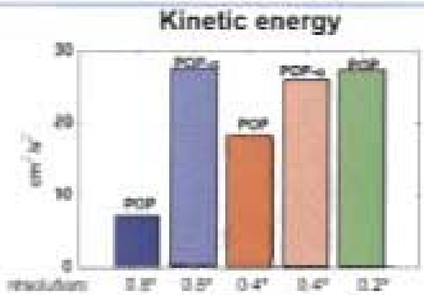
1. Two landmark papers by Andrews and McIntyre (1978)
   - Eulerian means commute with spatial gradients
   - Lagrangian means commute with advection operators.
   - The difference between the Eulerian mean and the Lagrangian mean is the 'Stokes Drift'.
2. GLM is closed provided the statistical properties of the Lagrangian disturbance are prescribed.
3. LANS-α closes GLM when the nature of the fluctuations are not known
4. **Uses nonlinear dispersion versus dissipation**

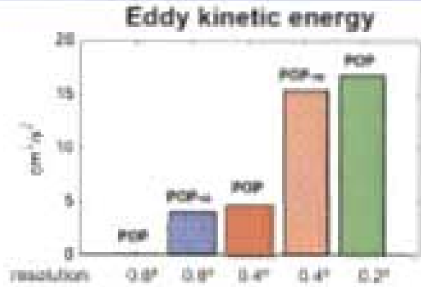


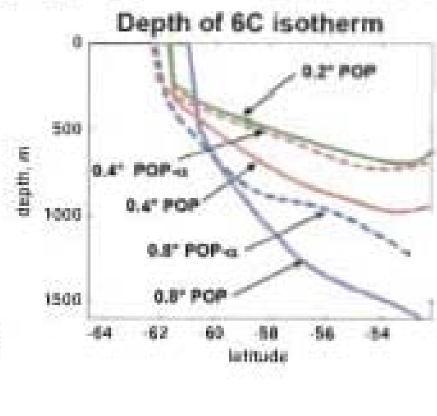
Andrews, D.G. and McIntyre M.E. "An exact theory for nonlinear waves on a Lagrangian mean flow" J. Fluid Mech, 89, 609-646, 1978
Andrews, D.G. and McIntyre M.E. "On wave-action and its relatives", 89, 647-664, 1978
Holm, D. D "Averaged Lagrangians and the mean effects of fluctuations in ideal fluid dynamics" Physica D, 170, 253-86, 2002

Example POP-α Results

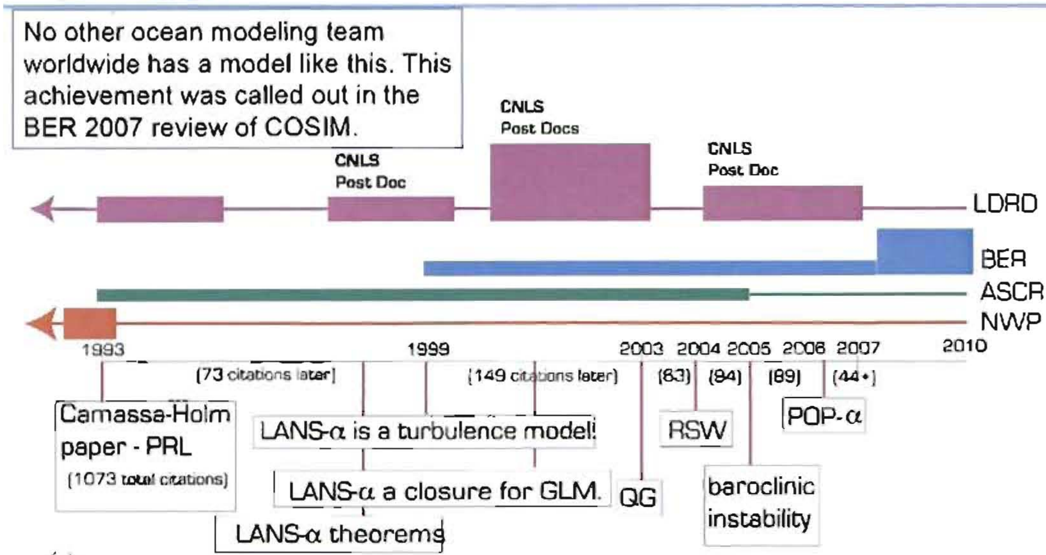
Hecht *et al.*, 2008 *Journal of Computational Physics,227,pp* 5691
Petersen *et al.*, 2008 *Journal of Computational Physics,227,pp* 5717







The example of POP-α: green line ¼ FTE, blue line ¼ FTE



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The rest of this talk: Slow dynamics in the Arctic

- Motivation for using multiscale in time methods – high latitudes
- Show that in the Arctic the slow dynamics evolves independently of the fast
- Derive new equations for the slow dynamics using a *projection operator* and show they are nonhydrostatic
- Show high resolution numerical solutions and observations in the Arctic to support the theory
- Suggest a path forward for investigating both the climate science implications and the derivation of new numerical schemes.

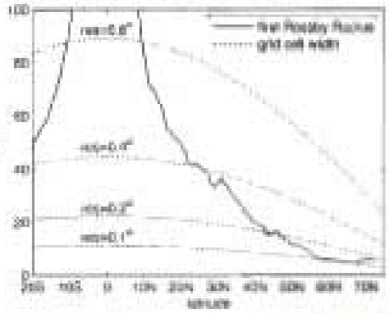
Motivation: IPCC class ocean models – a matter of convergence under grid refinement

Boussinesq equations and the hydrostatic primitive equations

$$\frac{D}{Dt}\mathbf{v}_H + f\hat{\mathbf{z}} \times \mathbf{v}_H + \rho_o^{-1}\nabla_H\, p = \nu\Delta\mathbf{v}_H$$
$$\frac{D}{Dt}w + \rho_o^{-1}\,\rho\, g + \rho_o^{-1}p_z = \nu\Delta w$$
$$\frac{D}{Dt}\rho - b\, w = \kappa\,\Delta\rho$$
$$\nabla\cdot\mathbf{v} = 0$$

State of the art IPCC class OGCMs

- In Models the flow is ***Hydrostatic*** – valid when horizontal grid spacing is much larger than vertical
- Important to resolve ***Deformation radius*** – gets smaller with latitude
- The higher the resolution, the harder it is to meet both these criteria.



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Dynamics at high latitudes

- Nearly solid body rotation
- Stratified flow, but weaker than stratification elsewhere.

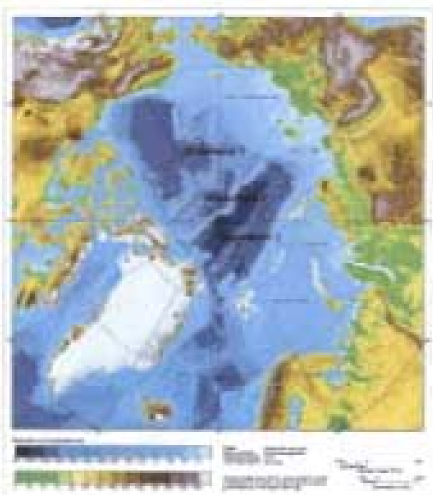


Image courtesy NOAA, 2007

Nondimensional Boussinesq Equations

$$\frac{D}{Dt}\mathbf{v} + \frac{1}{Ro}\hat{\mathbf{z}} \times \mathbf{v} + Eu\nabla\, p + \frac{1}{Fr}\rho\,\hat{\mathbf{z}} = \frac{1}{Re}\Delta\mathbf{v}$$

$$\frac{D}{Dt}\rho - \frac{1}{Fr}\,w = \frac{1}{Pr\,Re}\Delta\rho$$

$$\frac{D}{Dt}\,q = \frac{1}{Re}\left(-\frac{Ro}{Fr}\Delta\omega_3 + Ro\,\nabla\rho\cdot\Delta\omega\right) + \frac{1}{Pr\,Re}\left(\Delta\frac{\partial\rho}{\partial z} + Ro\,\omega\cdot\Delta(\nabla\rho)\right)$$

$$\begin{aligned} q &= \omega_{\mathbf{a}}\cdot\nabla\rho \\ &= \frac{\partial\rho}{\partial z} - \frac{Ro}{Fr}\omega_3 + Ro\,\omega\cdot\nabla\rho \end{aligned}$$

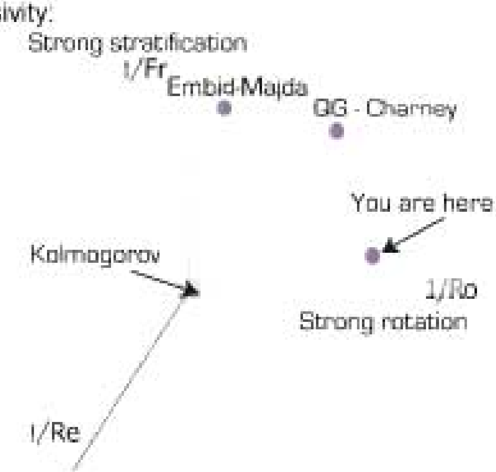
$$Ro = \frac{U}{fL},\quad Eu = \frac{P}{\rho U^2},\quad Re = \frac{UL}{\nu},\quad Pr = \frac{\nu}{\kappa},\quad Fr = \frac{U}{NL}$$

Conserved Quantities:
Total Energy and Potential Enstrophy

In the absence of viscosity and diffusivity:

$$\frac{1}{2}\frac{d}{dt}\langle|\mathbf{v}|^2 + \rho^2\rangle = 0$$

$$\frac{1}{2}\frac{d}{dt}\langle q^2\rangle = 0$$



where

$$\begin{aligned} q &= \omega_{\mathbf{a}}\cdot\nabla\rho \\ &= \frac{\partial\rho}{\partial z} - \frac{Ro}{Fr}\omega_3 + Ro\,\omega\cdot\nabla\rho \end{aligned}$$

Nonlocal form

$$\mathbf{u} = \begin{pmatrix} \mathbf{v} \\ \rho \end{pmatrix}$$

Embid and Majda, 1996, 1997
Schochet, 1994
Babin, Mahalov, Nicolaenko, 1996

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{1}{Ro} L_{Ro}(\mathbf{u}) + \frac{1}{Fr} L_{Fr}(\mathbf{u}) + B(\mathbf{u},\mathbf{u}) = \frac{1}{Re} D(\mathbf{u})$$
$$\mathbf{u}|_{t=0} = \mathbf{u}_0(\mathbf{x})$$

$$L_{Ro}(\mathbf{u}) = \begin{pmatrix} \widehat{\mathbf{z}} \times \mathbf{v} + \nabla\Delta^{-1}\omega_3 \\ 0 \end{pmatrix} \quad L_{Fr}(\mathbf{u}) = \begin{pmatrix} \widehat{\mathbf{z}}\ \rho + \nabla\Delta^{-1}(\frac{\partial \rho}{\partial z}) \\ -w \end{pmatrix}$$

$$B(\mathbf{u},\mathbf{u}) = \begin{pmatrix} \mathbf{v}\cdot\nabla\mathbf{v} - \nabla\Delta^{-1}(\nabla\cdot\mathbf{v}\cdot\nabla\mathbf{v}) \\ \mathbf{v}\cdot\nabla\rho \end{pmatrix} \quad D(\mathbf{u}) = \begin{pmatrix} \Delta\mathbf{v} \\ 1/Pr\Delta\rho \end{pmatrix}$$

Method of Multiple Scales

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_{\text{slow}}} + \frac{1}{\epsilon}\frac{\partial}{\partial t_{\text{fast}}} = \frac{\partial}{\partial t} + \frac{1}{\epsilon}\frac{\partial}{\partial \tau}$$

$$\mathbf{u}(\mathbf{x},t) = \mathbf{u}^0(\mathbf{x},t,\tau) + \epsilon\, \boxed{\mathbf{u}^1(\mathbf{x},t,\tau)}$$

To avoid secularity the second order term must be smaller than the leading order term.

$$|\mathbf{u}^1(\mathbf{x},t,\tau)| = o(\tau)$$

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Abstract form with slow and fast time scales

$$\frac{\partial \mathbf{u}^0}{\partial t} + \frac{\partial \mathbf{u}^1}{\partial \tau} + \mathcal{L}_{Ro}(\mathbf{u}^1) + \frac{1}{\epsilon}\left(\frac{\partial \mathbf{u}^0}{\partial \tau} + \mathcal{L}_{Ro}(\mathbf{u}^0)\right) = -\mathcal{L}_{Fr}(\mathbf{u}^0) - B(\mathbf{u}^0, \mathbf{u}^0) + D(\mathbf{u}^0) + \text{ hot}$$

To lowest order

$$\frac{\partial \mathbf{u}^0}{\partial \tau} + \mathcal{L}_F(\mathbf{u}^0) = \mathbf{0}$$

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Solve for the fast leading order solutions

$$\frac{\partial \mathbf{u}^0}{\partial \tau} + \mathcal{L}_F(\mathbf{u}^0) = \mathbf{0}$$

$$\mathbf{u}^0(\mathbf{x}, t, \tau) = e^{-\tau \mathcal{L}_F}\, \overline{\mathbf{u}}(\mathbf{x}, t).$$

The order 1 solution is a function of the leading order solution:

$$\frac{\partial \mathbf{u}^1}{\partial \tau} + \mathcal{L}_F(\mathbf{u}^1) = -\left(\frac{\partial \mathbf{u}^0}{\partial t} + \mathcal{L}_S(\mathbf{u}^0) + B(\mathbf{u}^0, \mathbf{u}^0) - D(\mathbf{u}^0)\right)$$

Solve with Duhammel's formula:

$$\begin{aligned} e^{-\tau \mathcal{L}_F} \mathbf{u}^1 &= \mathbf{u}^1(\mathbf{x}, t, \tau)|_{\tau=0} - \tau \frac{\partial \overline{\mathbf{u}}}{\partial t}(\mathbf{x}, t) \\ &\quad - \int_0^\tau e^{s \mathcal{L}_F} \left[\mathcal{L}_S(e^{-s\mathcal{L}_F}\overline{\mathbf{u}}) + B(e^{-s\mathcal{L}_F}\overline{\mathbf{u}}, e^{-s\mathcal{L}_F}\overline{\mathbf{u}}) - D(e^{-s\mathcal{L}_F}\overline{\mathbf{u}})\right] ds) \end{aligned}$$

Then use the method of fast wave averaging

Where $\overline{\mathrm{u}}$ solves:

$$\frac{\partial \overline{\mathrm{u}}}{\partial t}(\mathrm{x}, t) = -\lim_{T\to\infty}\frac{1}{T}\int_0^T e^{-s\mathcal{L}_F}\left[\mathcal{L}_S(e^{-s\mathcal{L}_F}\overline{\mathrm{u}}) + B(e^{-s\mathcal{L}_F}\overline{\mathrm{u}}, e^{-s\mathcal{L}_F}\overline{\mathrm{u}}) - D(e^{-s\mathcal{L}_F}\overline{\mathrm{u}})\right] ds,$$
$$\overline{\mathrm{u}}(\mathrm{x}, t)|_{t=0} = \mathrm{u}_0(\mathrm{x}).$$

And therefore, the solution to leading order is

$$\mathbf{u}^{\epsilon}(\mathbf{x}, t) = e^{-t/\epsilon \mathcal{L}_F}\overline{\mathrm{u}}(\mathbf{x}, t) + o(1).$$

And since the fast linear operator is skew-Hermitian, $\overline{\mathrm{u}}$ has an orthogonal decomposition into fast and slow components:

$$\overline{\mathrm{u}}(\mathbf{x}, t) = \overline{\mathrm{u}}^S(\mathbf{x}, t) + \overline{\mathrm{u}}^F(\mathbf{x}, t)$$

Using the fact that $\mathcal{L}_F(\overline{\mathrm{u}}^S) = 0$, the leading order solution looks like,

$$\mathbf{u}^{\epsilon}(\mathbf{x}, t) = \overline{\mathrm{u}}^S(\mathbf{x}, t) + e^{-t/\epsilon \mathcal{L}_F}\overline{\mathrm{u}}^F(\mathbf{x}, t) + O(1).$$

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The eigenvalues and eigenfunctions of the leading order equations

Therefore, study the solutions of the linear problem:

$$\frac{\partial \mathrm{u}^0}{\partial \tau} + \mathcal{L}_F(\mathrm{u}^0) = 0$$

$$\mathbf{u} = \mathbf{r}\ exp\left[i\mathbf{k}\cdot\mathbf{x} - i\omega(k)t\right]$$

$$\omega = 0, 0, \pm\frac{m}{|k|}$$

Notice that there is a dispersive mode with zero frequency.

By direct computation here is the fast wave averaged equation:

$$\bar{\mathbf{u}}(\mathbf{x},t) = \sum_{\mathbf{k}} \sum_{\alpha=-1}^{1} e^{i\mathbf{k}\cdot\mathbf{x}} \sigma_{\mathbf{k}}^{(\alpha)}(t)\mathbf{r}_{\mathbf{r}}^{\alpha}.$$

Compute the evolution equation for the Fourier amplitudes

$$\frac{d\sigma_{\mathbf{k}}^{\alpha}}{dt} + \sum_{\mathbf{k}_i,\ \alpha\ \text{resonant}} B_{(\mathbf{k}',\mathbf{k}'',\mathbf{k})}^{(\alpha',\alpha'',\alpha)} + \sum_{\omega_{(\mathbf{k})}^{(\alpha')}=\omega_{(\mathbf{k})}^{(\alpha)}} L_{(\mathbf{k})}^{(\alpha,\alpha')}\sigma_{(\mathbf{k})}^{(\alpha')} = \sum_{\omega_{(\mathbf{k})}^{(\alpha')}=\omega_{(\mathbf{k})}^{(\alpha)}} D_{(\mathbf{k})}^{(\alpha,\alpha')}\sigma_{(\mathbf{k})}^{(\alpha')}$$

The slow dynamics evolves independently of the fast

$$B_{(k',k'',k)}^{(\alpha',\alpha'',\alpha)} = \frac{i}{2}\left[(\mathbf{v}_{\mathbf{k}'}^{\alpha'}\cdot k'')(\mathbf{r}_{\mathbf{k}''}^{\alpha''},\mathbf{r}_{\mathbf{k}}^{\alpha}) + (\mathbf{v}_{\mathbf{k}''}^{\alpha''}\cdot k')(\mathbf{r}_{\mathbf{k}'}^{\alpha'},\mathbf{r}_{\mathbf{k}}^{\alpha})\right] \qquad (\mathbf{k}\neq\mathbf{0})$$
$$B_{(k',k'',k)}^{(\alpha',\alpha'',\alpha)} = \frac{i}{2}\left[(\mathbf{v}_{\mathbf{k}'}^{\alpha'}\cdot k'')\theta_{\mathbf{k}''}^{\alpha''} + (\mathbf{v}_{\mathbf{k}''}^{\alpha''}\cdot k')\theta_{\mathbf{k}'}^{\alpha'}\right]\theta_{\mathbf{k}}^{\alpha} \qquad (\mathbf{k}=\mathbf{0})$$

Three wave resonances means we must choose k' and k" such that

$$\mathbf{k}' + \mathbf{k}'' = \mathbf{k}, \quad \omega_{\mathbf{k}'}^{\alpha'} + \omega_{\mathbf{k}''}^{\alpha''} = 0.$$

You can show that the interaction coefficients are zero for the fast-fast interaction. Which means that the *slow dynamics evolves independently of the fast*.

Derive the equation for the slow dynamics

Knowing the slow dynamics evolves independently of the fast we can find the equations for the slow dynamics by projecting the solution and the equations onto the null space of the fast operator $\mathcal{N}(L_F)$. Then the fast wave averaged equation for the slow modes becomes,

$$\frac{\partial \overline{\mathbf{u}}}{\partial t} + P\Big(L_S(\overline{\mathbf{u}}) + B(\overline{\mathbf{u}}, \overline{\mathbf{u}}) - D(\overline{\mathbf{u}})\Big) = \mathbf{0}$$
$$\overline{\mathbf{u}}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) \in \mathcal{N}(L_F),$$

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The null space of the fast operator

$$\begin{aligned} -v + p_x &= 0, \\ -u + p_y &= 0, \\ p_z &= 0, \\ \nabla_H \cdot \mathbf{v}_H &= 0. \end{aligned}$$

$$\mathbf{u}^S = P\mathbf{u} = \begin{pmatrix} \langle \mathbf{v}_H \rangle_z - \nabla_H \Delta_H^{-1} (\nabla_H \cdot \langle \mathbf{v}_H \rangle_z) \\ \langle w \rangle_z \\ \rho \end{pmatrix}$$

where

$$\langle f \rangle_z = \frac{1}{2\pi} \int_0^{2\pi} f(x, y, z)\, dz$$

The new slow equations challenge our ideas of fast and slow dynamics in the ocean. They are:

$$\frac{\partial \mathbf{v}_H}{\partial t} + \mathbf{v}_H \cdot \nabla_{\mathbf{H}} \mathbf{v}_H + \nabla_{\mathbf{H}} p = \frac{1}{Re} \Delta_H \mathbf{v}_H \qquad \text{2-D}$$

$$\frac{\partial w}{\partial t} + \mathbf{v}_H \cdot \nabla_{\mathbf{H}} w = \frac{1}{Re} \Delta_H w - \frac{1}{Fr} \langle \rho \rangle_z \qquad \text{2-D}$$

$$\frac{D\rho}{Dt} - \frac{1}{Fr} w = \frac{1}{Re} \frac{1}{Pr} \Delta \rho \qquad \text{3-D}$$

$$\nabla_{\mathbf{H}} \cdot \mathbf{v}_H = 0 \qquad \text{2-D}$$

$$\mathbf{u}^S(\mathbf{x}, 0) = \mathbf{u}_0^S(\mathbf{x}) \in \mathcal{N}(L_F)$$

$\mathbf{v} = \mathbf{v}(x, y, t), \rho = \rho(x, y, z, t)$, and $\nabla_H\, p = \nabla_H \Delta_H^{-1} \left(\nabla_H \cdot (\mathbf{v}_H \cdot \nabla_H \mathbf{v}_H) \right)$

With Conservation Laws

$$\frac{1}{2} \frac{d}{dt} \int_A |\mathbf{v}_H|^2 = 0$$

$$\frac{1}{2} \frac{d}{dt} \int_A \omega_3^S = 0$$

$$\frac{1}{2} \frac{d}{dt} \int_A (w^2 + \langle \rho \rangle_z^2) = 0$$

$$\frac{1}{2} \frac{d}{dt} \int_V q^2 = 0$$

$$\frac{1}{2} \frac{d}{dt} \int_V \hat{\rho}^2 = 0$$

where:

$$\hat{\rho} = \rho - \langle \rho \rangle_z$$

$$q = \frac{\partial \rho}{\partial z}$$

Conservation of the ratio of slow to fast energy:

Using the same arguments as Embid and Majda, 1997, there is *conservation in time of the slow to fast energy ratio*. This means the total energy conservation is composed of both slow and fast dynamics.

But the leading order potential enstrophy is composed only of the slow dynamics.

$$\frac{1}{2}\,\frac{d}{dt}\int_V (q^S)^2 = \frac{1}{2}\,\frac{d}{dt}\int_V (q)^2 = 0.$$

High resolution numerical simulations

White noise forcing. **Smith and Waleffe, JFM, 2002**

Hyperviscosity:

$$\text{momentum:} \qquad (-1)^{p+1}\nu_h(\Delta)^p \mathbf{v}$$

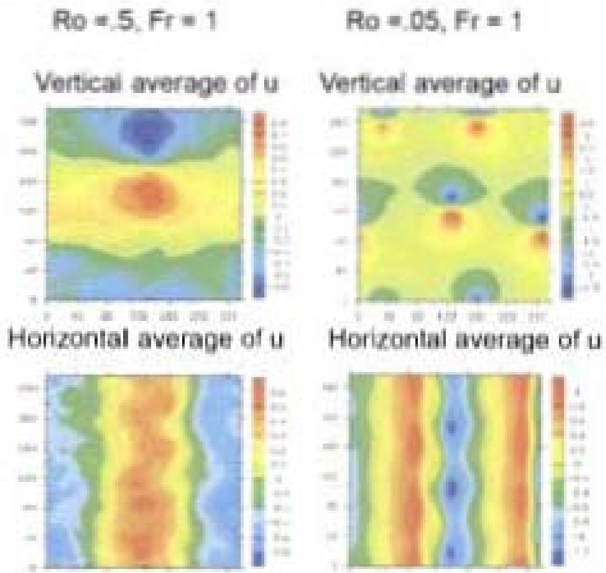
$$\text{buoyancy:} \qquad (-1)^{p+1}\kappa_h(\Delta)^p \rho$$

$$\nu_h = 2.5\left(\frac{E(k_m,t)}{k_m}\right)^{1/2} k_m^{2-2p}$$

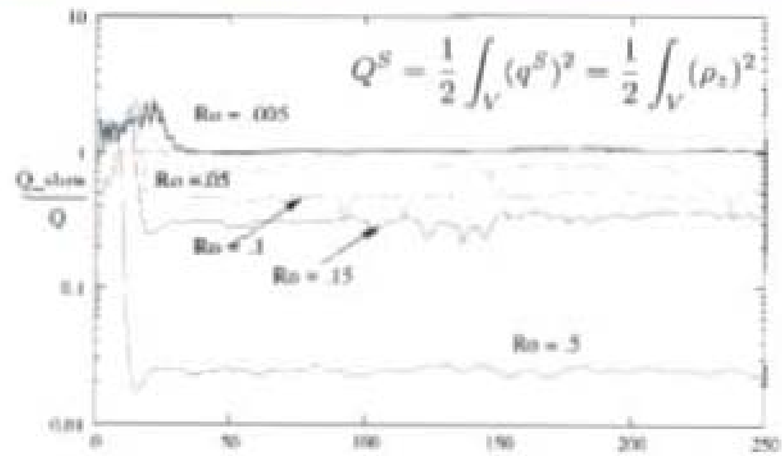
Random Forcing:

$$F(k) = \epsilon_f \frac{\exp(-.5(k-k_f)^2/s^2)}{(2\pi)^{\frac{1}{2}} s}$$

Forcing wave number 3

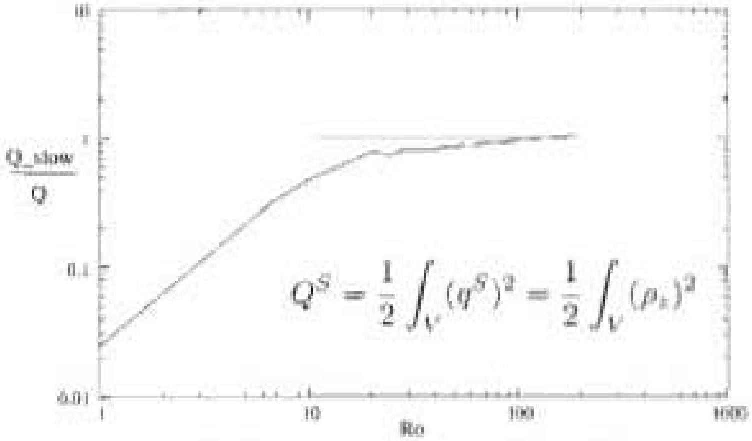


Ratio of Slow to Fast Potential Enstrophy



$$Q = \frac{1}{2}\int_V q^2 \qquad q = \frac{\partial \rho}{\partial z} - \frac{Ro}{Fr}\omega_3 + Ro\,(\omega \cdot \nabla \rho)$$

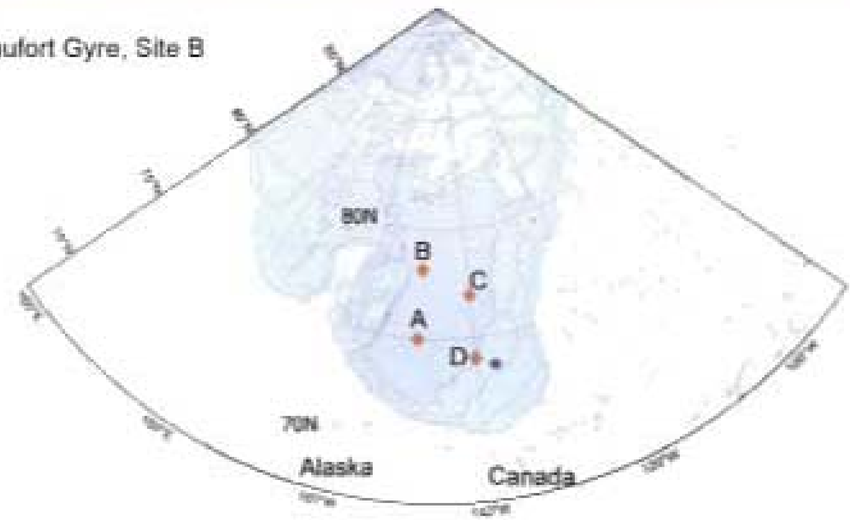
Dependence on Rotation Rate



$$Q = \frac{1}{2}\int_V q^2 \qquad q = \frac{\partial\rho}{\partial z} - \frac{Ro}{Fr}\omega_3 + Ro\,(\omega\cdot\nabla\rho)$$

Observations in the Arctic Basin
Mary Louise Timmermans, Yale University

Beaufort Gyre, Site B



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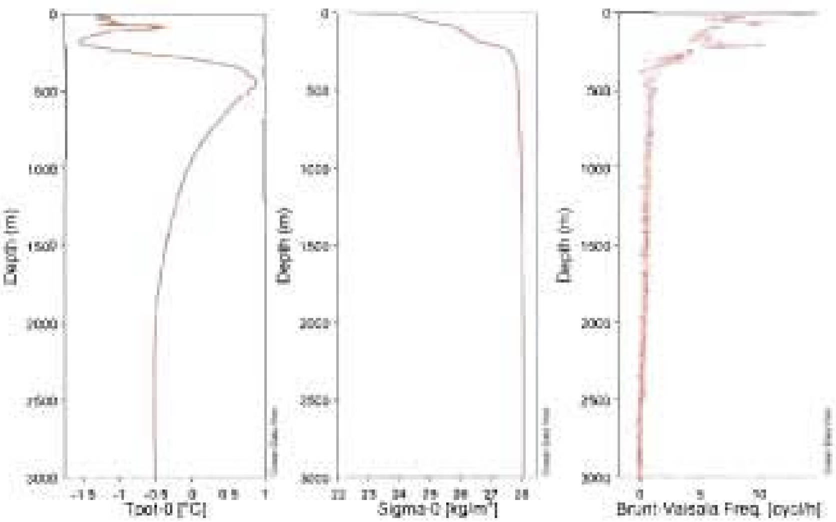
Typical Oceanic Conditions at site B



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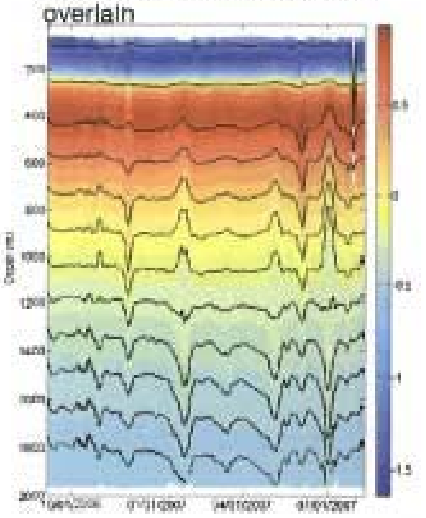
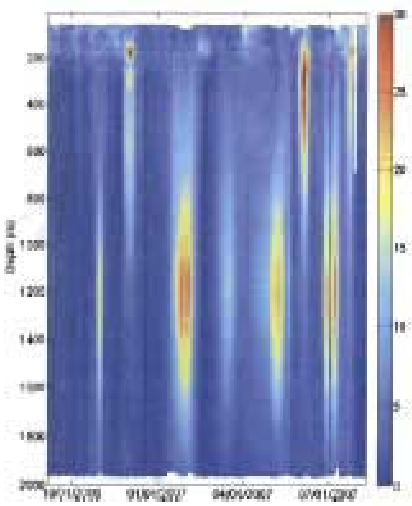
Mooring data show strong, deep vorticies in the Arctic.

depth-time section of potential temperature with isopycnals overlain



depth-time section of speed



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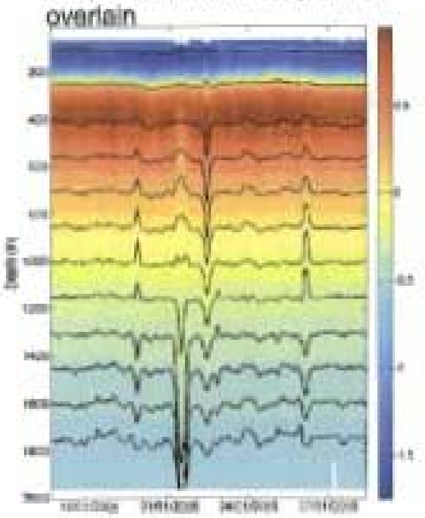
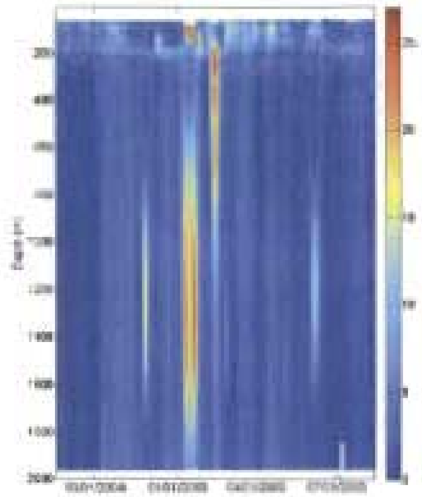
Mooring data: another time frame

depth-time section of potential temperature with isopycnals overlain



depth-time section of speed



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The projection operator could be the key to taking large time steps in a nonhydrostatic model of the future

- The slow dynamics evolves independently from the fast.
- New equations for the slow dynamics that predicts deep columns and new dynamics between the vertical kinetic energy and the buoyancy
- The theory is supported by numerical simulations and observations in the Arctic
- New operators that project any solution onto the null space of the fast operator (for new numerical schemes)

Future Directions

- Development of new asymptotic preserving *numerical schemes* with Rob Lowrie (LANL), Kate Evans (ORNL), Mark Taylor (SNL)
  - First Shallow Water Equations
- Investigation of high resolution hydrostatic numerical simulations with Mat Maltrud (LANL) & Wieslaw Maslowski (NPGS)
- Where in the world is Quasi-Geostrophy?
- Development of non hydrostatic numerical problems to test new parameterizations and study the fundamentals of the problem with Kate Hedstrom (IARC), Nicole Jeffery (LANL), Mary-Louise Timmermans (Yale)
- Refine Arctic parameterizations in current climate models with the CCSM polar climate working group ... because where there's a theory, there's a model
- Climate Science about the impact of the Arctic water mixmaster dynamics on deep water formation and the MOC.

Slow dynamics evolves independently of the fast

Triply periodic rotating and stratified Boussinesq equations

$$\frac{D}{Dt}\mathbf{v} + f\ \hat{\mathbf{z}} \times \mathbf{v} + \rho_o^{-1}\rho g\hat{\mathbf{z}} + \rho_o^{-1}\nabla p = \nu\Delta\mathbf{v},$$

$$\frac{D}{Dt}\rho - b\ (\hat{\mathbf{z}} \cdot \mathbf{v}) = \kappa\Delta\rho,$$

$$\nabla \cdot \mathbf{v} = 0,$$

$$\tilde{\rho} = \rho_o - b\ z + \rho$$

Alexander

Monte Carlo Methods

Francis J. Alexander / Institutes Office Division

Applied Mathematics and Computational Physics
Capability Review June 8-10, 2010

Applied Mathematics and Computational Physics
Capability Review
June 8-10, 2010

Monte Carlo methods are vital for many LANL applications

- This talk will focus on the MC algorithm development efforts at LANL
- Funding Sources:
  - ASC, LDRD, Office of Science (BES, ASCR ...), NIH, Gates Foundation ...
- MC supports numerous missions in the laboratory
  - BioSecurity (phylogenetics)
  - Energy Systems Modeling (rare events)
  - Materials
  - ASC
  - Nonproliferation
  - ... and many more
- MC is an integral tool for supporting all of the Science Pillars of the Laboratory:
  - Integrating Information Science and Technology for Prediction
  - Science of Signatures
  - Materials for the Future
- Algorithm Development Capability Extends Across the Laboratory
  - CCS, T, XCP, XTD, D
- Competitors:
  - Universities, LLNL, SNL

Applied Mathematics and Computational Physics Capability Review

Monte Carlo has a long history and rich tradition at LANL

- MC capability is both very broad and very deep
  - Supports a number of traditional enterprises
- Moving into exciting, new areas
  - Quantum inspired MC for classical optimization.
  - Optimal estimation
- Tight connection and collaborations to external community
- Synergy among / across disciplines
  - Physics + Biology + Control Theory + Math + Chemistry + ...

Applied Mathematics and Computational Physics Capability Review

Monte Carlo Research is being carried out across application domains

- Optimization
- Materials / Condensed Matter
- Optimal Estimation
- Transport
- Phylogenetics
- Systems Biology
- Statistical Sampling
- Kinetic MC
- Lattice QCD

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LANL is working with universities on the development of MC methods

- Brown (Faculty)
- MIT (Faculty, Postdocs, Students, MOU, Information Science, Algorithms and Methods Institute)
- Boston University (Faculty, Students)
- UCSB (Faculty, Postdoc)
- Johns Hopkins (Faculty)
- Indiana University (Faculty, Postdoc)
- Texas A&M (Faculty)
- Univ of New Mexico (Faculty)
- And others

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Sampler of MC research at LANL

- Brief overview of upcoming detailed talks
- Large Scale Eigenvalue Problems
- MC in HIV research
- Recent results in Lattice QCD
- Classical MC inspired by Quantum Mechanics
- Database Monte Carlo
- Optimal Estimation

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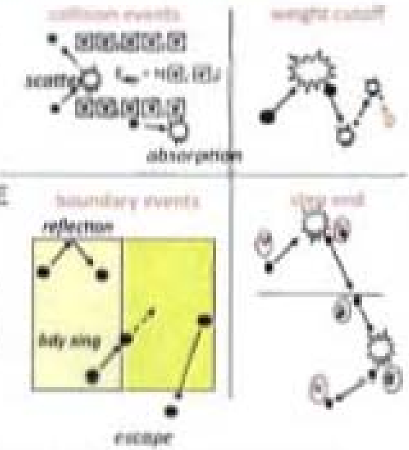
Implicit Monte Carlo (IMC) simulates thermal X-ray transport for nonlinear, time-dependent problems

- Material emits x-rays as T^4 and cools; transported x-rays reabsorb, heat material
- IMC tracks independent particles through mesh, tallies interactions with material in linearized, operator-split time step
- Roadrunner version preserves high-level distributed parallel structure; each Cell SPE tracks particles one at a time
- Challenges
  - random physical paths→random execution paths: hard to vectorize
  - randomly access mesh & material data sets too large for SPE local store
  - branch-heavy code
  - performance depends on physical state



McClarren and Urbatsch, "A modified implicit Monte Carlo method for time-dependent radiative transfer with adaptive material coupling," Journal of Computational Physics 228 (2009) 5669-5686

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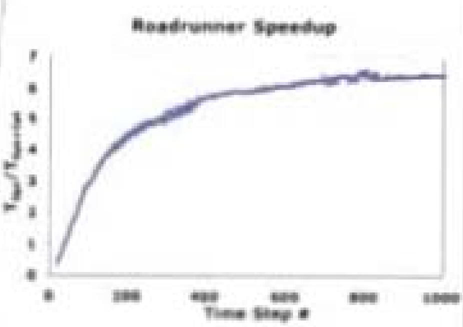
Test problem "double bend"
6x speedup over homogeneous machine



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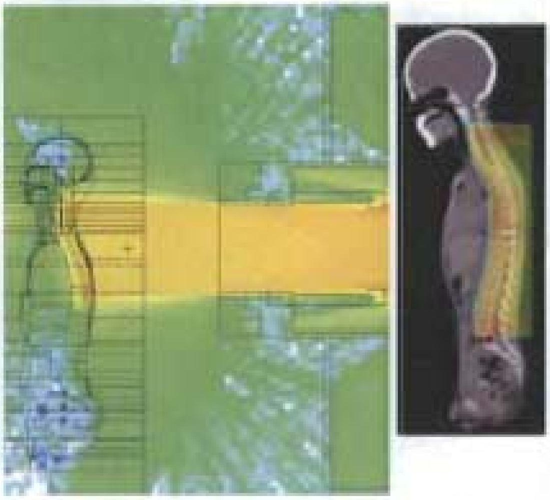
MCNP is used in Radiation Therapy Decisions

MCNPX is the most widely used general purpose Monte Carlo code for research in radiation cancer therapy.

The code is ideally suited for use in medical applications because of the accuracy of its physics models, the unique set of clinically relevant features, and the responsive support provided by the developers and the user community.

We used MCNPX to verify the Mass General Hospital Proton Center, and this information has gone into the design of the MDACC proton center and others, which are used to treat > 5K people a year.

Wayne Newhauser, Ph. D.
Dept of Radiation Physics
THE UNIVERSITY OF TEXAS
MD ANDERSON
CANCER CENTER



proton fluence and dose contours (arb units)

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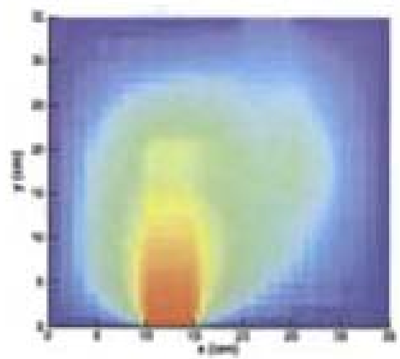
Hybrid Transport-Diffusion Methods for Implicit Monte Carlo Radiative-Transfer Simulations

- Realistic problems have both optically thick and thin regions



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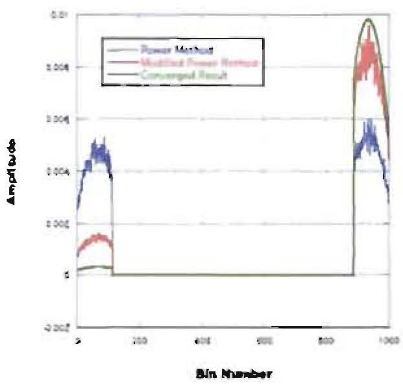
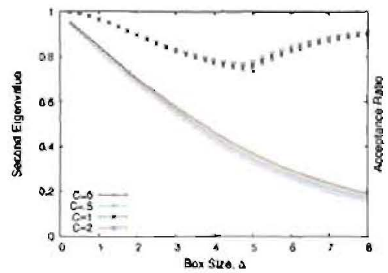
LANL has developed a new power method to calculate multiple extremal eigenvalues

T. E. Booth and J. E. Gubernatis, "Monte Carlo Determination of Multiple Extremal Eigenpairs," Phys. Rev. E, Volume 80, Issue 4, (2009)

Ultra-dimensional Matrices: 10^14 x 10^14





Monte Carlo Methods

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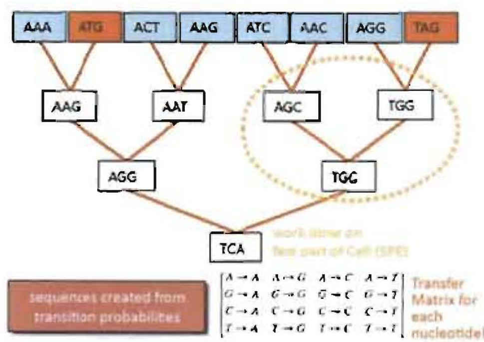
Viral Phylogenetics: Inheritance vs. Adaptation? HIV Vaccine design?

- Seeking correlation patterns of HIV viruses that are immunologically potent; giant "family tree" of HIV sequences
- 4000 HIV sequences (and more!)
- Each 10,000 nucleotides (HIV genome)
- Binary Trees built additively
  - Solve {s_1, s_2, s_3, s_4} then
  - Solve {s_1, s_2, s_3, s_4, s_5} ...
  - Work per tree: N^{3-4}
  - Search subset of *(2N-5)!!* trees
- For each set of sequences
  - Generate neighboring binary trees
  - Each tree communicated to Cell
  - Evaluate likelihood (p) on Blade
  - Move to a better neighborhood
- Aim: Find the most likely phylogenetic tree containing all *N* sequences

BILL & MELINDA GATES *foundation*

CHAVI



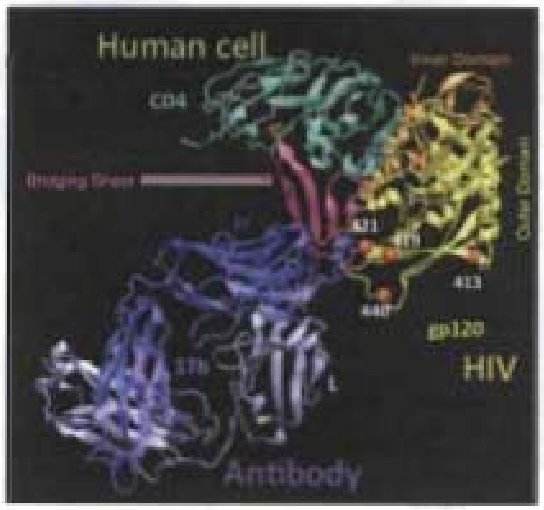
200,000 CPU hours on Roadrunner (continuing)

Future: Quantifying uncertainty propagation
Bayesian statistics
Parallel tree generation

Monte Carlo Methods

Preliminary Result: HIV Vaccine Implications

- CD4i region of viral envelope important for good immune response (inducing antibodies).
- Experiments underway to verify directly.



DataBase Monte Carlo for Variance Reduction

Estimate an expectation

$$J(\theta) = E[Y(\theta)]$$

θ is a parameter. We are under computational constraints described by:

- **Real-time:** Problem is known in advance, but θ is not known precisely. When θ is revealed, we must estimate $J(\theta)$ quickly
  - e.g. financial portfolio management, weather forecasting, radiation therapy, etc

OR

- **Repeated:** Estimate $J(\theta)$ for many different values of θ
  - e.g. financial portfolio risk assessment, uncertainty quantification, "what if" scenarios

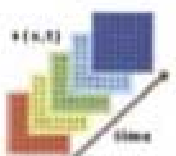
DBMC Strategy

- **Investment stage.**
  - Gathering information by brute force MC sampling at one or more nominal parameters $\theta_0, \theta_1, \dots \theta_M$
  - Information can be samples $Y(\theta_0)$, pathwise derivatives $Y'(\theta_0)$, etc.
- **Payoff stage.**
  - Estimation at θ in proximity of nominal $\theta_0, \theta_1, \dots \theta_M$.
  - Use much fewer samples at θ
  - Leverage investment stage information by use of variance reduction (e.g. Importance Sampling, Control Variates, Stratification).

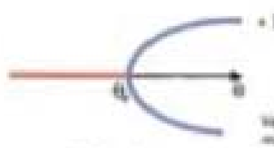
DBMC reduces variance even across phase transitions

2D Time-Dependent Ginzburg-Landau Model

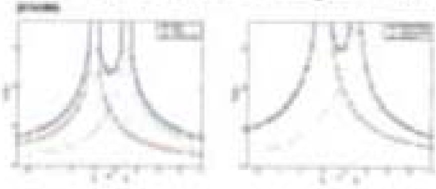
$$\frac{\partial\phi(x,t)}{\partial t} = D\Delta\phi(x,t) - V'(\phi(x,t)) + \eta(x,t)$$



(a) ϕ in space-time



(b) in phase space



Quantum Annealing for Classical Optimization

Optimization – Statistical Mechanics

- Optimization
  - Traveling Salesman, K-SAT, Graph Partitioning
  - Minimize Cost Function: min[H]
- Statistical Mechanics
  - Thermodynamics of Frustrated Systems, Spin Glass Ground State, Strongly Correlated Systems
  - Calculate the partition function: Z=Tr[exp(- H/kT)]

Typically hard computationally!

R. D. Somma, C. D. Batista, and G. Ortiz, A Quantum Approach to Classical Statistical Mechanics , Phys. Rev. Lett. 99, 030603 (2007)
R.D Somma, S. Boixo, H. Barnum, and E. Knill, Quantum Simulations of Classical Annealing Processes, Phys. Rev. Lett. 101, 130504 (2008)

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Quantum Annealing increases the effective dimension by one

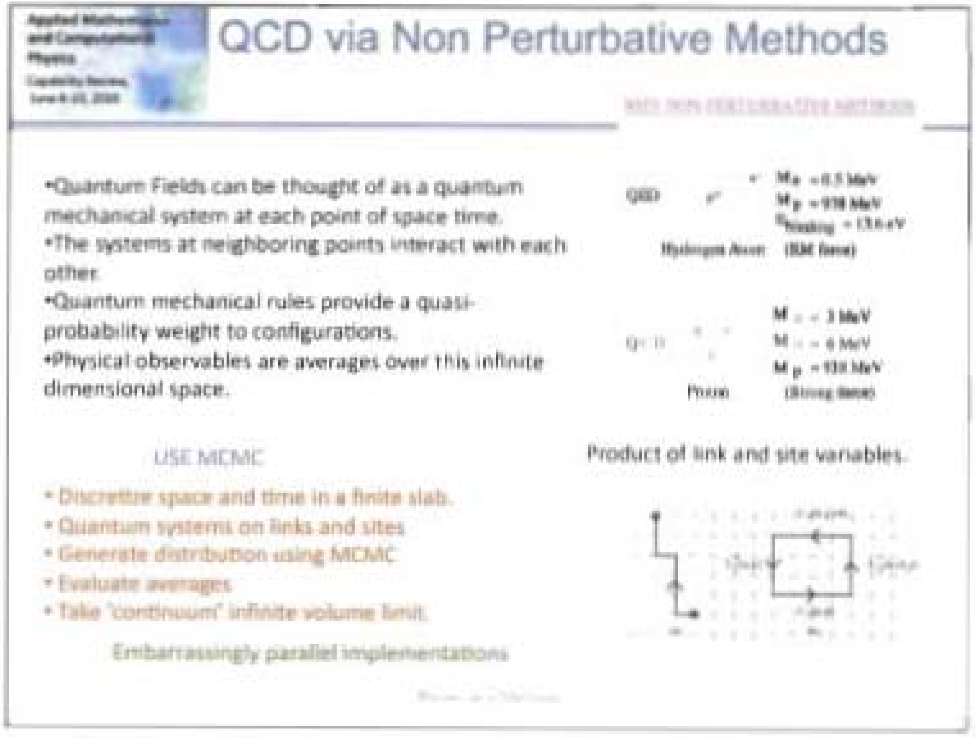
Map classical optimization/statistical mechanics problem to a quantum problem of the same spatial dimension D

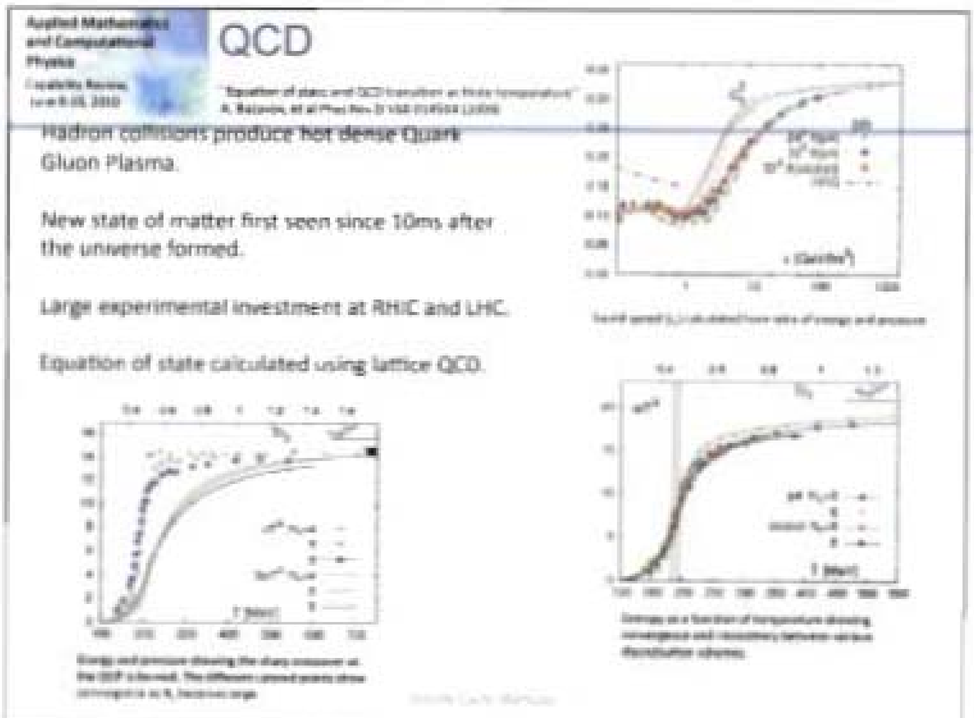
A D-dimensional quantum problem is equivalent to an effective D+1 dimensional classical problem

This mapping yields a better sampling/annealing strategy

$$H'_q(\gamma) = H - \gamma \sum_j \sigma^j_x \qquad (\gamma(\text{time}))$$

γ is decreased from a very large value (corresponding to $T \to \infty$) to $\gamma \approx 0$


QCD via Non Perturbative Methods
•Quantum Fields can be thought of as a quantum mechanical system at each point of space time.
•The systems at neighboring points interact with each other.
•Quantum mechanical rules provide a quasi-probability weight to configurations.
•Physical observables are averages over this infinite dimensional space.
Hydrogen Atom
Proton
Product of link and site variables.
USE MCMC
• Discretize space and time in a finite slab.
• Quantum systems on links and sites
• Generate distribution using MCMC
• Evaluate averages
• Take "continuum" infinite volume limit.
Embarrassingly parallel implementations


QCD
Hadron collisions produce hot dense Quark Gluon Plasma.
New state of matter first seen since 10ms after the universe formed.
Large experimental investment at RHIC and LHC.
Equation of state calculated using lattice QCD.

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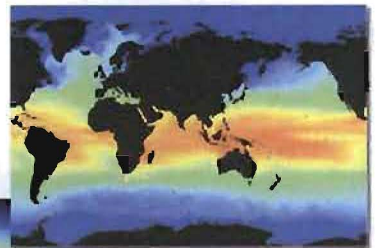
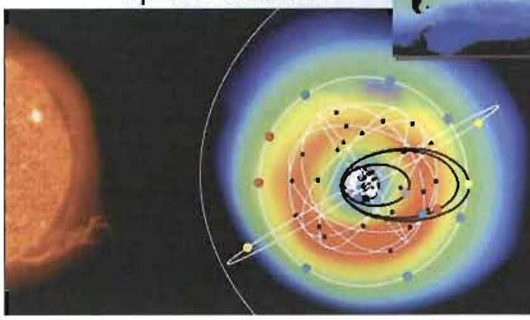
Optimal Estimation: Motivation

- Examples
  - Time Series
  - Ocean / Climate
  - Space Weather





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Optimal Estimation: Problem Statement

$$\mathbf{dx}(t) = \mathbf{f}(\mathbf{x}(t), t)dt + (2D)^{1/2}(\mathbf{x}, t)\,\mathbf{dW}(t)$$
$$\mathbf{x}(t_0) = \mathbf{x_0}.$$

$$\mathbf{y}(t_m) = \mathbf{h}(\mathbf{x}_m) + \boldsymbol{\epsilon}_m$$

$$\mathbf{x}_S(t) = E[\mathbf{x}(t)|\mathbf{y}_1, \ldots, \mathbf{y}_M]$$

Monte Carlo Methods

The standard approach has limitations

- Kalman/Bucy solved problems exactly for linear systems, Gaussian noise, additive Gaussian observation errors
- Scales badly with system size
- Ensemble Methods are popular– we're taking a different (complementary) approach
- Embrace the data
  - Use as much data as possible
  - Use complex dynamical models if necessary

LANL has developed a variety of new sampling algorithms to speed up inference

- Idea is to Map to the following form for likelihood (not a new idea!)

Prob(of a given history)= exp(-A(history))/Z

- Sampling techniques are new
  - Multigrid Monte Carlo
  - Langevin Monte Carlo
  - Fourier-Langevin
  - Hybrid Monte Carlo
  - Generalized Hybrid Monte Carlo
  - Adjoint Driven Monte Carlo
  - Cluster Algorithms

N. Gulbahce, F. J. Alexander, and G. Johnson, "Statistical Mechanics of Histories: a Cluster Monte Carlo Algorithm," Phys. Rev. E, **73, 026701, (2006)**

The future holds exciting, new directions to explore and exploit in MC research and development

- Certainly continue pursuing the methods described here
- More Hybrid MC /Deterministic Algorithms
  - Generalized Belief Propagation + MC for inference on large graphs
  - MC to inform Master equations (avoiding MC!)
    (poster session)
- Heterogeneous / Multicore systems
  - Can MC make a comeback in solving PDE's?
  - Computational Co-design
- Data Intensive Scientific Computing

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Thank you

Densmore

5/27/10

Hybrid Transport-Diffusion Methods for Implicit Monte Carlo Radiative-Transfer Simulations

Jeffery D. Densmore and Todd J. Urbatsch/CCS-2

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Accurately simulating radiative transfer is challenging.

- Implicit Monte Carlo (IMC) is an effective technique for simulating x-ray regime radiative transfer.
- However, radiative-transfer problems typically contain optically thick regions.
  - The mean-free path between collisions is small.
  - Collisions are primarily effective scatters (which represent radiation absorption and re-emission).
  - Particle histories consist of an excessive number of steps, and the resulting Monte Carlo simulation is inefficient.
- In contrast, the diffusion approximation is inexpensive and accurate in optically thick regions (but not in optically thin regions).

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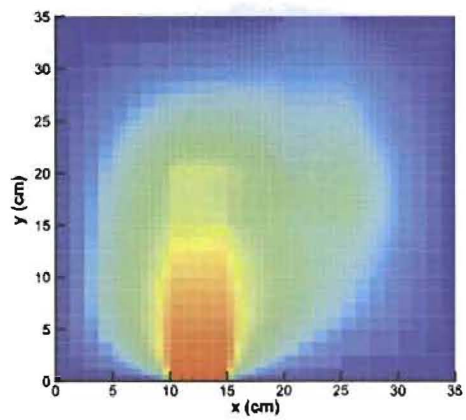
Realistic problems have both optically thick and thin regions.



At LANL, we have developed DDMC to increase the efficiency of IMC.

- One approach to improving the efficiency of IMC is a hybrid transport-diffusion method.
  - Use Monte Carlo simulation in optically thin regions.
  - Use the diffusion approximation in optically thick regions.
- This idea has led to our development of Discrete Diffusion Monte Carlo (DDMC).
  - Particles take discrete steps between spatial cells according to a discretized diffusion equation.
  - Each discrete step replaces many smaller Monte Carlo steps, resulting in a more efficient calculation.
  - DDMC is employed in optically thick regions and combined with Monte Carlo simulation in optically thin regions to form a hybrid method.

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Relevant LANL Publications

- J.D. Densmore, T.M. Evans, and M.W. Buksas, "A Hybrid Transport-Diffusion Algorithm for Monte Carlo Radiation-Transport Simulations on Adaptive-Refinement Meshes in *XY* Geometry," *Nucl. Sci. Eng.* **159**, 1-22 (2008).
- J.D. Densmore, T.J. Urbatsch, T.M. Evans, and M.W. Buksas, "A Hybrid Transport-Diffusion Method for Monte Carlo Radiative-Transfer Simulations," *J. Comp. Phys.* **222**, 485-503 (2007).
- G. Davidson, J.D. Densmore, A.K. Prinja, and J.E. Morel, "Asymptotically Correct Angular Distributions for Monte Carlo-Diffusion Interfaces," *Trans. Am. Nucl. Soc.* **94**, 517-520 (2006).
- J.D. Densmore, G. Davidson, and D.B. Carrington, "Emissivity of Discretized Diffusion Problems," *Ann. Nucl. Energy* **33**, 583-593 (2006).
- J.D. Densmore, "Interface Methods for Hybrid Monte Carlo-Diffusion Radiation Transport Simulations," *Ann. Nucl. Energy* **33**, 343-593 (2006).
- J.E. Morel and J.D. Densmore, "A Two-Component Equilibrium-Diffusion Limit," *Ann. Nucl. Energy* **31**, 2049-2057 (2004).
- T.J. Urbatsch, J.E. Morel, and J. Gulick, "Monte Carlo Solution of Spatially-Discrete Transport Equations, Part II: Diffusion and Transport-Diffusion," *Proc. Int. Conf. Mathematics and Computation, Reactor Physics, and Environmental Analysis in Nuclear Applications*, Madrid, Spain, September 27-30, 1999.

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DDMC allows order-of-magnitude efficiency gains for important multiphysics calculations.

- The Jayenne Project consists of
  - Todd Urbatsch, team leader
  - Jeff Densmore
  - Tim Kelley
  - Gabe Rockefeller
  - Kelly Thompson
- This project provides production-level, massively parallel IMC software for simulating high energy density physics phenomena:
  - supernova explosions
  - inertial confinement fusion
  - radiation flow experiments (Z, Omega, NIF)
- The hybrid transport-diffusion methods resulting from our research are being implemented into Jayenne Project software, enabling efficiency gains of up to several orders of magnitude while retaining the accuracy of IMC.

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DDMC is more efficient and accurate than competing methods.

- Random Walk (RW)
  - This is a well-known technique used in most IMC codes.
  - In RW, particles take macrosteps within a spatial cell according to an analytic diffusion solution.
  - Near cell boundaries or after certain events, RW is disabled and Monte Carlo simulation is employed instead.
  - Thus, RW provides smaller efficiency gains than DDMC.
- Implicit Monte Carlo Diffusion (IMD)
  - This method is under active development at LLNL.
  - IMD is similar to DDMC, except
    - it is based on a time-discretized diffusion equation, while DDMC is temporally continuous
    - the coupling to Monte Carlo simulation is less accurate than in DDMC

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Radiative Transfer

- The frequency-independent radiative-transfer equations are

$$\frac{1}{c}\frac{\partial I}{\partial t} + \Omega \cdot \nabla I + \sigma I = \frac{1}{4\pi}\sigma a c T^4$$

$$C_v \frac{\partial T}{\partial t} = \int \sigma I d\Omega - \sigma a c T^4$$

- Here,
  - $I(\mathbf{r},\Omega,t)$ is the radiation intensity
  - $T(\mathbf{r},t)$ is the material temperature
  - $\sigma(\mathbf{r},T)$ is the opacity
  - $C_v(\mathbf{r},T)$ is the heat capacity
  - a is the radiation constant
  - c is the speed of light

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Implicit Monte Carlo

- To simulate radiative transfer using IMC
  - the temporal domain is divided into a time-step grid $0<t_0<t_1<t_2\ldots$
  - the emission source is semi-implicitly approximated within each time step $t_n<t\le t_{n+1}$ using the material energy equation, which helps stabilize the calculation
  - the opacity is evaluated explicitly (i.e., at t_n)

Implicit Monte Carlo (continued)

- The resulting equations governing IMC are

$$\frac{1}{c}\frac{\partial I}{\partial t}+\Omega\cdot\nabla I+\sigma_a I=$$
$$\frac{1}{4\pi}\int(1-f_n)\sigma_a I(\mathbf{r},\Omega',t)d\Omega'+\frac{1}{4\pi}f_n\sigma_a acT_n^4$$

$$C_v\frac{\partial T}{\partial t}=\int f_n\sigma_a I d\Omega-f_n\sigma_a acT_n^4$$

where $0<f_n<1$ is the *Fleck factor.*

- Note that a fraction $1\text{-}f_n$ of collisions are now effective scatters.

Asymptotic Description of Optically Thick Regions

- Optically thick regions in radiative transfer are represented by the equilibrium diffusion limit:

$$\sigma \to \frac{\sigma}{\varepsilon}$$
$$c \to \frac{c}{\varepsilon}$$
$$C_v \to \varepsilon C_v$$
$$\varepsilon \to 0$$

- In this limit
  - the mean-free path is an $O(\varepsilon)$ quantity
  - the Fleck factor is an $O(\varepsilon^2)$ quantity, and thus most collisions are effective scatters

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Diffusion Approximation

- The asymptotic solution of the IMC equations under the equilibrium diffusion limit scaling yields the diffusion approximation,

$$\frac{1}{c}\frac{\partial \phi}{\partial t} - \nabla \cdot \frac{1}{3\sigma_n}\nabla\phi + f_n\sigma_n\phi = f_n\sigma_n acT_n^4$$

- Here, we have defined the scalar intensity as

$$\phi(\mathbf{r},t) = \int I(\mathbf{r},\Omega,t)d\Omega$$

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Asymptotically Correct Boundary Condition

- The corresponding boundary condition is

$$2\int_{\Omega\cdot\mathbf{n}<0} W(|\Omega\cdot\mathbf{n}|)I(\mathbf{r},\Omega,t)d\Omega = \phi + \frac{d}{\sigma_t}\mathbf{n}\cdot\nabla\phi$$

where **n** is the unit-outward normal vector on the boundary of the optically thick region, *d≈0.7104* is the *extrapolation distance* and *W* is a transcendental function well approximated by

$$W(\mu) \approx 0.91\mu + 1.635\mu^2$$

- This boundary condition can produce accurate solutions in the interior of optically thick regions regardless of the angular distribution of incident radiation.

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Discrete Diffusion Monte Carlo

- To develop the equations governing DDMC in an optically thick region
  - subdivide the region into a set of spatial cells (in most calculations this step has already been done)
  - apply a standard cell-centered discretization to the diffusion approximation
  - give the resulting equations a Monte Carlo interpretation

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DDMC for Interior Cells

- For a cell in the interior of the region, we have

$$\frac{1}{c}\frac{\partial \phi_i}{\partial t} + \left(\sum_j \sigma_{i\to j} + f_{n,i}\sigma_{n,i}\right)\phi_i = f_{n,i}\sigma_{n,i}acT_{n,i}^4 + \frac{1}{V_i}\sum_j \sigma_{j\to i}\phi_j V_j$$

where

- $\Phi_i(t)$ is the cell-averaged scalar flux
- the summations are over neighboring cells
- $\sigma_{i\to j}$ is the *leakage opacity* from cell i to cell j, for example in planar geometry,

$$\sigma_{i\to j} = \frac{2}{3\Delta x_i}\frac{1}{\sigma_{n,i}\Delta x_i + \sigma_{n,j}\Delta x_j}$$

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DDMC for Interior Cells (continued)

- This equation can be viewed as representing a time-dependent, infinite-medium transport problem.
  - Particles have no position or angular information but always know their current cell and time.
  - Particles can undergo "leakage" reactions to neighboring cells or be absorbed.
  - The source term consists of not only the usual IMC explicit emission source but also particles experiencing leakage reactions from neighboring cells.

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DDMC for Boundary Cells

- When a cell face coincides with the boundary of the region, the corresponding equation is instead

$$\frac{1}{c}\frac{\partial\phi_i}{\partial t}+\left(\sum_j\sigma_{i\to j}+\sigma_{i\to b}+f_{n,i}\sigma_{n,i}\right)\phi_i=f_{n,i}\sigma_{n,i}acT_{n,i}^4$$

$$+\frac{1}{V_i}\left(\sum_j\sigma_{j\to i}\phi_jV_j+\int_{A_{i,b}}\int_{\Omega\cdot\mathbf{n}<0}P_{i,b}(|\Omega\cdot\mathbf{n}|)\,|\Omega\cdot\mathbf{n}|\,I(\mathbf{r},\Omega,t)\,d\Omega\, d^2r\right)$$

DDMC for Boundary Cells (continued)

- Here,
  - $\sigma_{i\to b}$ is the leakage opacity for the face on the boundary
  - $P_{i,b}(\mu)$ is the *conversion probability*
- For example, in planar geometry

$$\sigma_{i\to b}=\frac{1}{\Delta x_i}\frac{2}{3\sigma_{n,i}\Delta x_i+6d}$$

$$P_{i,b}(\mu)=\frac{4}{3\sigma_{n,i}\Delta x_i+6d}\frac{W(\mu)}{\mu}$$

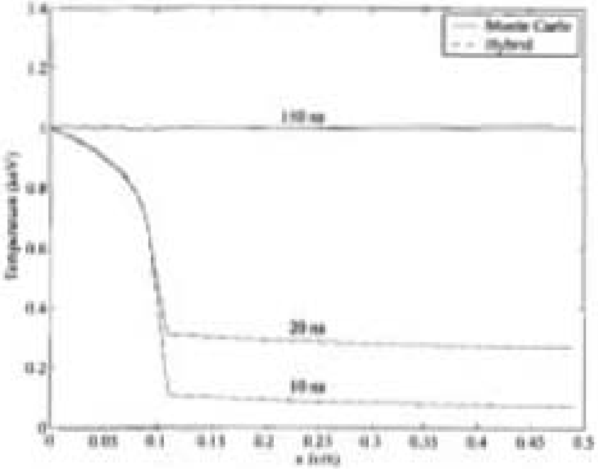
DDMC for Boundary Cells (continued)

- This equation shows how DDMC is coupled to Monte Carlo simulation, i.e., how "DDMC" particles are converted into "Monte Carlo" particles and vice versa.
  - DDMC particles leave the optically thick region and are converted into Monte Carlo particles according to $\sigma_{i\to b}$.
  - A Monte Carlo particle with direction $\mathbf{\Omega}$ incident on the boundary of the optically thick region enters the optically thick region and is converted into a DDMC particle with probability $P_{i,b}(|\mathbf{\Omega}\cdot\mathbf{n}|)$.
  - Unconverted Monte Carlo particles are returned to the adjacent optically thin region.

Numerical Results

- We now demonstrate the accuracy and increased efficiency, as compared to pure Monte Carlo simulation, of the hybrid transport-diffusion method based on DDMC with several test problems.
- First problem:
  - one-dimensional planar geometry
  - the leftmost region is optically thick, followed by an optically thin region
  - an isotropic intensity is incident on the left boundary
  - the hybrid method was approximately 20 times faster than pure Monte Carlo simulation

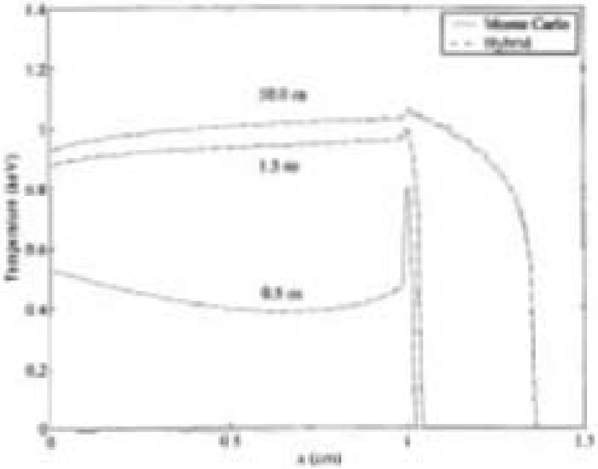
Numerical Results (continued)



Numerical Results (continued)

- Second Problem:
  - one-dimensional planar geometry
  - the leftmost region is optically thin, followed by an optically thick region
  - a normally directed intensity is incident on the left boundary, which tests the coupling between DDMC and Monte Carlo simulation
  - the hybrid method was over 10 times faster than pure Monte Carlo simulation

Numerical Results (continued)



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Numerical Results (continued)

- Third problem:
  - Two-dimensional Cartesian geometry
  - Steady state
  - Entire problem is optically thick except for an embedded void duct
  - An isotropic intensity is incident at the entrance of the duct
- This problem features an adaptive-refinement mesh.
  - Spatial cells may have multiple neighboring cells across each face.
  - This type of mesh is commonly employed in Eulerian hydrodynamics calculations.

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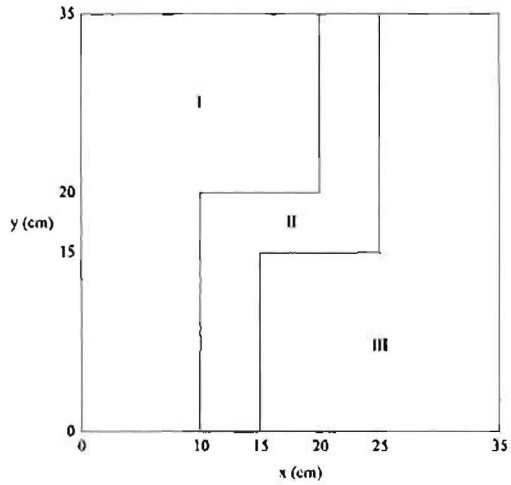
Numerical Results (continued)



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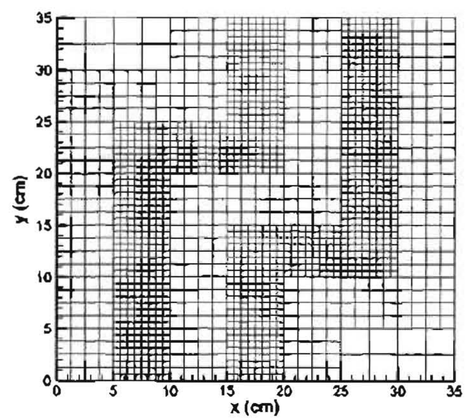
Numerical Results (continued)



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Numerical Results (continued)

- We also simulated this problem using RW with two different minimum step sizes.
  - λ = 5 mean-free paths (more efficient)
  - λ = 20 mean-free paths (more accurate)
- The hybrid method was over 300 times faster than pure Monte Carlo simulation.
- In contrast, RW was 4 (λ = 5) and approximately 1.5 (λ = 20) times faster than pure Monte Carlo simulation.
- We examine the radiation intensity in the row of cells just after the duct makes a turn to the right.

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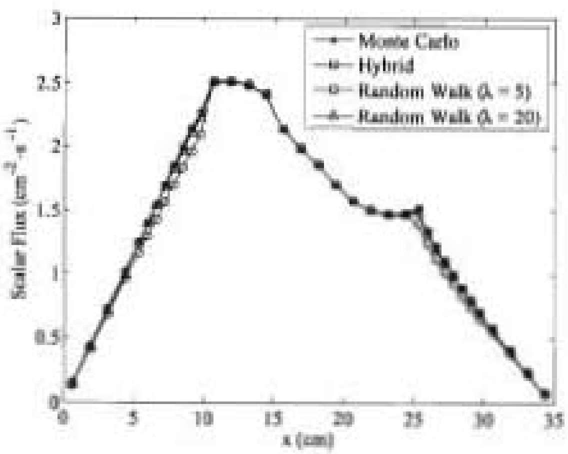
Numerical Results (continued)



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Conclusions

- We have developed a family of hybrid transport-diffusion methods for IMC radiative-transfer simulations.
- These hybrid methods combine DDMC in optically thick regions with Monte Carlo simulation in optically thin regions.
- We have specifically examined
  - one-dimensional planar geometry
  - two-dimensional Cartesian geometry (including adaptive-refinement meshes)
- We have demonstrated order-of-magnitude efficiency gains while retaining the accuracy of IMC.
- In addition, our hybrid methodology is more efficient than the commonly employed RW technique.
- We expect similar performance for realistic multiphysics applications.

Funding Sources, Status, and Future Work

- We are currently halfway through a 3-year LDRD.
  - Previous sources of funding include ASC and Weapons Supported Research.
- In the past 18 months, we have:
  - extended DDMC to one-dimensional spherical and two-dimensional cylindrical (including adaptive-refinement meshes) geometries
  - implemented the resulting hybrid transport-diffusion methods into Milagro, the Jayenne Project's stand-alone radiation-only IMC code

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Funding Sources, Status, and Future Work (continued)

- For the remainder of this fiscal year, we plan on:
  - extending DDMC to include multigroup frequency dependence
  - developing an automatic domain decomposition method for determining where to use DDMC instead of Monte Carlo simulation
  - also implementing this work into Milagro
- Next fiscal year, we plan on continuing our implementation through to Wedgehog
  - Wedgehog is the Jayenne Project's callable library that provides IMC capability to multiphysics application codes.
  - Wedgehog uses many of the same underlying components as Milagro, so this integration should be straightforward.

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Kelley

Implicit Monte Carlo Radiation Transport for Roadrunner

Tim Kelley
Applied Computer Science (CCS-7)
Los Alamos National Laboratory

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Roadrunner is enabling more accurate transport methods in simulations

- Monte Carlo is an essential transport simulation method
  - Often considered too expensive to use regularly
- Heterogeneous computing architectures like Roadrunner reduce the runtime costs of Monte Carlo simulation
  - These performance gains require code changes
- Joint effort between CCS-2 IMC team (Urbatsch, Densmore, Rockefeller, Thomson) and CCS-7 (Kelley, Henning)

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Outline

- description of Roadrunner architecture
  - changes it reflects in microarchitecture
  - changes it engenders in code
- overview of *Milagro* Implicit Monte Carlo transport
- adapting core particle transport to the Cell processor
  - dealing with memory hierarchy
  - adapting to instruction set architecture
- integrating Cell transport into regular MPI application

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Roadrunner combines Opteron CPUs with Cell coprocessors

- #1 on Top500
- first to sustained petaflop
- also very efficient— #3 on Green500
- hybrid processor architecture
  - Opteron server chips + FP-intensive Cell accelerators
  - usual hype: video game chips in supercomputer!
  - more accurate hype: SC chips in video games!!
- a glimpse of the near future

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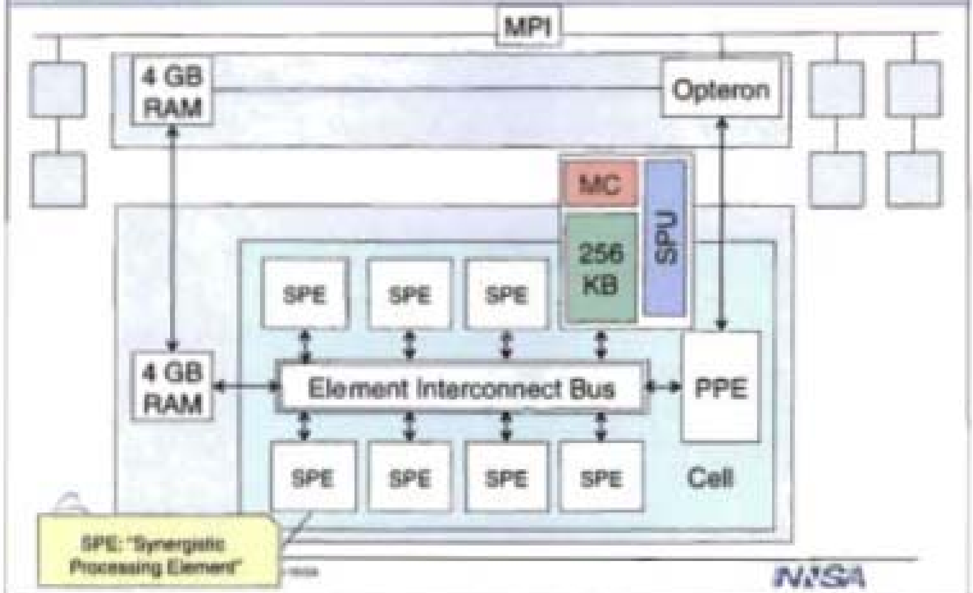
An app programmer's view of Roadrunner hybrid node: one Opteron + one Cell



Roadrunner gives us a jump on advanced architectures

- hierarchical concurrency on many cores and threads
  - how to partition and control programs over hybrid resources?
  - mix MPI, threads
  - other approaches: Map-Reduce, functional languages, PGAS?
- complex memory hierarchies
  - With RR, one *must* program the data motion (both weakness & strength)
- vectors are back
  - 128b now, 256-512b soon
  - much wider on GPUs (nearly—"SIMT" instead of SIMD)
- simple core architectures
  - little hardware tolerance for inexperienced programming
- limited support for established languages, paradigms

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Roadrunner challenges for codes

- find and implement hierarchical concurrency
- "strong" memory hierarchy: explicitly programmed memory control
  - disadvantage: you *must* program the data motion
  - advantage: you *can* program the data motion
- Cell SPE cores
  - limited address space—256 KB (code + data!)
    - exchange data with main memory
    - mfc_get(local, remote, how much, tag)
    - cf. MPI_Recv(local, how much, type, source, tag, comm, status)
  - instruction set architecture (almost) all vector
  - lots of registers
  - doesn't like branches

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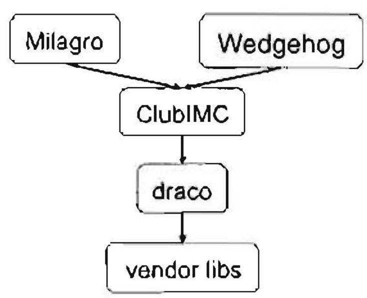
Implicit Monte Carlo simulates thermal X-ray transport for time-dependent, nonlinear problems

- Fleck & Cummings time discretization
  - effective scattering even in purely absorbing media
- object-oriented, generic C++
  - templated on mesh type, freq. type, particle type.
- transports particles 3D, meshes articulated in 1, 2, 3D
- supports Rage AMR
- two distributes parallel modes: mesh replicated, decomposed



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Heterogeneous reimplementation of production code began as a research project

- Two approaches:
  - evolve incrementally ("bottom up")
  - freely rewrite structures & algorithms ("top down")
- both kept existing large-scale MPI structure on hosts
- both decoupled particle generation from particle tracking
- similar performance gains at assessment
- different approaches to work
  - bottom up: Cell SPEs push particles one at a time
  - top down: Opterons generate work packets, any available processor pulls work from queues

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Cell challenges for Milagro

Worst Cell code ever?

- random access into large data sets
  - opacities, emission CDF, mesh connectivity
  - random, but slowly changing in (CPU) time
    - mean free path, ~1/[illegible]_a
  - strategy: proxy large data objects on SPE
    - just enough data for one mesh cell
- scalar code: one particle at a time
  - particles follow different physical paths, thus different execution paths
  - strategy: explicitly use half-full vectors
- much branching, conditional assignment
  - as much as ~1 branch/flop
  - strategy: eliminate branches

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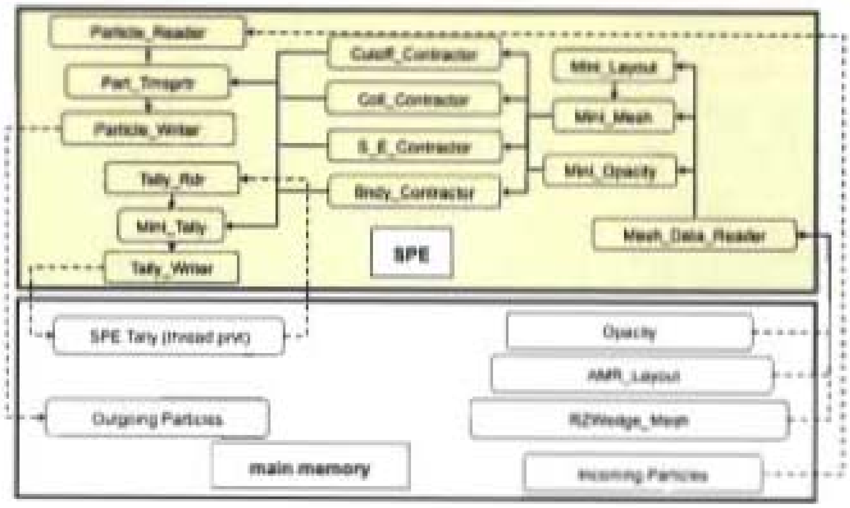
Proxies represent large data structures in SPE local store

core objects don't know about DMA



simplified view of data flow

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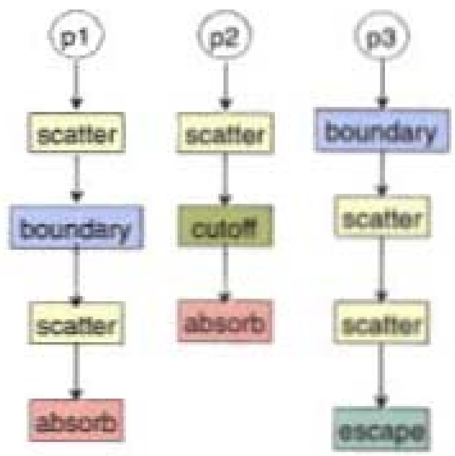
MC particles follow different execution paths

this is difficult to vectorize



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Avoid branches by computing both legs, then masking

simple changes lead to large performance gains

```
for i in (0,1):
  if a[i] > b[i]:
    c[i] = a[i]
  else:
    c[i] = b[i]
```

3.14159265359	5.43656365918	a
6.28318530718	2.71828182846	b

`cmpgt(a,b)` produces mask

00000...0000000	1111111...1111111

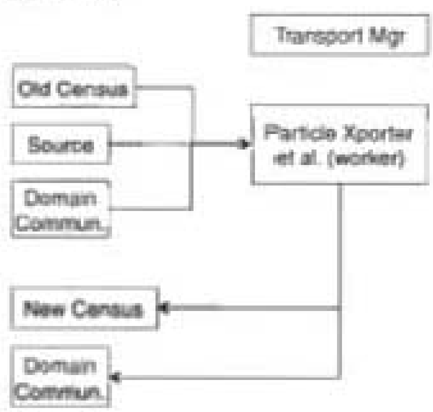
`(a AND mask) OR (b AND ~mask)` produces c:

6.28318530718	5.43656365918

To a full, heterogeneous application

how it works at present (roughly)

- transport manager coordinates the generation and transport of one particle at a time



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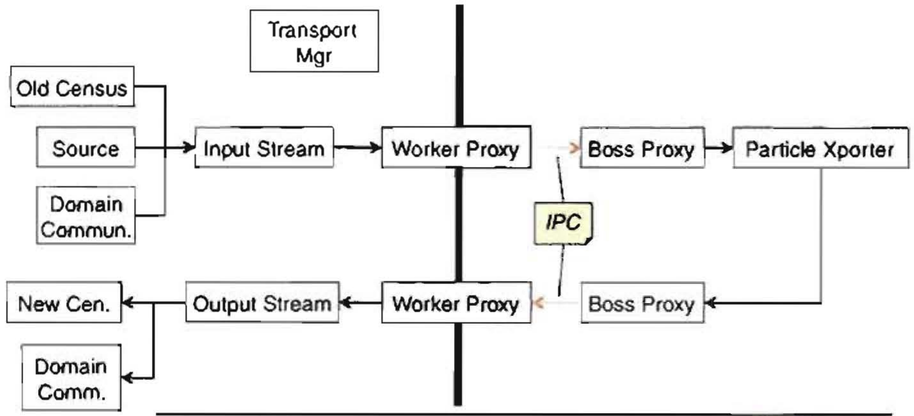
To a full, heterogeneous application
streams allow logical, physical decoupling

- Insert streams, proxies to decouple particle generation from transport
  - transport mgr no longer knows anything about pushing particles



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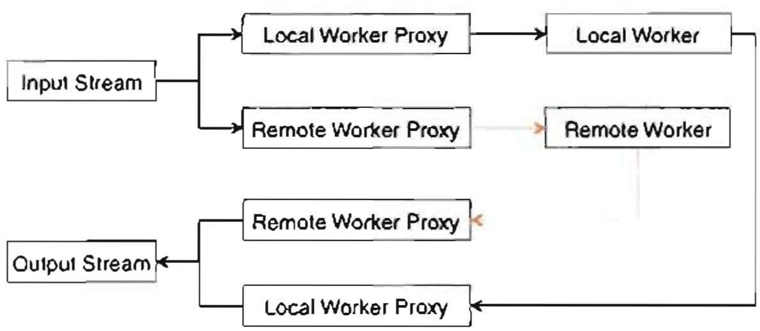
To a full, heterogeneous application
streams allow logical, physical decoupling

- streams form unified interfaces, accommodate multiple workers
- workers can be local, remote, or both
- this architecture extends well beyond Roadrunner



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Hybrid time step

who does what in each phase of a time step

	Opteron: host	PPE: manager	SPE: worker
initialize	• signal Cell to begin time step • prep sources, mesh, opacity • send mesh, opacity to Cell	• receive mesh/opacity • start SPE threads	• wait
transport	• generate particles (census, source, receive), send to PPE • recover spent particles from PPE, retire them (kill, census, send)	• synchronize particle I/O between host & workers	• load particles, mesh, opacity, tally data • transport particles – refresh mesh, tally, opacity data as needed • store particles, tallies
finalize	• signal Cell • wait for Tally finished signal • recover Tally, update material state	• join SPE threads • merge thread-private tallies • signal host	• idle

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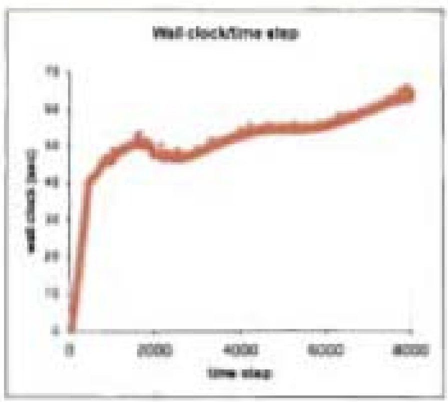
IMC performance depends on the problem

- different events take different times to process
  - cutoff event: a few stores
  - effective scatter event: thousands of instructions
- performance also varies within problem
  - number of MC steps & mix of step types changes as materials and fields evolve
- **this makes it difficult to summarize performance in a single number**



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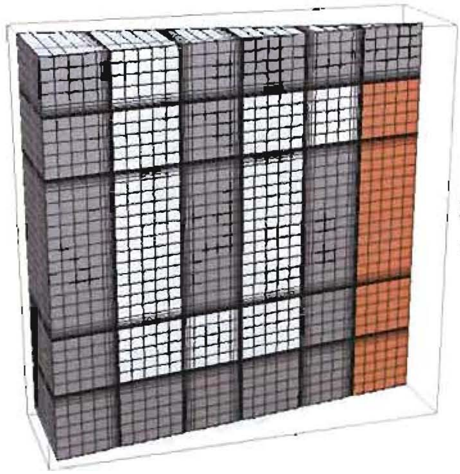
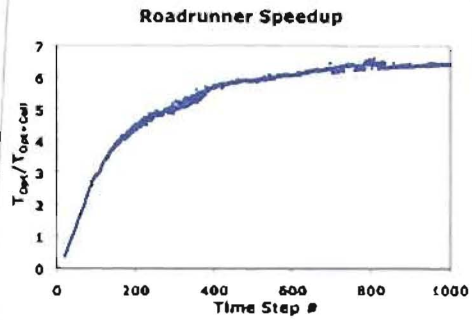
Success led to production code

6x speedup over homogeneous machine on "double bend" test problem





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Future work

- continue production code support
  - we have incorporated domain decomposition, random walk, material motion,
  - need to implement surface tallies, more mesh types
  - improve testing
- maintain our core capability
  - keep conventional implementation for methods R&D, next big transition
  - merge stream architecture back into trunk
- investigate advanced approaches, new platforms
  - Vector Monte Carlo for improved performance
  - advanced programming models: OpenCL
  - new languages: parallel Haskell? domain-specific languages?

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Applied Computer Science group

leading computational science onto novel computing architectures

- Four mutually-supporting teams:
  - algorithm+architecture co-design
    - jointly design machines and architectures
  - collaborative development
    - teach code teams to design and code for new architectures
  - programming models and languages
    - develop tools and domain-specific languages to ease architecture migration
  - data science at scale
    - large scale data-mining and data-intensive problems
- ***Actively training students, postdocs for a LANL & national pipeline to support DOE exascale initiative!***

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The End

- more Roadrunner information: http://www.lanl.gov/roadrunner
  - technical talks on system, all assessment codes
- thank you

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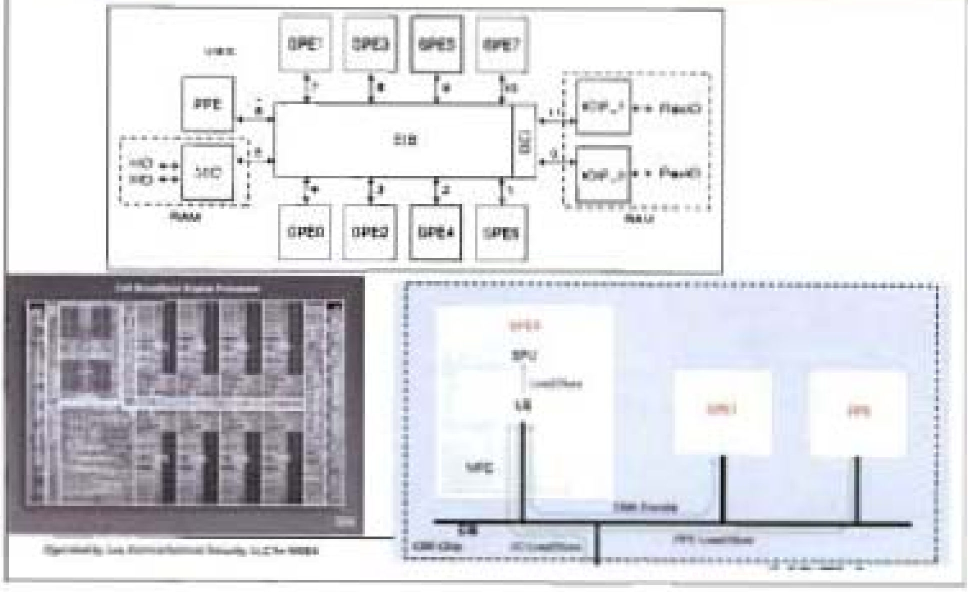
Cell Broadband Engine: hardware overview
from CBE programmer's Handbook, v. 1.0



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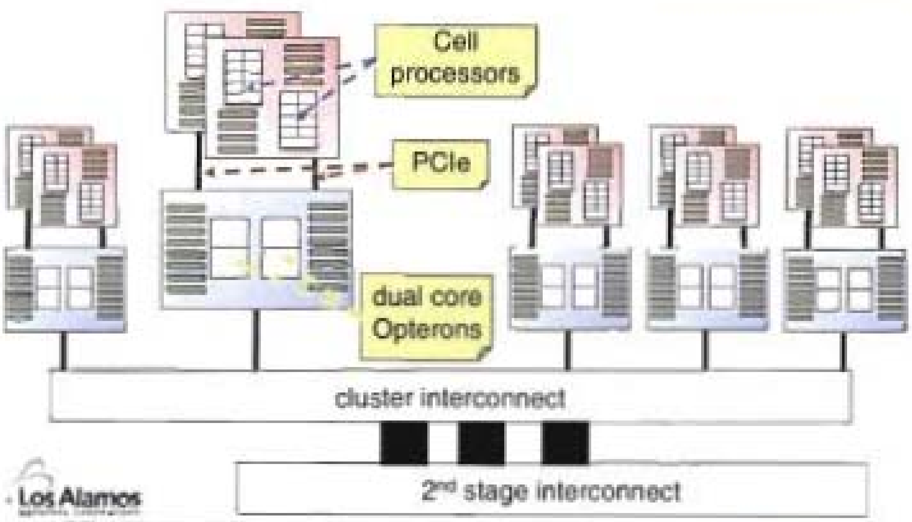
Cell processors accelerate an Opteron cluster



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The problem with SPE scalars...

compiler doesn't know where they are in vector, must shuffle & rotate

```
void add_two( double *a, double *b, double *c){
   *c = *a + *b;        // pointers, compiler doesn't know alignment of the doubles
   return;}
```

x86

```
movsd   (%rdi),  %xmm0
addsd   (%rsi),  %xmm0
movsd   %xmm0,  -8(%rsp)
ret
```

SPE

```
lqd $2,  0($3)
lqd $5,  0($4)
rotqby $2,$2,$3
rotqby $5,$5,$4
lqd $6,32($sp)
cdd $7,0($sp)
dfa $2,$2,$5
shufb  $6,$2,$6,$7
stqd   $6,32($sp)
bi $lr
```

Goorley

The MCNP code: Overview and Highlights

Tim Goorley, XCP-3 GL

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Overview - Presentation

- MCNP Overview
  - What is MCNP?
  - Mission
  - Sponsors
  - LANL Staff Effort
  - Competitors
- MCNP Applications Highlights & KUDOS Slides
  - How accurate simulations change decision making
- Future Development Efforts
  - MCNP will continue to develop to meet new sponsor needs

MCNP – Monte Carlo N - Particle

- 3D Monte Carlo many particle transport
- Large energy range (eV – 100s of GeV)
- ~400 Man-years of development
- ~350K lines of code
- 10K+ users world wide
- Parallel (MPI and omp)
- PC, Mac, Linux, Unix, Sun support
- Substantial V&V
- ~15K reference citations
- Export controlled+
  - Big deal, limits use in universities

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MCNP contains a lot of physics

- Incorporates other codes as libraries:

– LAHET (High Energy transport)	LANL
– CEM & LAQGSM (High energy transport)	LANL
– CINDER (Unstable Nuclei Database)	LANL
– ITS (Electron Transport)	SNL
– MARS (High Energy transport)	FNAL
– HETC (High Energy transport)	ORNL

- Utilizes Nuclear and Atomic Data
  - LANL, LLNL, BNL, EU, Japan

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MCNP has lengthy history

- MCNP code now more than 30 years old.
- MCNPX developed from 4B in 1996.
- Multiple releases of both codes in 2000s
- Code Merger began in July 2006 from MCNPX 2.6.B
  - Steering Committee is addressing alignment of XPC-3 and D-5 projects
- After >$3M, code 98% merged
- MCNP6 has been beta released outside LANL.

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Stockpile Stewardship, Threat Reduction, Non-Proliferation, Radiation Protection Missions

The XCP-3 team provides Monte Carlo particle transport capability in support of lab missions including stockpile stewardship, nonproliferation, threat reduction, and energy and environmental science. We deliver technology, methods, production quality codes, and training to sponsors, primarily U.S. federal agencies, through research, development, and maintenance of high quality software and documentation so that we can accurately predict the interaction of radiation with matter. This predictive capability plays a central role in tying weapon output simulation to the NTS database and is the nations foremost predictive tool for nuclear criticality safety simulations. Our success is measured by comparison with physical measurements (validation) and with applicable test problems (verification); by acceptance, usage, and scientific citation of our products; and by satisfaction first of our sponsors and then of others.

ADC: RM
Nov 2009

Stockpile Stewardship, Threat Reduction, Non-Proliferation, Radiation Protection

Many Mission Examples

- Stockpile Stewardship
  - Criticality Safety
  - Radiography
- Threat Reduction
  - Urban Consequences
- Non-Proliferation
  - Reactor Actinide Inventories
  - Portal Monitors
  - Active Interrogation
- Medical & Health Physics
  - Shielding Design
  - Radiology, Radiation Therapy

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$8.7M from Sponsors in FY10

- In FY2010 (in $K):

ASC-IC	3360
DHS-DNDO	1500
DTRA	1000
NA-42/24/other	800
NNSA (Criticality Safety)	600
NNSA-DTRA MOU	550
Campaign – 7	400
ASC-Capability	200
ASC- Urban Consequences	200
NEAMS (ANL)	100

Significant LANL Staff Effort

- Code Development (FTEs)
  - XCP-3: 11
  - D-5: 8
  - T-2: 1.5
  - LLNL: <1
  - AWE: proposed
- Code Reviewers
  - XCP-7, N, P, LANSCE, ISR (~ 2-3 FTE)
- Users:
  - 10K worldwide
  - ~1K @ US Gov agencies

Numerous Competitors

- Competitors

GEANT	CERN	many particle, high energy
TRIPOLI	CEA	electron & photon
PHITS	JAPAN	many particle
COG/TART	LLNL	neutron & photon
FLUKA	CERN	many particle, high energy
EGS 4.0	CANADA-NRC	electron & photon
ITS 5.0	SANDIA	electron & photon
SCALE	ORNL	criticality

- Spin Off Competitors

MCNP-BRL	ORNL	CAD geometry
MCNP-POLIMI	ORNL	decay data
A^3MCNP	Florida State U	SN Hybrid

MCNP Influencing Decisions

- Threat Reduction
  - Radiation Effects of 10 kT IND are manageable
- Non-Proliferation
  - Better Distinguish False Alarms
  - Detectable Quantities of materials
- Medical & Health Physics
  - Analysis of proposed therapies, general & specific
  - Shielding / Detector re-design to reduce dose
- Nuclear Regulation
  - Verify requests from industry
- Nuclear Rector Design and Analysis
  - Acceptability tests of faster design codes

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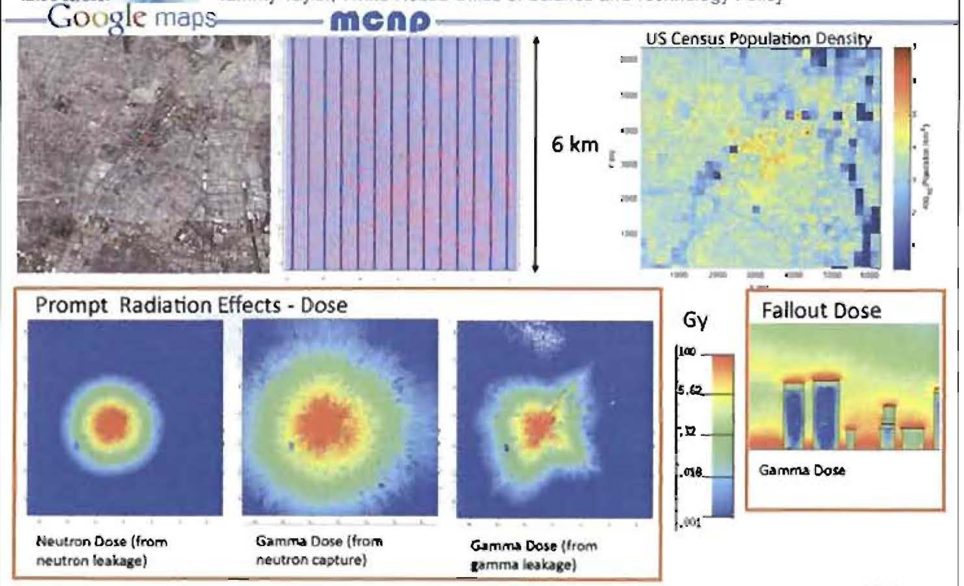
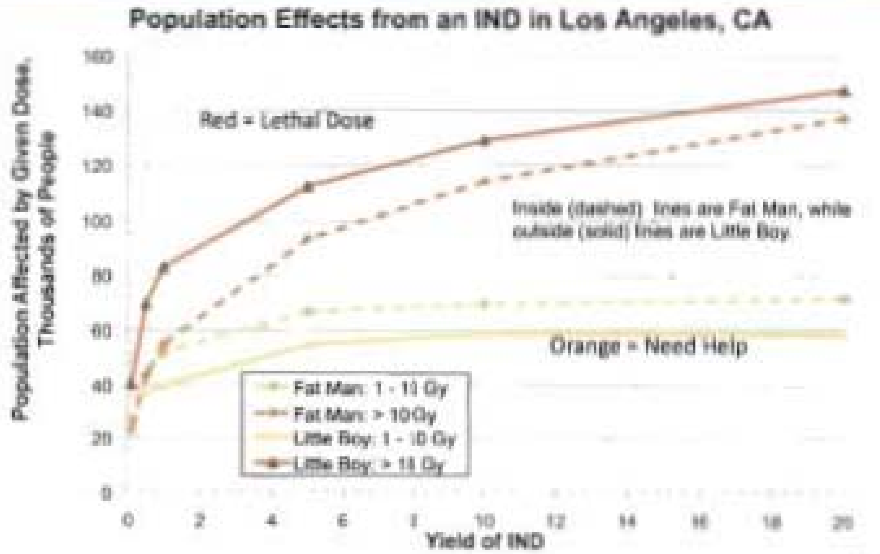
IND Dose Effects Manageable

Input into FEMA's "Planning Guidance for Response to a Nuclear Detonation", 2nd Ed.
Tammy Taylor, White House Office of Science and Technology Policy

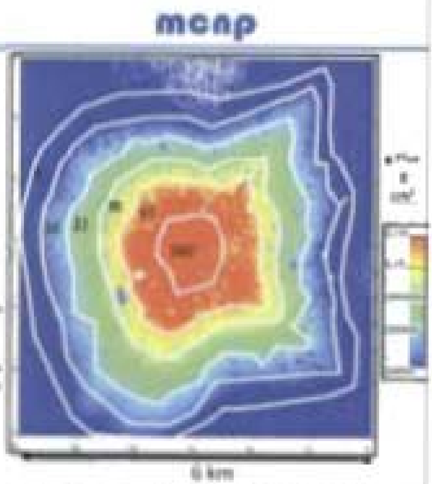


Dose contours from a 20 kT Little Boy device in downtown LA

IND Dosed Populations Manageable



IND Circuit Effects Manageable



- The results presented here are based on source region simulation levels from MCNP. This is part of the LANL EMP start-up project's goal of incorporating first physics principle source region calculations into legacy EMP code and then migrating to a fully integrated EMP physics package.
- note: these calculations are going to be given to the NISAC systems analyst team to produce an more representative evaluation of equipment/infrastructure failure.

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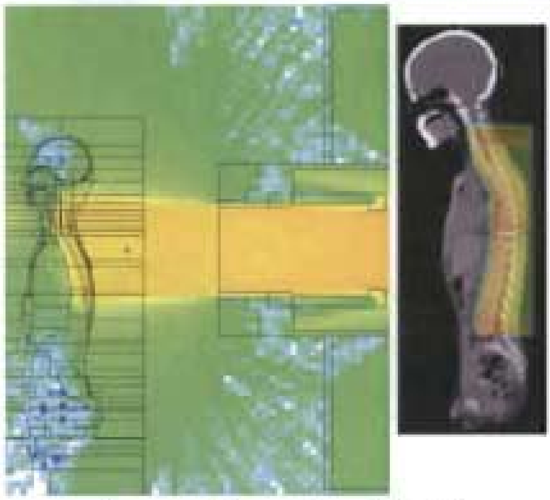
MCNPX is the most widely used general purpose Monte Carlo code for research in radiation cancer therapy.

The code is ideally suited for use in medical applications because of the accuracy of its physics models, the unique set of clinically relevant features, and the responsive support provided by the developers and the user community.

We used MCNPX to verify the Mass General Hospital Proton Center, and this information has gone into the design of the MDACC proton center and others, which are used to treat > 5K people a year.

Wayne Newhauser, Ph. D.
Dept of Radiation Physics
MD ANDERSON CANCER CENTER



proton fluence and dose contours (arb units)

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Nuclear Regulatory Commission Use of MCNP

Criticality Safety:

1) To assess the criticality safety of licensed facilities that handle fissionable materials.

Radiation Shielding:

1) To benchmark other shielding and dose calculation computer codes and methods used by NRC staff.

2) To verify licensees' shielding and dosimetry calculations.

Radiation Dosimetry:

1) Assess planned and unplanned worker radiation exposures.

2) Assess public exposure from planned licensing actions.

Medical:

1) To understand the radiation safety implications of using radiation in medical diagnosis and treatments.

Continuing development of MCNP capabilities is important to improve the code's ability to model situations that currently are modeled only approximately, particularly in the area of electron transport, which is a very important consideration in NRC's dosimetry work. - Sami Sherbini, Nuclear Material Safety and Safeguards, NRC

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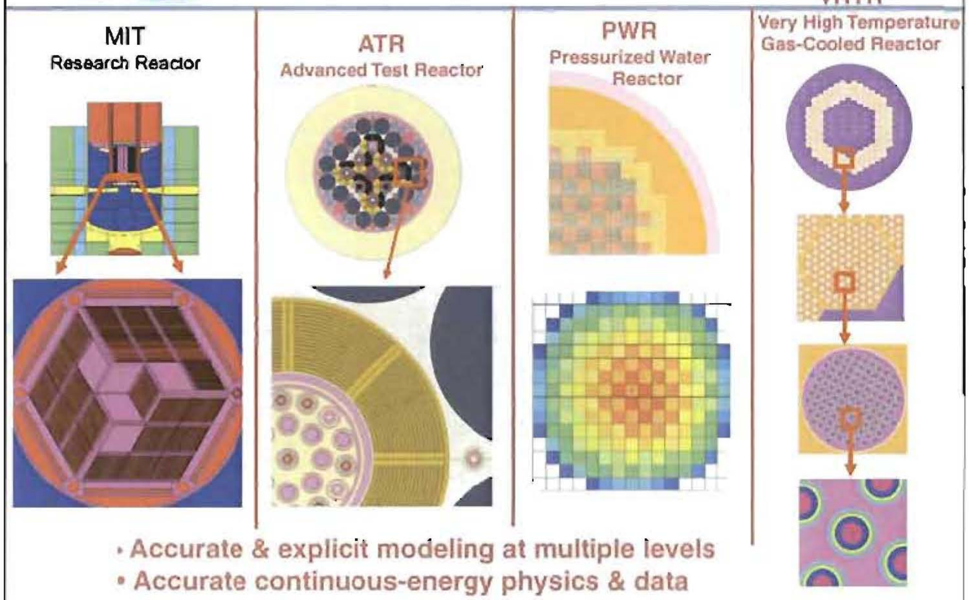
MCNP is benchmark for Nuclear Reactor Design codes



- Accurate & explicit modeling at multiple levels
- Accurate continuous-energy physics & data

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Future Vision – Top Ten List

1. Monte Carlo Applications ToolKit (MCATK)
2. Unstructured Meshes (CAD/CAE)
3. Lower Energy Thresholds
4. Next Generation of Parallel Capability
5. Temperature Effects
6. Damage Effects
7. Better physics
8. Improved variance reduction
9. Criticality Efforts
10. Maintenance & Support

- Half are funded (shown in green)
- Several of them could involve University R&D efforts / partnerships
  - U. Michigan
  - U. New Mexico
  - Texas A&M
  - West Point / AFIT
- Brings "in-house" capabilities third parties have been developing for years
  - Visual Editor
  - U. Wisconsin
  - Oak Ridge
  - Japan Atomic Energy Agency

Theme Area 3: Monte Carlo Methods

The MCNP code and teams are world leaders in particle transport

- MCNP is a widely used and respected many-particle transport code.
  - Extensive physics over large energy range
  - Extensive V&V efforts spanning many applications
- MCNP has a large sponsor / stakeholder base, which drives the addition of new features.
  - Potential to find and develop synergies between sponsors
  - Furthering the ability to provide answers that affect decision making.
- MCNP has a large code development team of internationally known experts, which strengthen its position for the future.

Jones

Climate Models: A Complex Integrated Application

Phil Jones
Fluid Dynamics and Solid Mechanics (T-3)
Climate, Ocean and Sea Ice Modeling (COSIM)

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Los Alamos is a climate modeling center

- Climate, Ocean and Sea Ice Modeling (COSIM)
  - Develops advanced ocean, ice models
  - ~15 staff
  - $6.8M/year and growing rapidly (mostly DOE-SC)
  - Part of larger Community Climate System Model (CCSM) – largest of three centers in US
- Since 1989
  - DOE Computer Hardware, Advanced Mathematics, Model Physics (CHAMMP), the original co-design
  - Built on earlier reputation in nuclear winter

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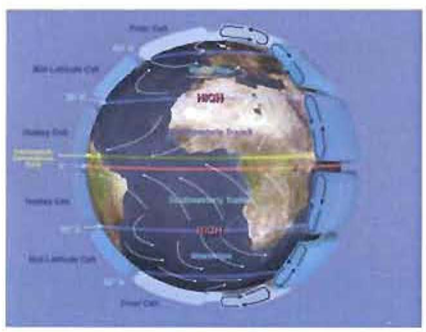
Outline

- Climate complexity – the real climate
- Climate model applications – how do we use the models?
- Climate model development
- Computing implications
- Coming soon

What do we mean by climate?

- *Not* weather
  - Weather = properties at a specific place and time
  - Typically daily to 10 days
- Climate
  - Earth system works to distribute heat (temp), water, tracers
  - Mean, variability (including extremes)
  - Multiple time and space scales



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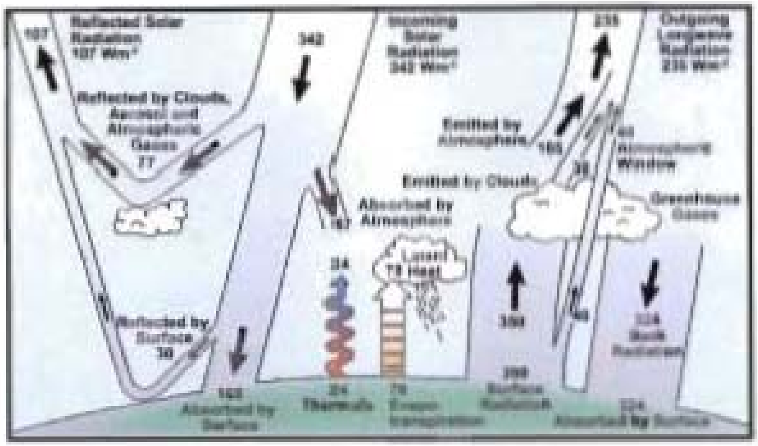
Climate change governed by energy balance



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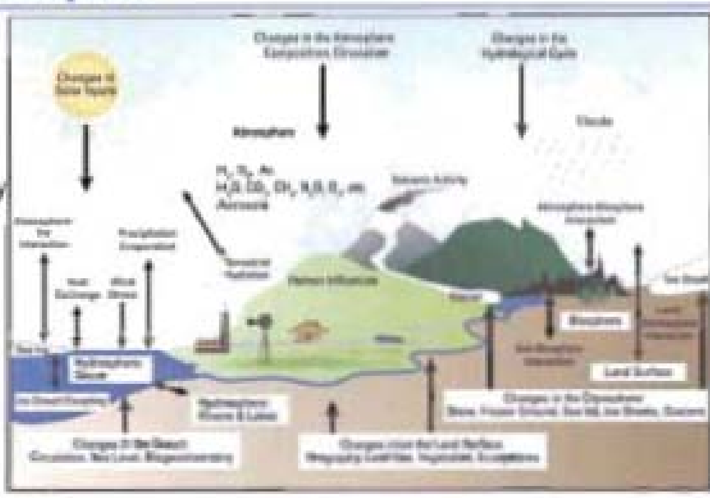
Climate details are more complex

Dynamics
Physics
Biogeochemistry

Human
Interactions



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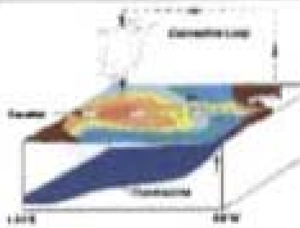
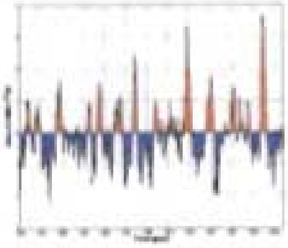
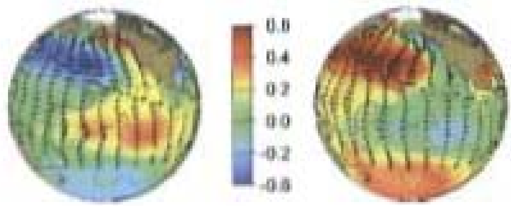
Climate variability and response spans many timescales

- Interannual
  - ENSO
- Decadal
  - PDO
  - NAO
  - AMO
  - BYO

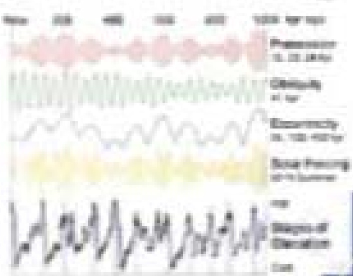


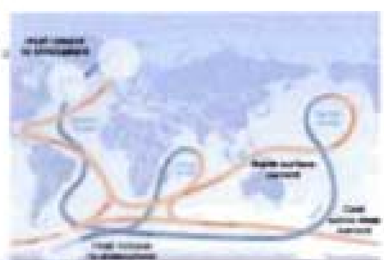




Climate variability and response spans many timescales

- Centennial
- Millenial
- Paleo





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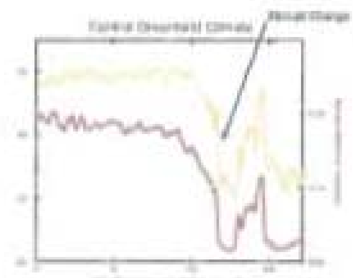
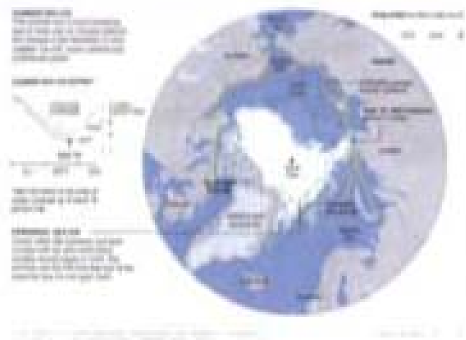
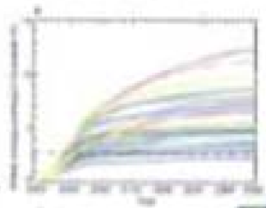
Climate dynamics includes thresholds and abrupt change

- Thresholds in climate system







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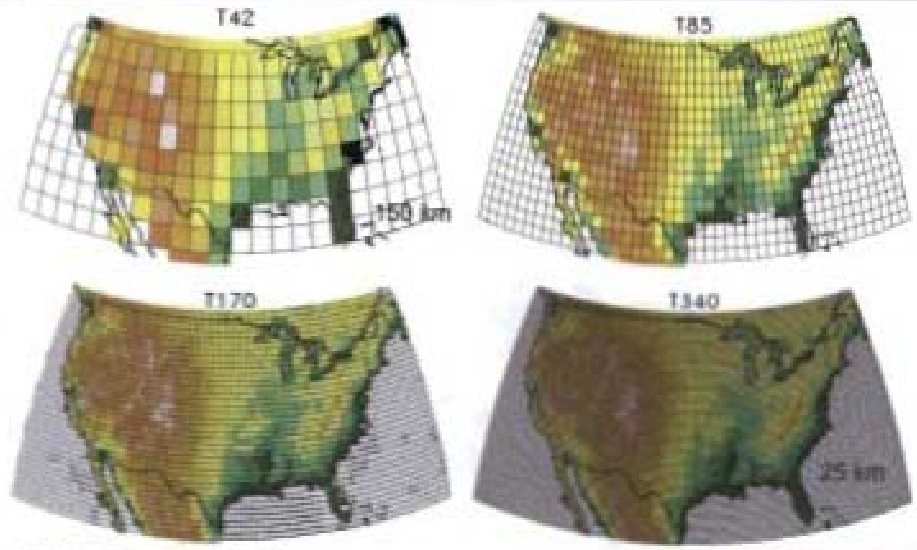
Climate dynamics spans many spatial scales



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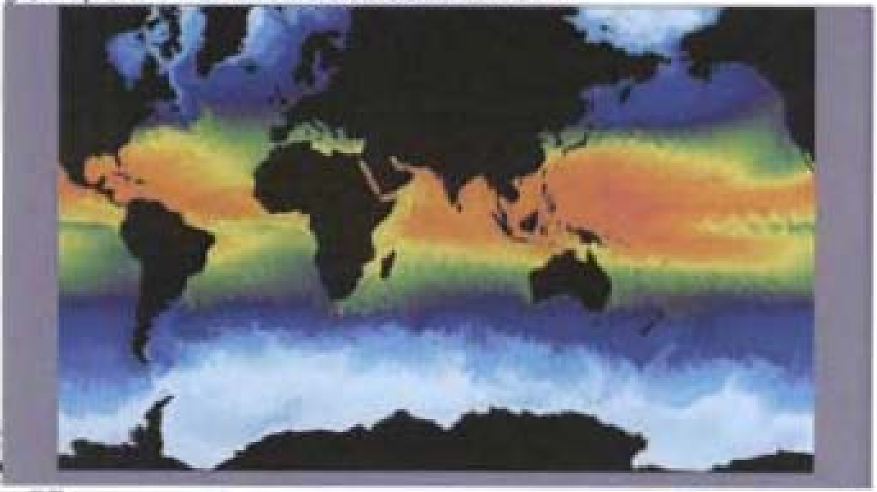
Ocean mesoscale eddies impact global circulation

Resolving eddies necessary for accurate simulation of currents and their role in sea ice edge, deepwater formation and thermohaline circulation.



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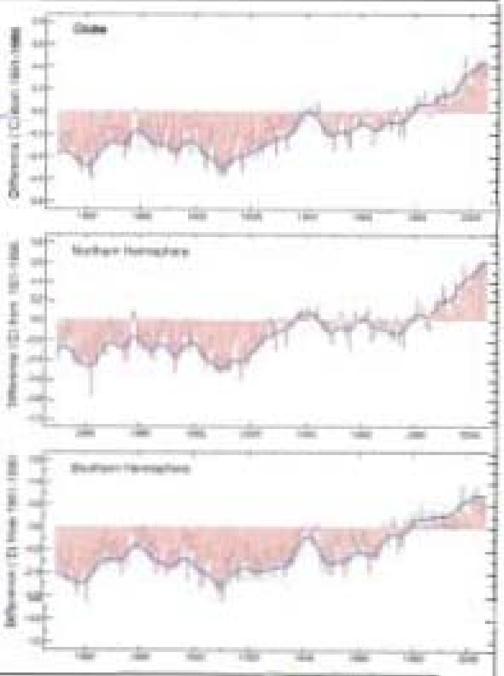
Instrumental record reveals warming climate



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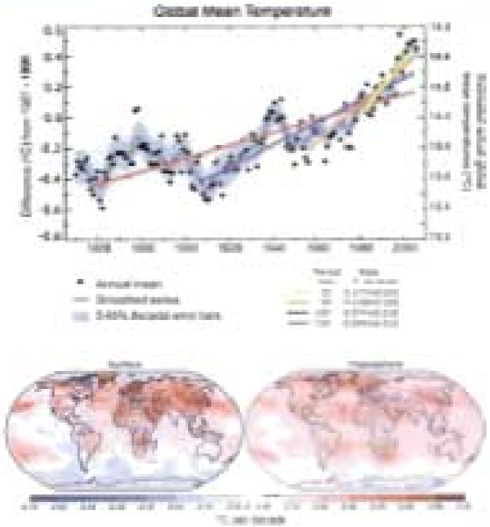
Warming not uniform in space or time



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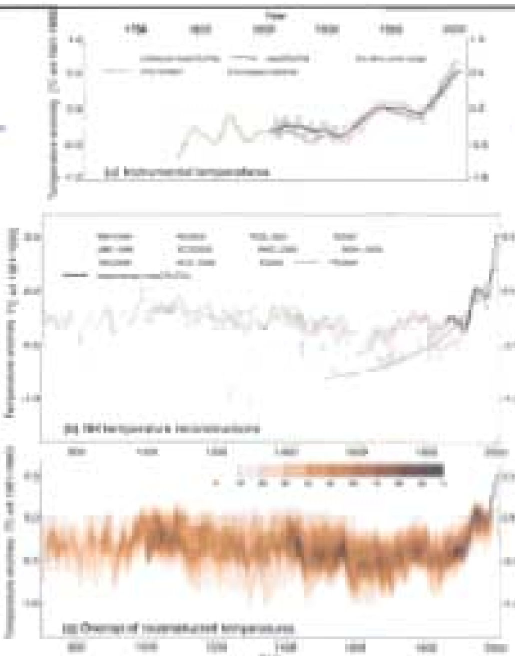
Paleoclimate record shows warming is unusual



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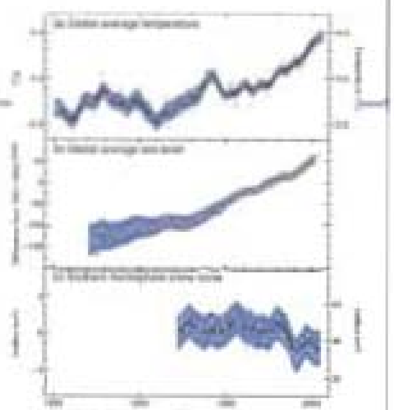
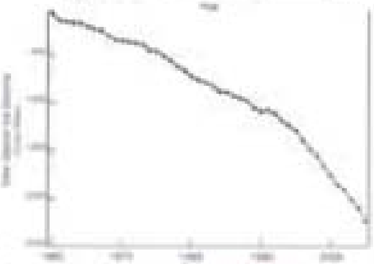
Other observations

- Arctic warming 2x faster
- Ocean warming to 3000m depth
- Glaciers, snow cover declined
- Ice sheet losses accelerated
- Sea ice decreased
- Changes in precipitation patterns (poleward and upward, snow pack)
- More intense, longer droughts in tropics, subtropics
- Freq. of heavy precip events increased
- Cold days, nights, frost decreased; hot days increased
- Increased water vapor
- 29,000 time series, 75 studies





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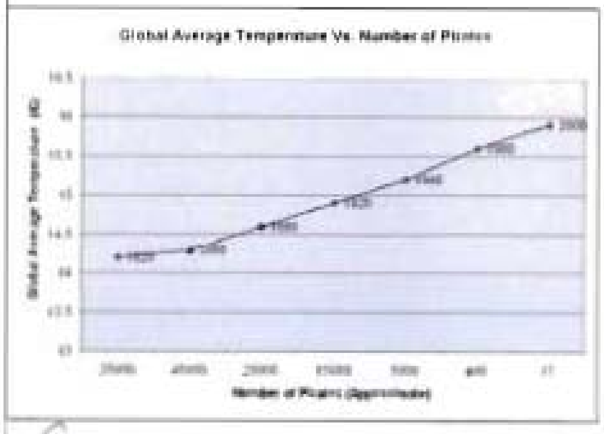
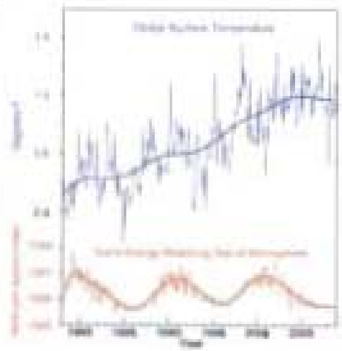
Attribution: Recent warming is not caused by…





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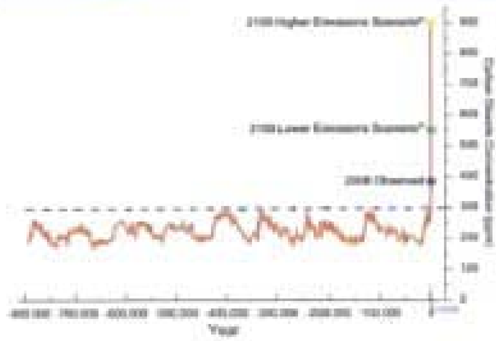
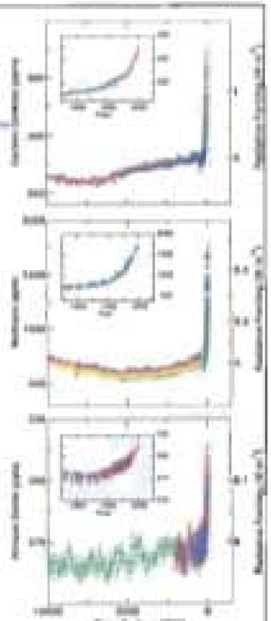
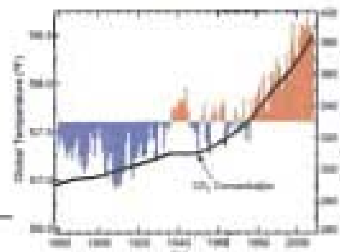
Greenhouse gas concentrations are high





Isotopes: human emissions and land use change



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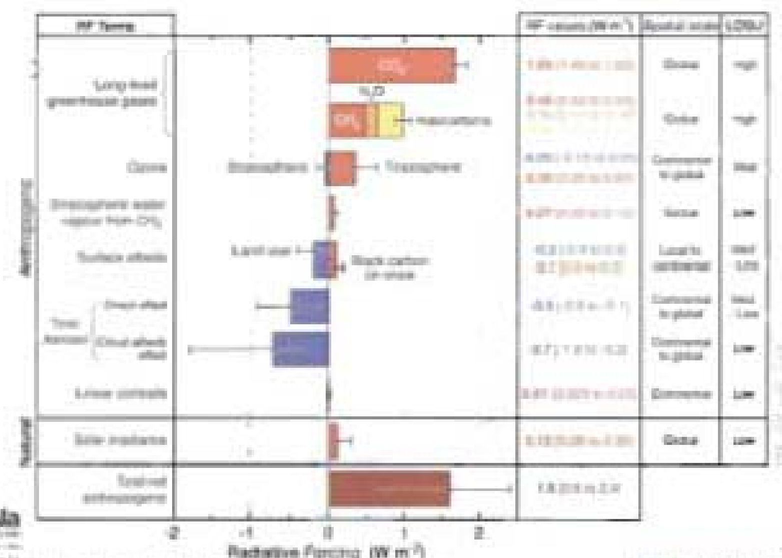
Other forcings can supply positive or negative feedbacks



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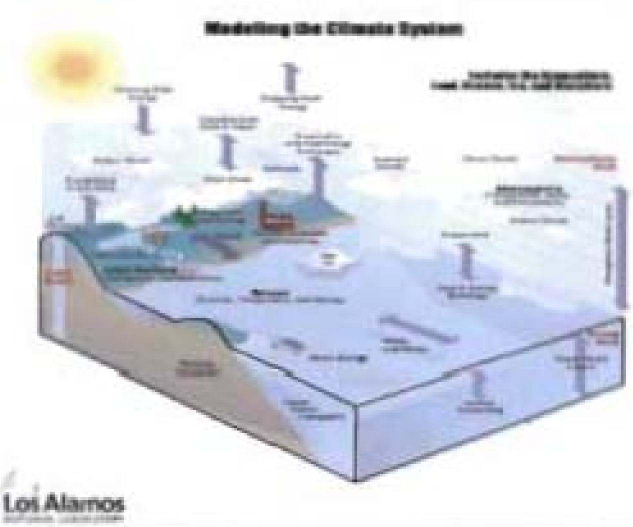
Climate models used for many applications



- Integrates knowledge of climate system
- Used to understand and quantify feedbacks
- Attribution
- Projecting future change

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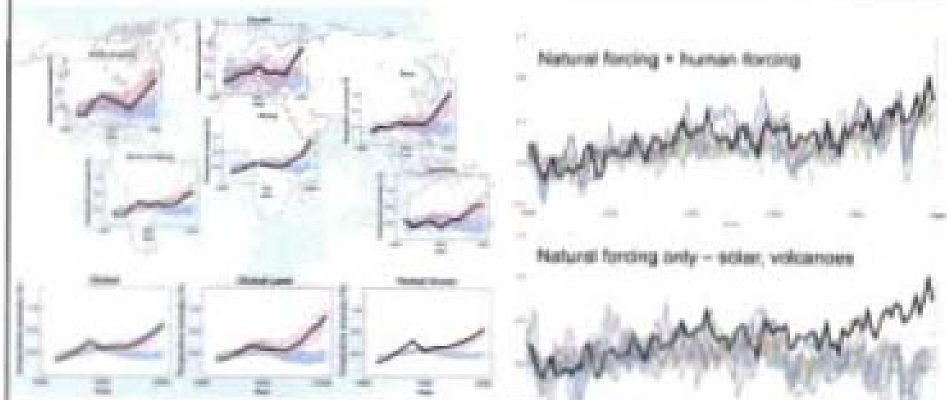
Models are used for attribution



Solid black line is observational record
Other lines are ensembles of model results
Observations can only be explained by increased human influence

From Stott et al. 2006

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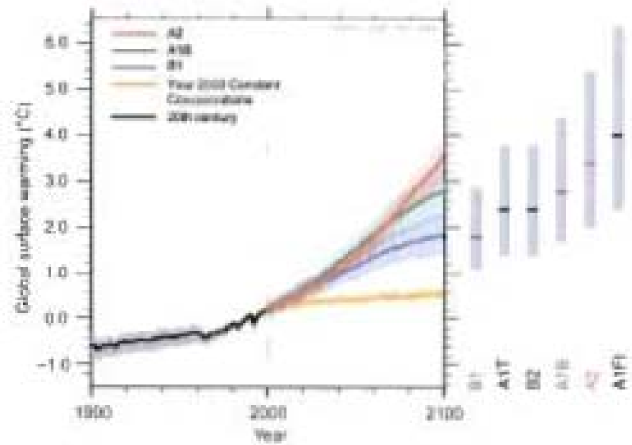
Models are used to project future climate change

- Multiple modeling groups
- Ensembles
- Emissions scenarios



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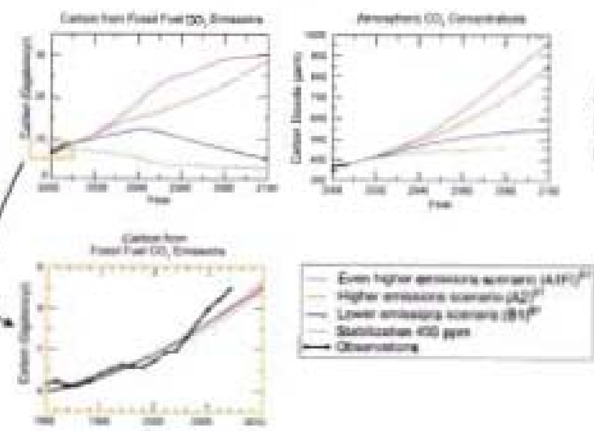
Emissions scenarios project future GHG concentrations



Scenarios generated from integrated assessment models

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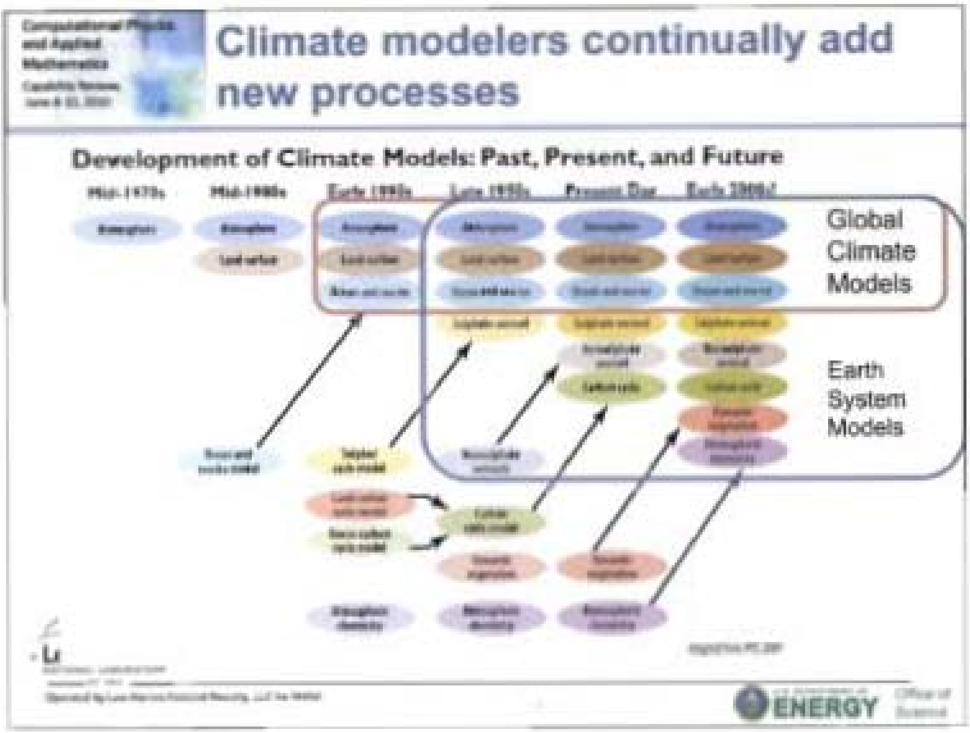
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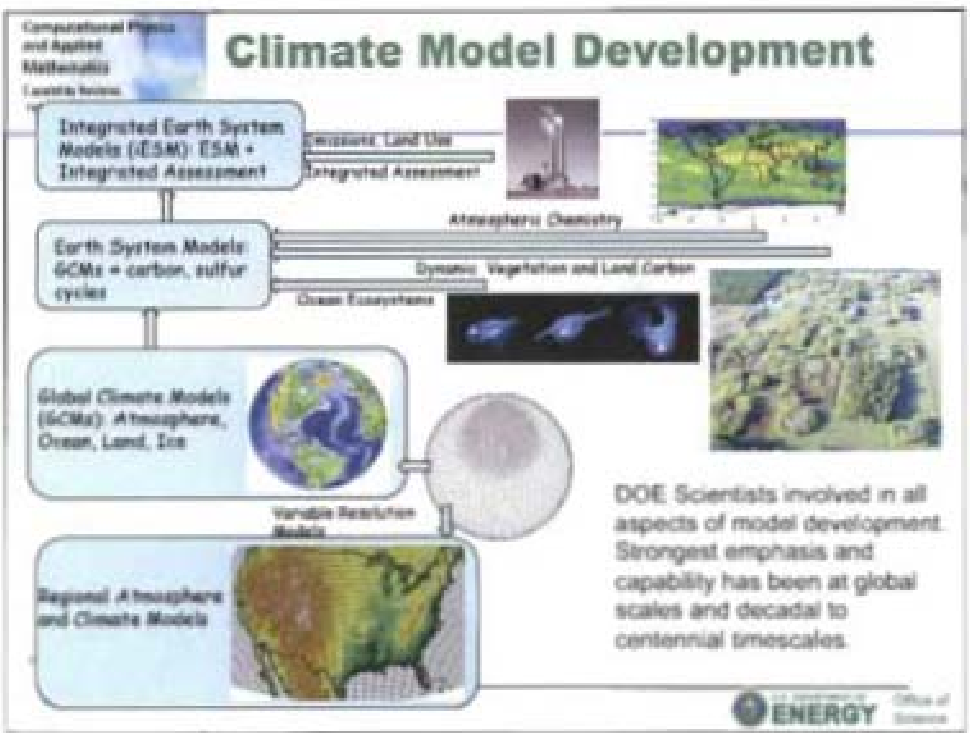
Climate modelers continually add new processes
Development of Climate Models: Past, Present, and Future
Global Climate Models
Earth System Models
ENERGY


Computational Physics and Applied Mathematics
Climate Model Development
Integrated Earth System Models (iESM): ESM + Integrated Assessment
Emissions, Land Use
Integrated Assessment
Atmospheric Chemistry
Earth System Models: GCMs + carbon, sulfur cycles
Dynamic Vegetation and Land Carbon
Ocean Ecosystems
Global Climate Models (GCMs): Atmosphere, Ocean, Land, Ice
Variable Resolution Models
Regional Atmosphere and Climate Models
DOE Scientists involved in all aspects of model development. Strongest emphasis and capability has been at global scales and decadal to centennial timescales.
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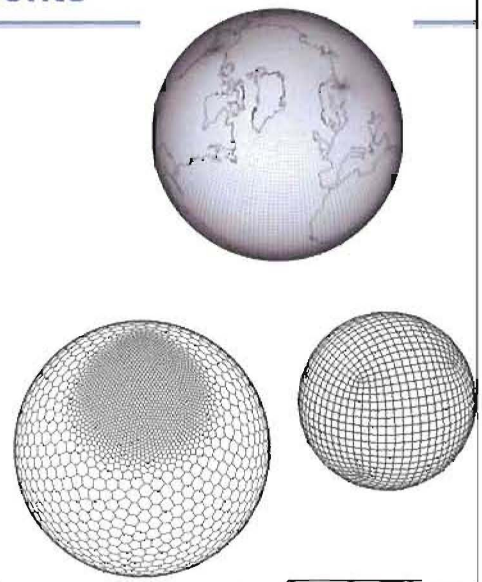
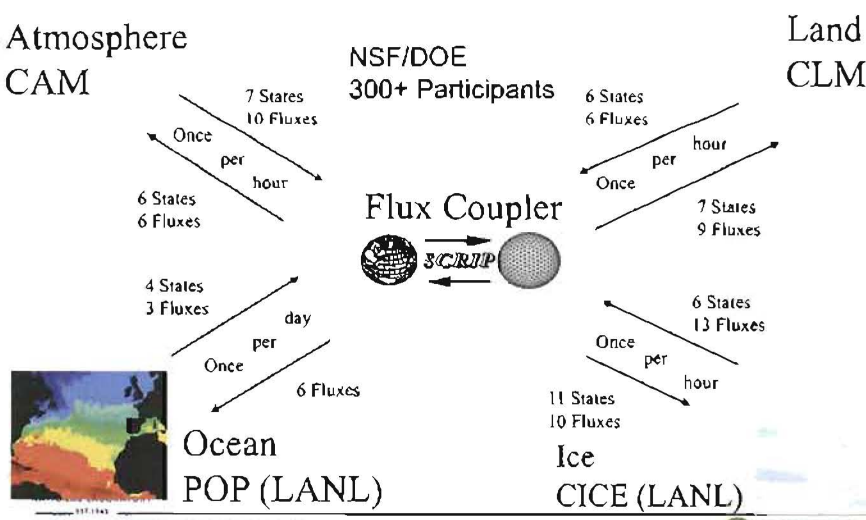
Climate models are built from base components

- Atmosphere
  - 3-d Fluid equations
  - Column physics (radiation, clouds, convection)
- Ocean
  - 3-d Fluid equations
  - EOS, mixing
- Sea Ice
  - Viscous-plastic
  - Thermodynamics
- Land Surface
  - Plant functional types
  - Surface water, energy

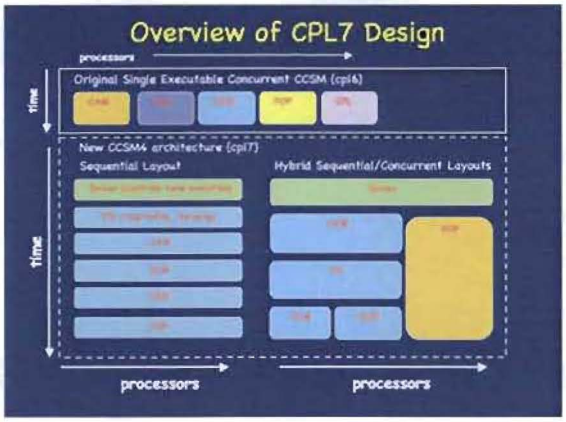


The Community Climate System Model is one example



Model components are joined by a coupler

CCSM as a typical coupled GCM architecture.

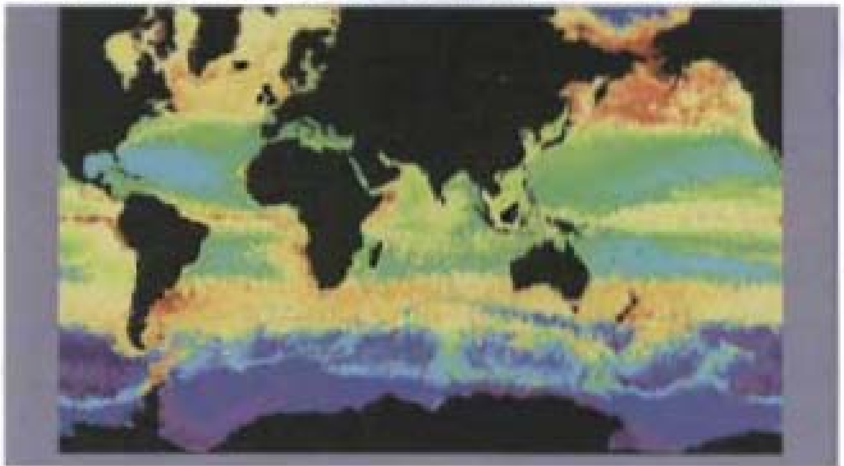


Climate, Ocean and Sea Ice Modeling (COSIM) Project

- Develop advanced ocean and ice models for climate science
- Focus on high latitude climate change and impacts throughout the globe
  - Ice sheets and sea level rise
  - Rapid ice retreat
  - Ocean circulation stability
  - High latitude biogeochemistry and clathrates

Eddy-resolving Ocean Modeling

In addition to circulation, eddies are important for nutrients and biogeochemistry



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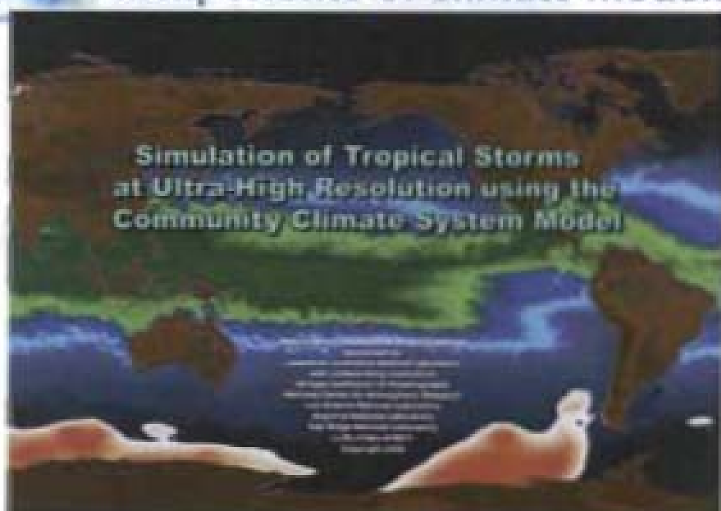
High resolution required for all components of climate models



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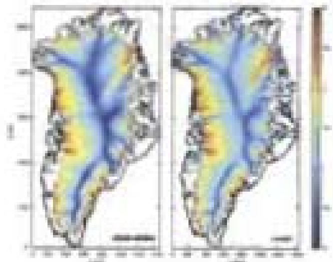
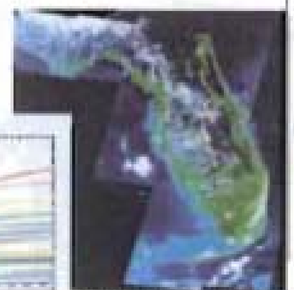
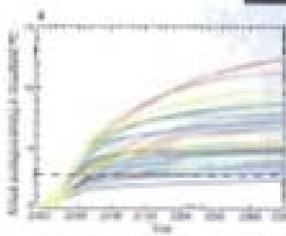
Ice sheets are new component

- Largest missing piece of physical climate in current models
- Needed for sea level rise prediction
- 6m of sea level rise if Greenland melts, 6m if W. Antarctic ice sheet melts
- Slow melt over 1000 years or more rapid?
- Threshold of no return?
- Small-scale ice sheet dynamics, ocean/ice interaction, disparate timescales
- Variable coastlines, topography





Stephen Leatherman



Gregory et al. 2004

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CICE used to understand ice loss

- Poles warm almost 2x faster
- Large ice feedbacks
- Ice free summer by 2050
- Record low arctic ice in 2007
- Impacts
  - Ecosystems (polar bears, walrus)
  - Oil, resource extraction
  - Ocean thermohaline circulation
- Need mechanisms for faster ice melt (algae, cracks, etc.)

NY Times, 10/1/07

Nearly ice-free summertime arctic predicted by CCSM (with LANL ocn and ice models) between 2000-2040, much of it within a decade due to ice thinning combined with pulse of warm water input (M. Holland et al.)

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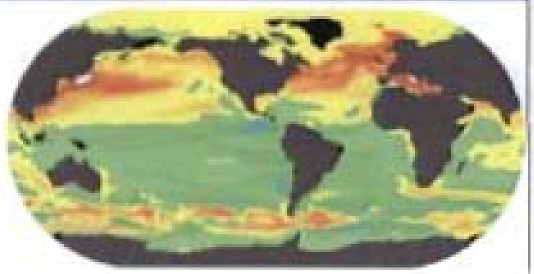
June 8-10, 2010

Earth System Models add biogeochemical processes

- Coupling ocean biogeochemistry with extensive atmospheric chemistry and land biogeochemistry
  - Carbon and sulfur cycles
  - Needed to assess ability of oceans and land to sequester carbon
  - Aerosol direct/indirect (reduced precipitation?)
  - Projections with specified emissions
  - Methane hydrates/clathrates
  - Ocean acidification
  - Engineered climate
- Many tracers
  - 100x atm, 20x ocean
  - Many reactions
  - Metagenomics



Flux of CO_2 at ocean surface
Red/yellow – CO_2 leaving ocean
Green/blue – ocean uptake of CO_2

Coral bleaching

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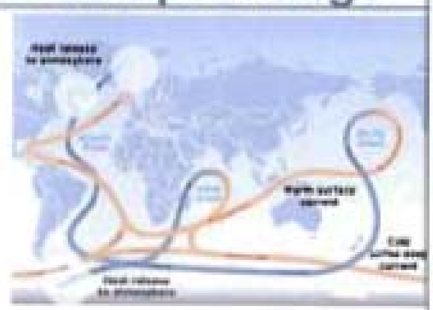
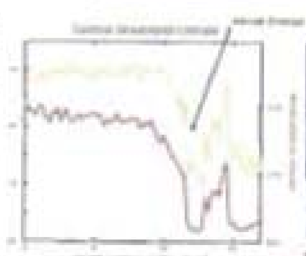
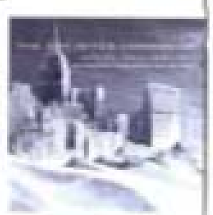
Capability Review
June 8-10, 2010

The thermohaline circulation may experience abrupt change

- Carries large fraction of heat from equator to poles
- Responsible for mild climate of Europe, NE US
- Driven by formation of cold, salty water in N. Atlantic and Antarctica
- Abrupt scenario:
  - Large influx of fresh water due to ice melt, increased precipitation
  - Prevents formation of dense water
  - THC slows/shuts down in response
  - Impacts on Europe, NE US and overa atmospheric circulation
- Implicated in past abrupt climate shift
- Current models predict weakening, then recovery
- Implicit models/parameter continuatio







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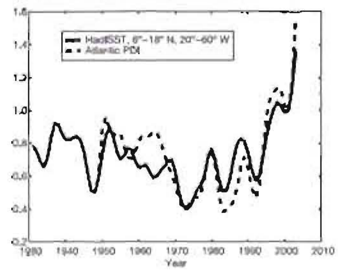
Climate change impact on hurricanes remains unclear

- Hurricane peak wind speeds increase due to ocean SSTs
- No evidence for increased hurricane frequency
  - Could change if ENSO changes
- Power dissipation (and damage) increases
  - Cube of peak wind speed
  - Longer duration of storms
- Other severe storms, flooding
- Falwell effect



Hurricane power dissipation index (v3. duration)
From Emanuel 2005

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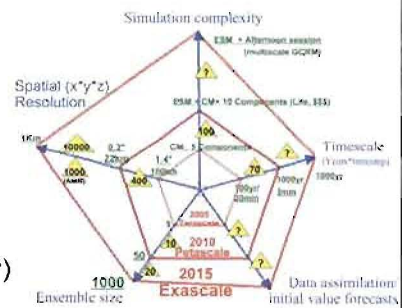
Climate simulations will continue to need computational power

- Resolution (10^3-10^5)
  - x100 horiz, x10 timestep, x5-10 vert
  - Regional prediction (10km)
  - Eddy resolving ocean (< 10km)
- Completeness (10^2)
  - Biogeochem (30-100 tracers, interactions)
  - Ice sheets
- Fidelity (10^2)
  - Better cloud processes, dynamic land, etc.
- Increase length/number of ensembles (10^3)
  - Run length (x100)
  - Number of scenarios/ensembles (x10)
  - Data assimilation (3-10x)
- Data requirements have similar factors
  - 35 TB currently, distributed
  - More for assimilation



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Computing transitions will provide new opportunities

- Hybrids – Back to the Future
  - Transition like early 1990s
  - Permits re-evaluation of approaches, algorithms
  - Co-design (see Andy White)
- Scaling
- Time Integration
- Ensembles
- Uncertainty quantification (Higdon)

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Future Directions

- Continued improvement
  - Reducing biases
  - Improving representations and accuracy
- Regional scales
  - Ultra high resolution
  - Variable resolution
- New processes
  - Ice sheets and sea level rise
  - Dynamic vegetation, disturbances, mortality
  - Integrated Earth System models

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Archer

Nuclear Weapons Applications (U)

Bill Archer*

Bob Weaver**

The Advanced Simulation and Computing (ASC) nuclear weapon applications are the focal point where science results are integrated together to provide tools that are useful to the analysis communities. This brief gives an overview for the Computational Physics and Applied Mathematics (CPAM) review of how various science results are being used to improve the analysis of various devices. (U)

*ACS-PO

**Laboratory Fellow

Higdon

Uncertainty Quantification

Dave Higdon/CCS-6 (Statistical Sciences)

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Uncertainty Quantification @ LANL

- UQ is the process of carrying out scientific inference (prediction uncertainties, parameter estimates, sensitivities, etc). UQ typically combines physical observations, computational models and high performance computing to make these inferences.
- UQ activities are funded by a variety of sources.
  - ASC Verification and Validation (~3.5 FTEs)
  - Enhanced Surveillance (~3 FTEs)
  - Advanced Certification (.75 FTEs)
  - Ice Sheet Modeling (Office of Science ASCR ~1 FTE)
  - Stochastic PDEs (Office of Science ASCR ~1.5 FTEs)
  - Cosmology (LDRD, Office of Science HEP, NASA ~ .5 FTEs)
  - DoD Joint Munitions Stockpile Management (Joint Munitions Project ~ .5 FTE)
  - Advanced Supercomputing for Environmental Management (~ .75 FTE)
  - Integrated Climate Systems (Office of Science BER ~2 FTEs)
  - Regional Climate Interactions (Office of Science BER ~ 2 FTE)
  - Nuclear Energy Advanced Materials (NEAMS ~1 FTE)
  - Greenhouse Gas Information System (GHGIS ~ 2 FTE) (Total = ~11.5 FTEs)
- UQ supports Stockpile Stewardship, Climate, Energy Security, Physical Sciences
- People Involved: Researchers from CCS-2, CCS-3, CCS-6, X-TD, X-CP, T-2,T-5, ISR-1, UNM, SFU, UCSC, UT
- Peers: Other National Labs, especially LLNL, NNSA PSAAP Centers, especially UT; UK academic/industrial consortium Managing Uncertainty in Complex Models

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Brief history: simulation-aided inference @ LANL

Implosion calculations motivate first physics computer simulations

Computing evolves to carry out complex implosion simulations

Analysis algorithms evolve from LANL computing (e.g. Monte Carlo method)

Supercomputing, ASCI, computational models in the era of no nuclear testing

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UQ is a fundamental integrator for science at LANL

- UQ has played a key role in LANL activities that combine physical experiments/observations, computational modeling, and high performance computing.
- UQ activities require in-depth collaboration between subject matter scientists, computational scientists, and statisticians (including machine learning, applied math, computer science).
- LANL's competitive advantage in this area stems from its broad range of experts and its ability to allow significant, and deep collaboration.
- Methods originally developed in Nuclear Weapon certification and assessment have been applied to a variety of scientific investigations (cosmology, nuclear energy, climate, ...)
- LANL UQ researchers are leaders in the broader UQ community (NRC study, UQ workshops, roadmapping research directions, invited talks,...)

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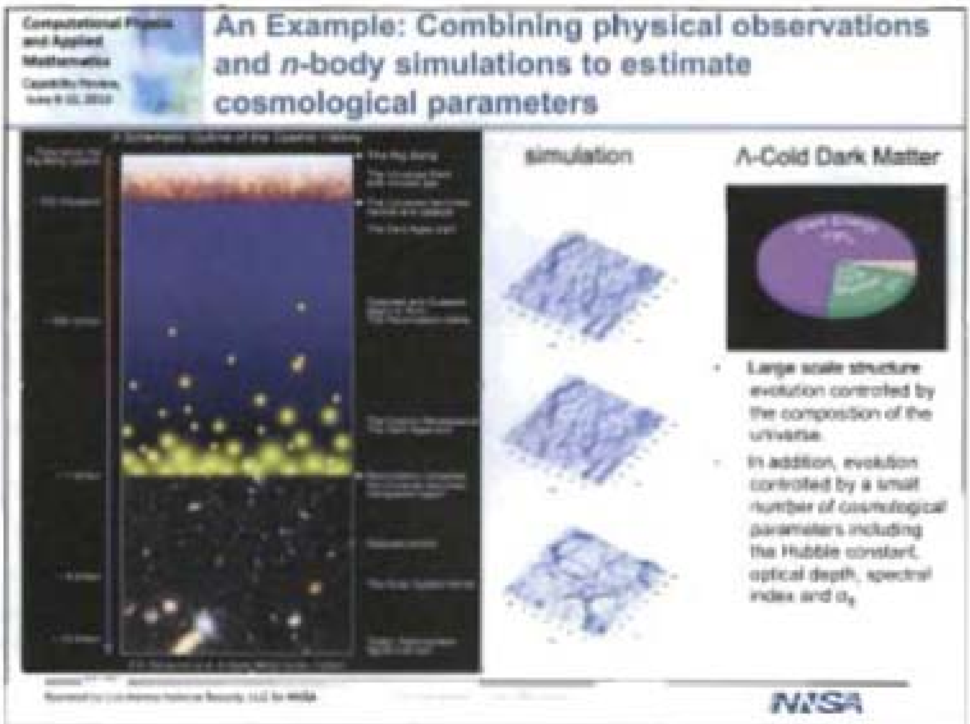
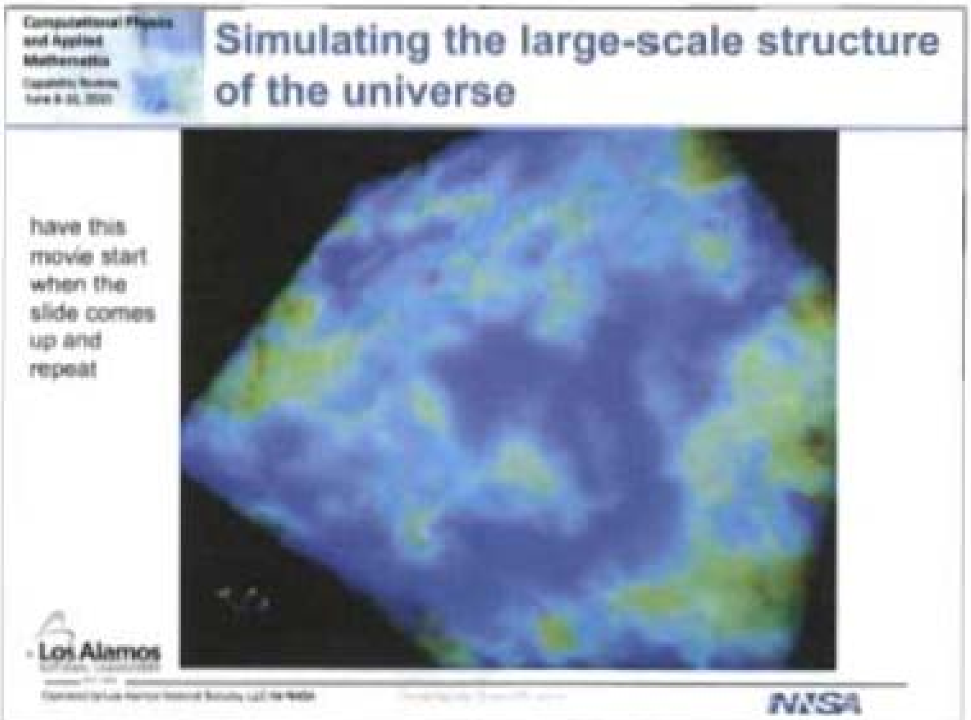

An Example: Combining physical observations and *n*-body simulations to estimate cosmological parameters
simulation
Λ-Cold Dark Matter
Large scale structure evolution controlled by the composition of the universe.
In addition, evolution controlled by a small number of cosmological parameters including the Hubble constant, optical depth, spectral index and σ_8
NNSA


Simulating the large-scale structure of the universe
have this movie start when the slide comes up and repeat
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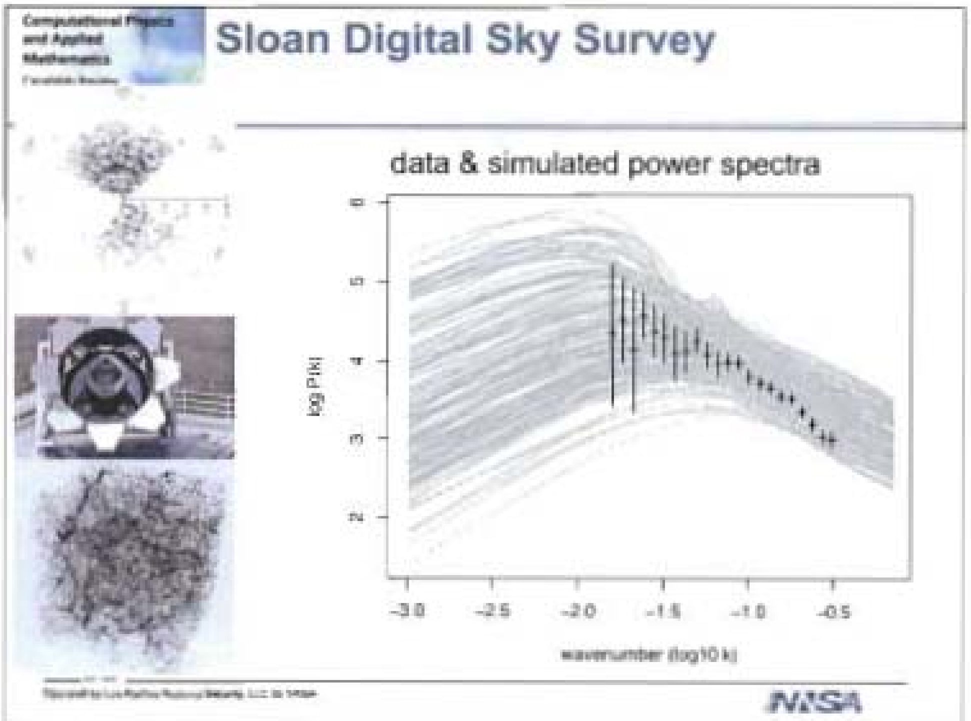

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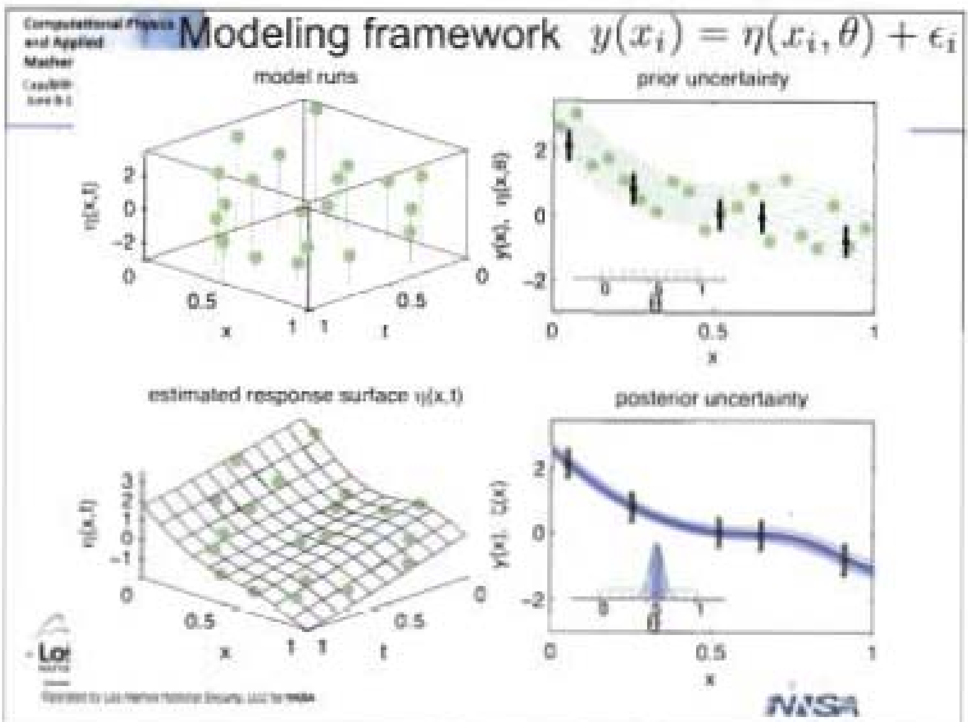
Sloan Digital Sky Survey
data & simulated power spectra
log P(k)
wavenumber (log10 k)
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5



Modeling framework $y(x_i) = \eta(x_i, \theta) + \epsilon_i$
model runs
prior uncertainty
estimated response surface η(x,t)
posterior uncertainty

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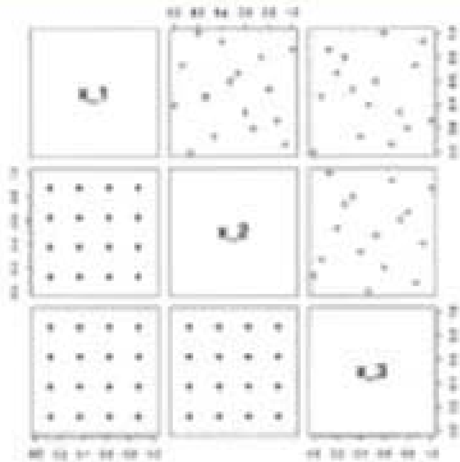
Determining input settings for model ensembles – an OA-based Latin Hypercube



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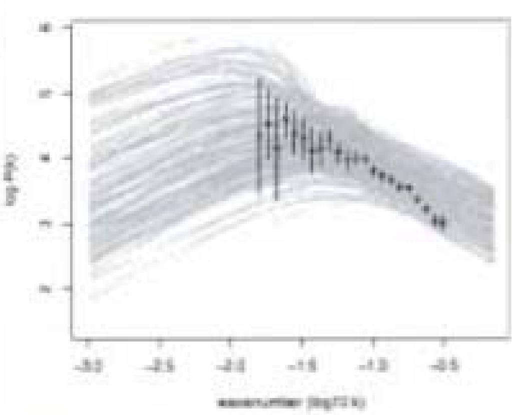
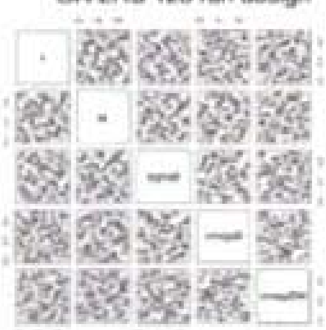
Data, parameter ranges, and simulations

Physical observations and simulations



OA-LHS 128 run design



Calibration parameter ranges

Spectral index	0.8 to 1.4
Hubble parameter	0.5 to 1.1
Sigma 8	0.6 to 1.6
Omega CDM	0.051 to 0.6
Omega baryon	0.02 to 0.12

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Inference uses joint model of the physical observations and computational model output

$$y(k) = \eta(\theta; k) + \delta(k) + \epsilon_k$$

Posterior density:

$$\pi(\eta(\cdot;k), \delta(k), \theta, \xi) \propto L(y|\eta(\cdot;k), \delta(k), \theta, \xi) \times \pi(\eta(\cdot;k)|\xi) \times \pi(\delta(k) \times \pi(\theta) \times \pi(\xi)$$

ξ controls statistical parameters governing likelihood and priors
Posterior explored via MCMC

$$\pi(\theta|y) = \int \pi(\eta(\cdot;k), \delta(k), \theta, \xi|y) d\eta \; d\delta \; \xi$$

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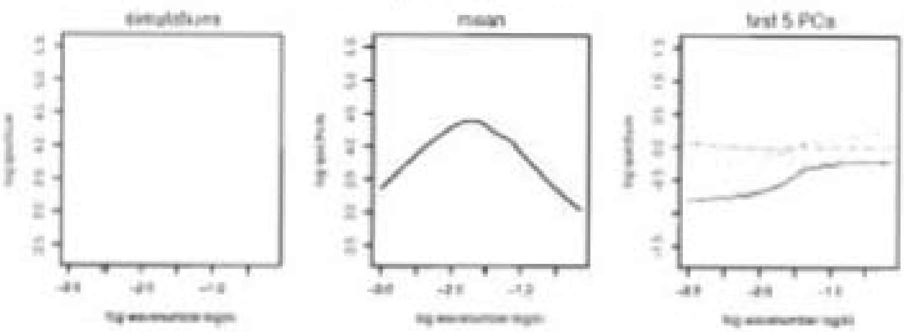
Basis representation of simulated spectra

Basis representation for matter power spectra.



Power spectra are represented as a function of the 5-d input parameters θ and PC basis functions $\phi_j(k)$:

$$\hat{\eta}(\theta; k) = \sum_{j=1}^{p_\eta} w_j(\theta) \phi_j(k)$$

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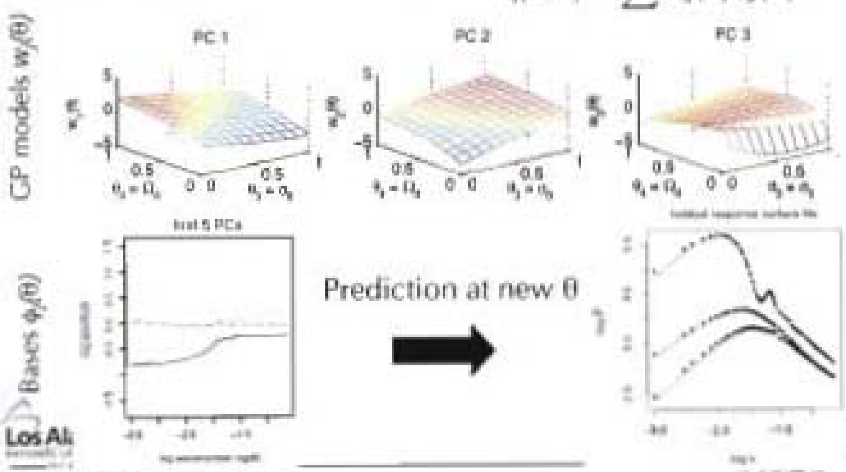
Gaussian process model to emulate simulation output

Gaussian process (GP) models are used to estimate the weights $w_j(\theta)$ at untried settings

$$\tilde{\eta}(\theta;k) = \sum^{p_\eta} w_j(\theta)\phi_j(k)$$



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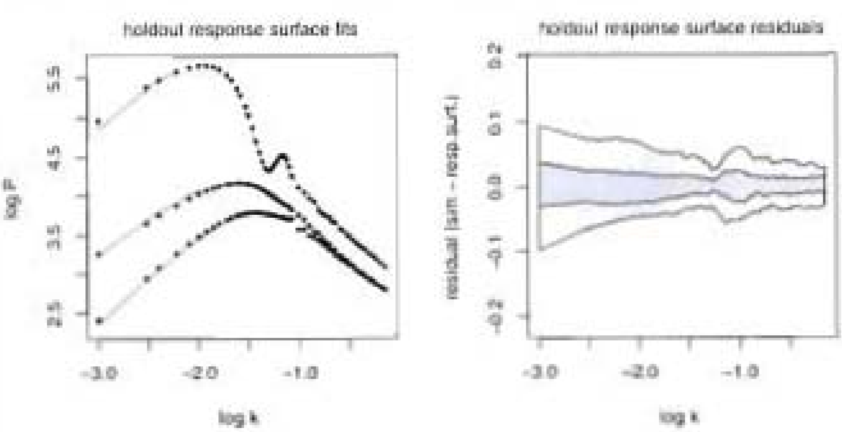
Response surface is sufficiently accurate for this application



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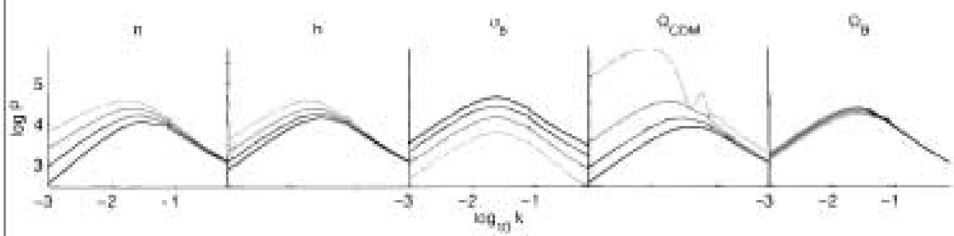
Simulator emulation and sensitivity



- Changes in emulator prediction as each parameter is varied while holding the others at their midpoint
- Note, σ8 ΩCDM have the largest effect on log P

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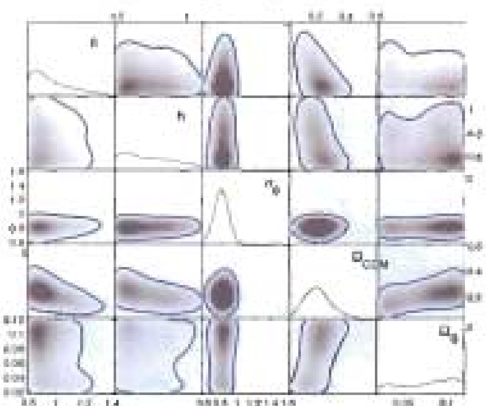
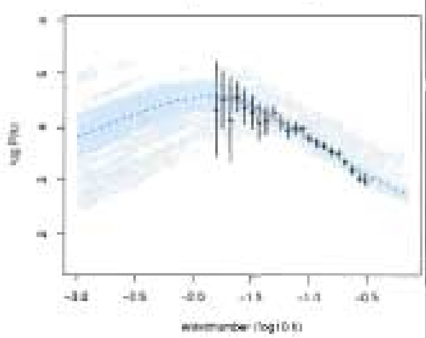
Calibration results using data from Tegmark et al (2004).

Posterior distribution of cosmological parameters



Resulting fit and uncertaintiy for the matter power spectrum



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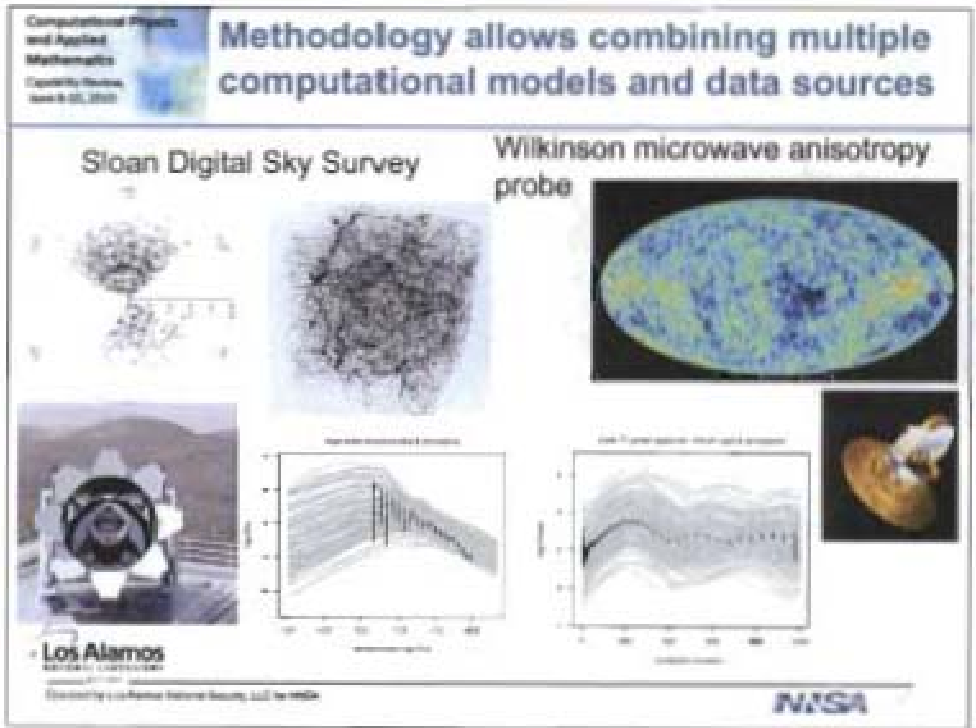
Methodology allows combining multiple computational models and data sources
Sloan Digital Sky Survey
Wilkinson microwave anisotropy probe
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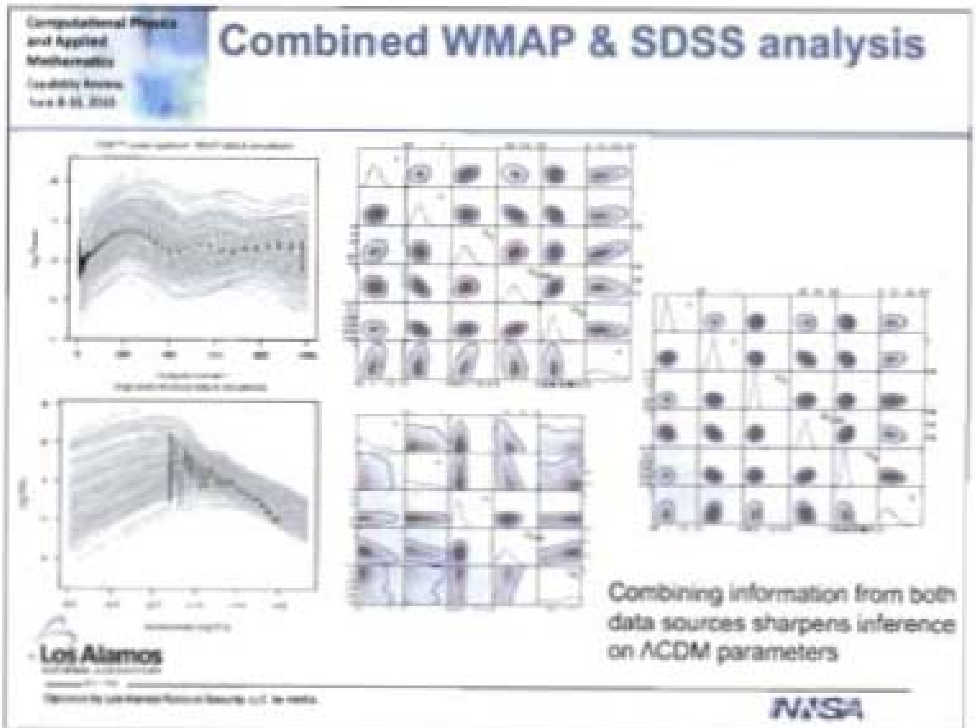
Combined WMAP & SDSS analysis
Combining information from both data sources sharpens inference on ΛCDM parameters
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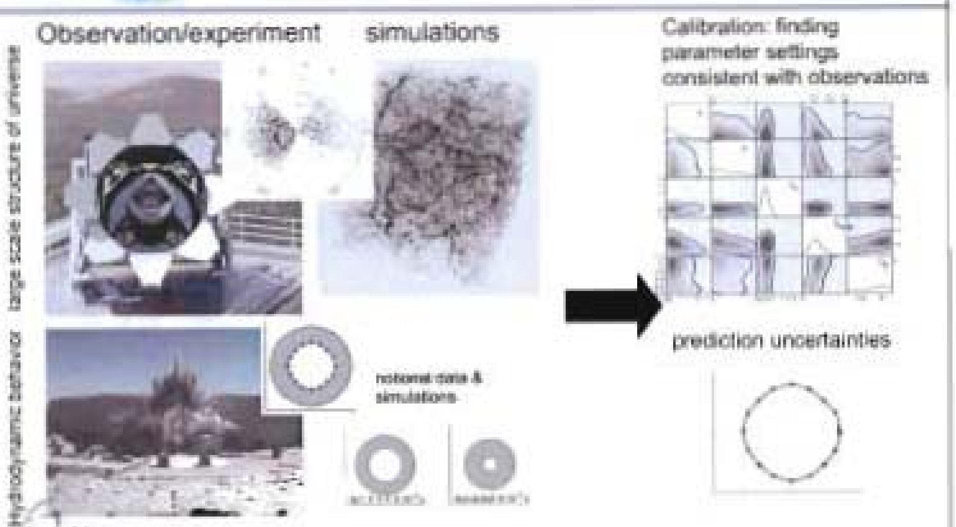
This basic template for cosmology is applicable in other scientific investigations



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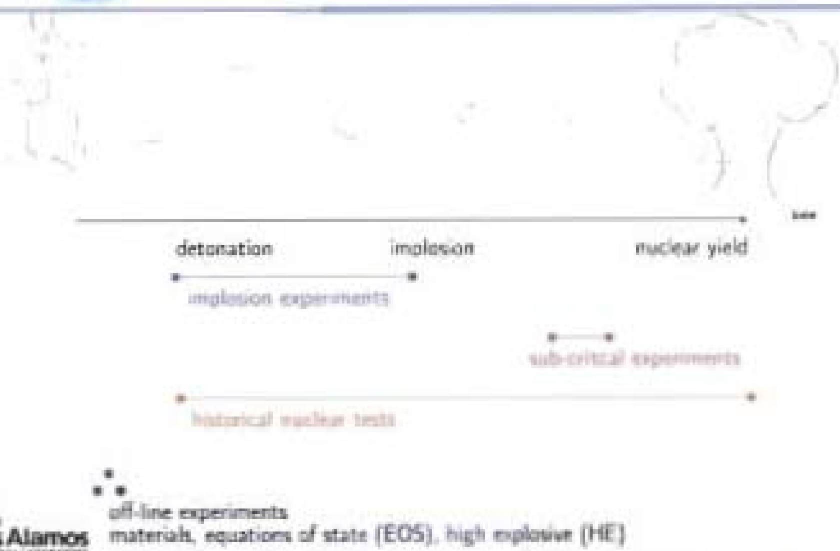
UQ in support of NW assessment combines information from many data sources



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Future Directions for UQ

- Continue engaging in well-chosen application areas
  - in LANL's wheelhouse, right people and resources available.
- Help broader UQ community map out research needs.
- Continue pursuing research directions that suit LANL activities
  - Foundational research
    - Linking model to reality, bounding small probabilities, formalism for dealing with extrapolations,...
  - Methods and algorithms
  - Applications with a 'data assimilation' flavor
    - Greenhouse Gas, Ocean Modeling, Space weather, non-proliferation, ...
  - Look for opportunities that combine novel approaches from computational modeling and high performance computing to enable UQ
- Future Funding opportunities
  - Climate, nuclear energy, material science, greenhouse gas monitoring, situational awareness, data assimilation

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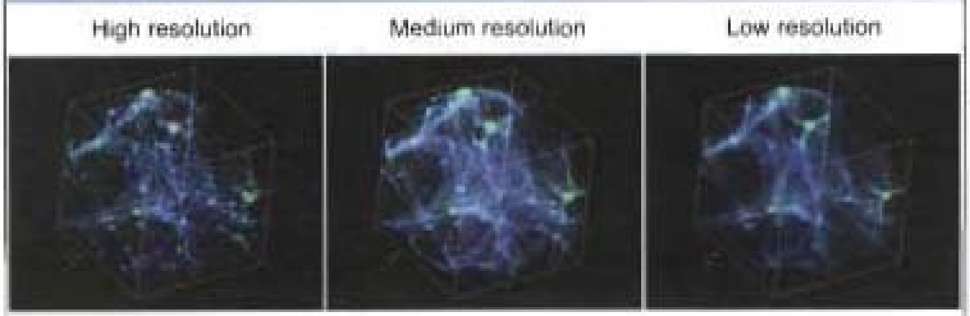
Making use of multiple model fidelities



- Infer about the physical system
- Make best use of limited computing resources
- May only need a few runs at highest fidelity

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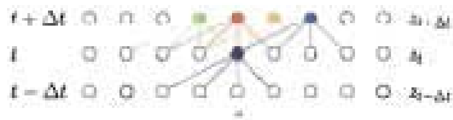
Exchange traditional computational models for UQ friendly implementations

PDE Solver

$$\frac{\partial}{\partial t} z(s,t) = [z(s+1,t) - z(s-2,t)]z(s-1,t) - z(s,t) + F$$

Markov Random Field



Constructing forward models and adjoints

- Very informative in high-dimensional problems
- Can help in building response surface
- Can facilitate MCMC or other UQ algorithms

Exploiting new, heterogeneous, high performance computing architectures

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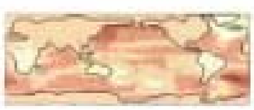
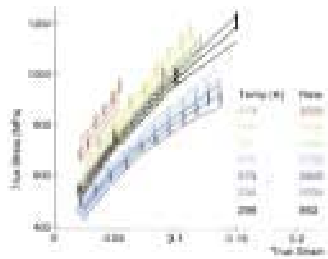
UQ approaches differ depending on the application

Physically based	⟷	Empirically based
Model rich – data poor	⟷	Data rich – model is weaker
Extrapolate?	⟷	Interpolate





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Future Directions for UQ

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- Future Funding opportunities
  - Climate, nuclear energy, material science, greenhouse gas monitoring, situational awareness, data assimilation

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Future Directions: Applications and Capabilities

Computational Physics and Applied Mathematics (CPAM)
Capability Review June 6-10, 2010

Andy White
Deputy Associate Director for
Theory, Simulation, and Computation

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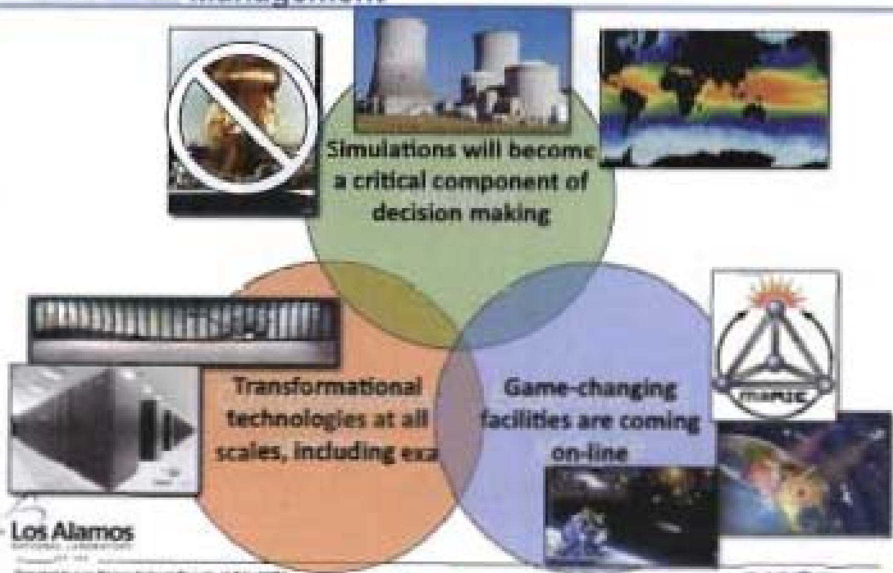
The Next Decade will be a Perfect Storm of Opportunity: Understanding, Prediction & Management



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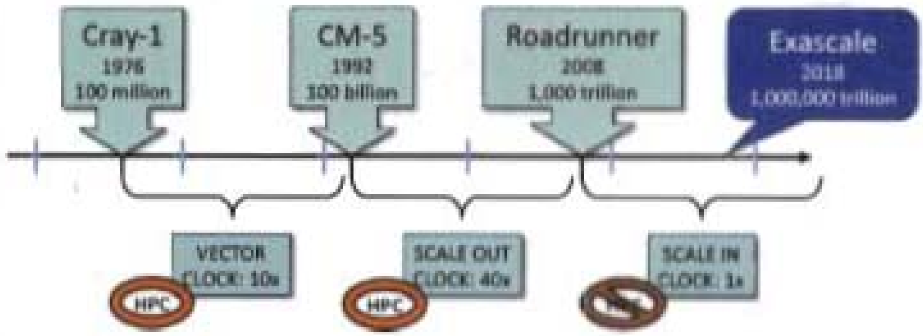
TRANSFORMATION OF APPLICATIONS & TECHNOLOGY

DOE mission and science imperatives require simulation and analysis for understanding, prediction, policy & decision making

- *Climate Change*: Understanding, mitigating and adapting to the effects of global warming
  - Sea level rise
  - Severe weather
  - Regional climate change
  - Geologic carbon sequestration
- *Energy*: Reducing U.S. reliance on foreign energy sources and reducing the carbon footprint of energy production
  - Reducing time and cost of reactor design and deployment
  - Improving the efficiency of the existing light water reactor fleet

- *National Nuclear Security*: Maintaining a safe, secure and reliable nuclear stockpile
  - Stockpile certification and management
  - Predictive scientific challenges
  - Real-time evaluation of urban nuclear detonation
- *Materials*: Understanding and design of materials in extreme conditions
  - Predictive multi-scale materials modeling: observation to control
  - Effective, commercial technologies in renewable energy, catalysts, and batteries

We are at the beginning of a technology transformation.



Computational physics is dependent on the enabling technologies that make it possible.

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This transformation provides challenges & opportunities.

System attributes	2010	"2015"		"2018"	
Performance	2 Peta	200 Petaflop/sec		1 Exaflop/sec	
Power	6 MW	15 MW		20 MW	
System memory	0.3 PB	5 PB		32-64 PB	
Node performance	125 GF	0.5 TF	7 TF	1 TF	10 TF
Node memory BW	25 GB/s	0.1 TB/sec	1 TB/sec	0.4 TB/sec	4 TB/sec
Node concurrency	12	O(100)	O(1,000)	O(1,000)	O(10,000)
System size (nodes)	18,700	50,000	5,000	1,000,000	100,000
Total Node Interconnect BW	1.5 GB/s	150 GB/sec	1 TB/sec	250 GB/sec	2 TB/sec
MTTI	days	O(1 day)		O(1 day)	

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Exascale Initiative Steering Committee

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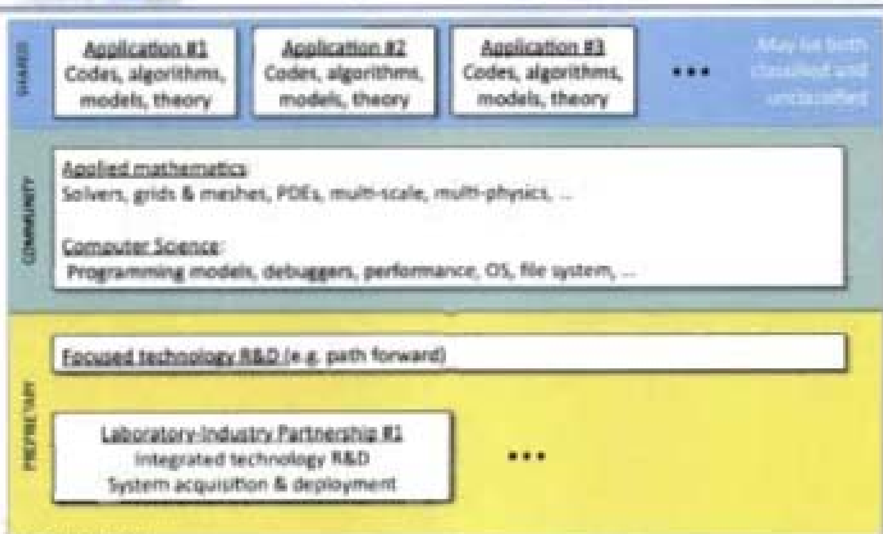
Applications & technologies come together @ exascale



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INTEGRATION & LEVERAGE

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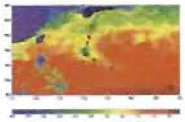
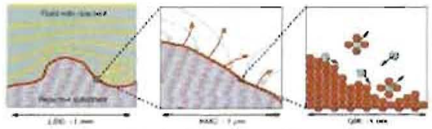
Integration and leverage are critical to success of CPAM.

- Uncertainty quantification
  - Predict climate response to energy technology
  - Certification of aging/evolving stockpile without nuclear testing
  - Energy security
  - Responding to natural and manmade hazards
  - Understanding and "predicting" rare events
- Multi-scale, multi-physics modeling
  - Multiple physics packages in earth system model: ocean, land surface, atmosphere, ice
  - Multiple physics packages in modeling reactor core: neutronics, heat transfer, structures, fluids
  - Atomistic to everyday scales in nuclear energy, materials, ICF & MCF, biology
  - Atomistic to universal scales in astrophysics and cosmology
- Co-design
  - Applications
  - Methods and physical models
  - Programming models
  - Operating systems
  - Memory hierarchy
  - Processors


Storm track in ESM


urban fire


Multi-scale physics modeling

Environmental Stewardship

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UNCERTAINTY QUANTIFICATION

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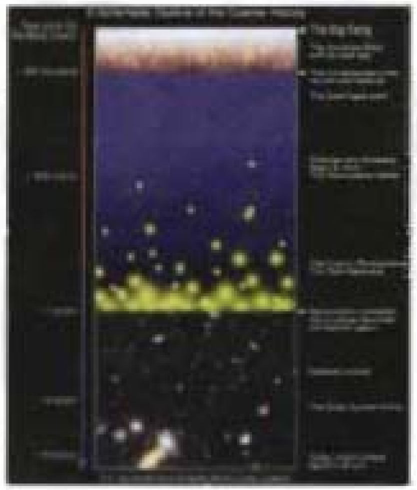
Uncertainty quantification is playing an increasingly key role at LANL.

- UQ has played a key role in LANL activities that combine
  - physical experiments/observations,
  - computational modeling
  - high performance computing
- UQ activities require in-depth collaboration
  - subject matter scientists
  - computational scientists
  - statisticians
- LANL's competitive advantage stems from its broad range of experts and its ability to allow significant, and deep collaboration.
- LANL UQ researchers are leaders in the broader UQ community



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Computational Physics and Applied Mathematics
Capability Review
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There are additional opportunities for uncertainty quantification

	Parametric	Structural	Relational
Theory & models	•Calibrated parameters in models	•Unknown effects omitted from models •Extrapolation	•Multi-scale, multi-physics effects
Algorithms	•Discretization error	•Extrapolation	•Multiple time scales in operator split algorithms
Applications code	•Convergence criteria	•Errors in apps code	•Data mapping among different components
Computation and communication	•Rounding errors	•Silent data corruption	•Race conditions among separate components of system
Operating system & environment	•ECC error rates (chip bit errors)	•System parameters set incorrectly •Chip temperature excursions	•System policy mis-match (e.g. memory management)
Observations & data assimilation	•Statistical variation in experimental data	•Unknown systematic errors in data	•Contextual mismatch of observational and computational data

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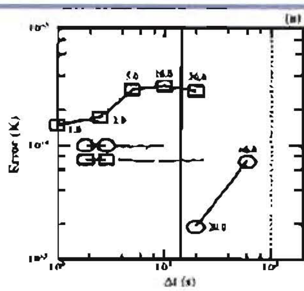
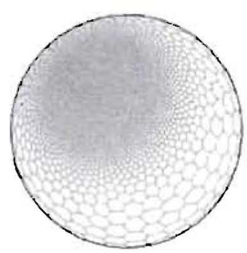
MULTI-SCALE MULTIPHYSICS

Multi-scale and multiphysics are key challenges for future.

- Multiphysics methods and time integration errors:
  - Accurate time integration for multiphysics systems.
  - Relationship between time integratior error, optimal UQ and co-design
- Scale-bridging algorithms on exascale platforms: a test bed for computational co-design
  - A finite-volume solver that is robust for climate applications
  - Particle pushing for Vlasov solve done on Cells to increase dynamic range





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CO-DESIGN

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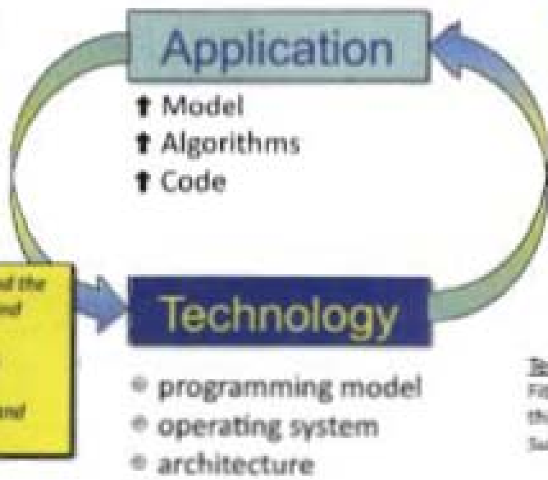
Traditional one-sided approaches will not work.

Application driven:
Find the best technology to run this code.
Sub-optimal



Best
Power?
Performance?
Price?
Prediction?
Productivity?

Now, we must expand the co-design space to find better solutions:
- *new applications & algorithms,*
- *better technology and performance.*

Technology driven:
Fit your application to this technology.
Sub-optimal

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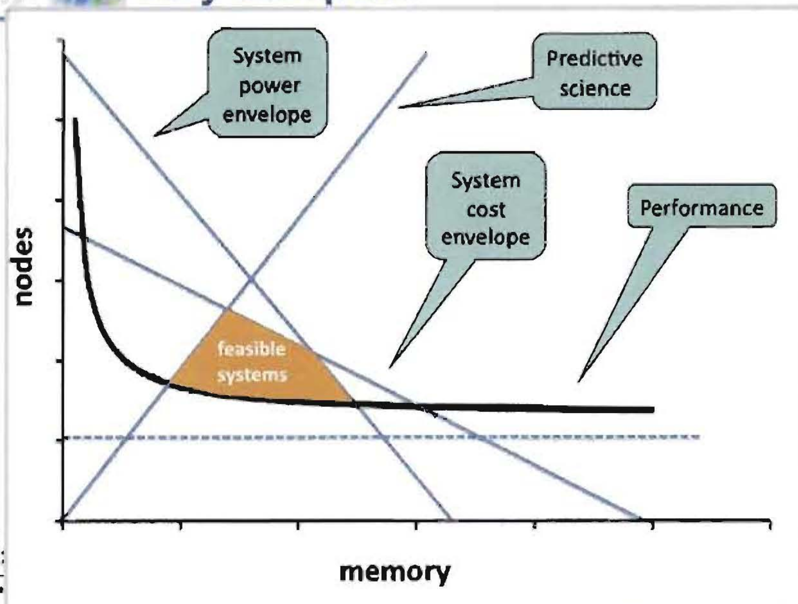
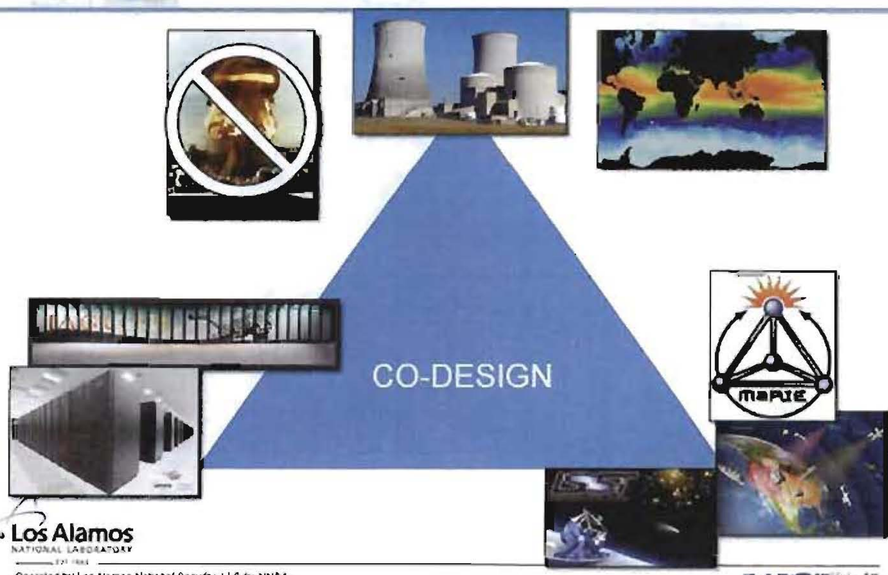
The trade space for exascale is very complex.



Co-design can integrate all aspects of mission & science.



Los Alamos is pursuing a wide variety of integrative activities

- Internal
  - Computational Science WG
  - Information, Science and Technology
  - Roadrunner open science projects
  - LDRD category in co-design
- External
  - Exascale Initiative Steering Committee
  - CASL: Consortium for Advanced Simulation of Light Water Reactors
  - SPEC: Science Partnership for Extreme-scale Computing
  - HMC: Hybrid Multicore Consortium