LA-UR- 10-03508

Approved for public release; distribution is unlimited.

Title:	Computational Physics and Applied Mathematics Capability Review June 8-10, 2010 (Advance Materials to Committee Members)
Author(s):	Various, Primary Responsible Author, Stephen R. Lee
Intended for:	Review Attendees and Committee Members

Los Alamos
NATIONAL LABORATORY
EST. 1943

Form 836 (7/06)

Computational Physics and Applied Mathematics
Self-Assessment Report

CPAM Capability Review

June 8-10, 2010

CY2009-2010

Table of Contents

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):

- *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, and 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 capability 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 5 themes). Yearly written status reports will be provided to the Capability Review 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 1-1 below is illustrative of our multi-programmatic approach, building from our science base.

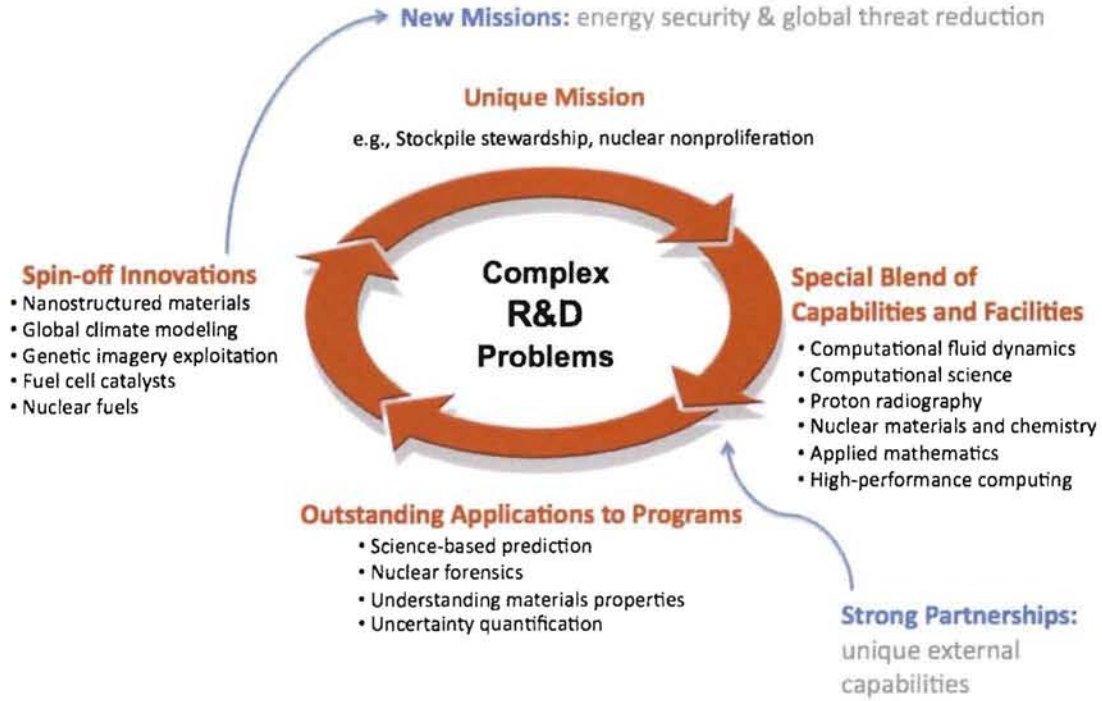


Figure 1. Spin-off innovations based on our core scientific capabilities in support of our unique mission space lead to growth as a capability-based national security laboratory and new mission areas.

We, as a Laboratory, seek 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 Assessment Document

The remainder of this self-assessment document, with the exception of the general challenges and issues section (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*: How the theme area is related 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*: In this section, the status of capabilities within the theme are discussed. 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*: In this section, 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 the document. A list of acronyms used in this document, posters, presentations and other related items are included in the full CPAM Capability Review materials provided separately.

Appendix A contains a document of 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 6 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 previously 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. Here we review some of the astrophysics applications Los Alamos is working on:

- *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; 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 regards 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, 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 Department of Energy 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; 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:

- 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 Sriram Swaminarayan and Tim Germann for molecular dynamics, and work done by Ben 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. Finally, the third thrust is Site Applications. This thrust 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. This is a diverse set of sub-topics. For some of these sub-topics the relevant Los Alamos community resides in one group. For other sub-topics the relevant Los Alamos 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 10 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, one 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-LDRD.

3.1.2 Deterministic Transport. Deterministic transport methods research, and the organizational thread it follows, has 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 the mission of the laboratory 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 90's 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.

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 collisionless 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 nations 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 (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.

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: I) the example of applied mathematics in climate modeling, II) the CNLS, III) the Los Alamos ASCR applied math program.

I. Applied Mathematics in Climate Modeling

(a) 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, DOE-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 [see 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.

(b) 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.

II. The Center for Nonlinear Studies

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 (joint T-5 and CNLS) 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 post-doc level, in addition to group hires, the CNLS have played a key role in providing the right multi-disciplinary post-doc environment combined with access to a variety of computing platforms, and compares well with some of the best post-doc programs in the nation. The CNLS is funded by several overlapping LDRD grants. Each post-doc is supported at the 50% funding level in conjunction with a host from one of the many groups around the laboratory. This ensures that the CNLS becomes involved in some programmatic effort right from the start.

Historically, the 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 who are playing important roles in Applied Math at Los Alamos, at other laboratories, and in academia.

The CNLS Annual Conference has often led to significant new developments in applied math. In the past 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. It can be viewed as nucleating several teams and led to the recruitment of many outstanding post-docs 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 with 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.

III. The Los Alamos ASCR Applied Mathematics program

Office of Science funding in this field is traditionally provided by the Office of Advanced Scientific Computing Research (ASCR). Los Alamos has a long history of ASCR funded projects, originally mostly in PDEs and their numerical analysis. The FY10 total 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 post-docs 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 (see the presentation of Misha Shashkov on ALE methods, and the poster presentation by Konstantin Lipnikov 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 stockpile 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, between Los Alamos and other national labs, as well as strong ties with academia in the US and Europe. It has attracted outstanding post-docs, some of whom 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 necessary capability has evolved through the years to keep pace with evolving requirements that arise from changing laboratory mission activities or out of scientific or technological concerns.

It may be categorized into the following general research areas:

- *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 with in both the computational mechanics and climate simulation communities at Los Alamos.

3.2.4 Computational Plasma Physics. VPIC [Bowers, 2008a], [Bowers,2008b] 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 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. This is carried out jointly by T-5 and XCP-6 plasma physicists. 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 at Los Alamos in the Plasma Physics Team of T-5 Applied Mathematics and Plasma Physics Group. The key Los Alamos 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; (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 just 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 the 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 method, level set method and immersed boundary method. 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 problems, 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 plasma physics team of the T-5 group 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 and 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.

Also, a collaboration team from the 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, England 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. The peer group to be considered in applied mathematics is other National Laboratories such as LLNL and SNL. Each has its strengths and weaknesses. Los Alamos's key strengths are in:

- 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 of the other laboratories. This multidisciplinary environment (of which the CNLS is a good example) provides an incubator for new methods in applied mathematics, especially in areas close to these fields. For example, in problems involving stochastic dynamics, fluctuations, and rare events, there is a very powerful local theoretical and computational expertise, and 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 (now 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 that is published as a result of research areas that impact the laboratory mission and capability has a far-reaching influence on the scientific community. University faculty visit on a frequent basis to conduct technical collaborations. Students seek temporary and permanent positions within the transport group on a regular basis. One of the group's distinguishing characteristics is that research takes place hand-in-hand with code development and implementation. This means that cutting-edge capabilities can be almost immediately leveraged for use in application simulations.

3.3.3 Solvers. As compared to our 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 at Los Alamos, non-Los Alamos packages provide the foundational solver needs is 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 research efforts have provided impact to the ASCI program, and various Office of Science programs is 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. Sandia is actively developing its Sierra framework collection of physics codes to address coupled physics problems. Livermore is also 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 the other NNSA labs, LLNL and SNL, although Los Alamos has not been as coordinated in developing well recognizable software packages for meshing. Of

these our efforts are closest to those of LLNL due to the emphasis of both labs on capturing complex physics in high-speed shock simulations. LLNL has a package called PMesh that has capabilities that are somewhat similar to the capabilities of the Setup team at Los Alamos. Also, the ITAPS (see section 3.1.6) 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. However, CUBIT is mainly focused on unstructured meshes for engineering type parts and is 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. Finally, 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 the Los Alamos it is difficult to assess its overall strength. However, the development of entirely new areas of application of applied mathematics, such as the new network capabilities, suggests overall health. However, two key issues, discussed in more detail below, prevail. The first is the loss of key applied math staff that participated strongly in the CNLS. The second is that not only do we need to replace those staff, but we also need to consider that the new demands faced by the DOE and our nation may require a new generation of applied mathematicians who are very different from what worked in the 80's and 90's. 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 project, 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 directly 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 at the laboratory for the last forty years in an ongoing effort to extend capability, methods and algorithms to meet the changing requirements that arise through continuing evolution of computer capacity and technical or scientific 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 6 years. The code framework includes the latest and most advanced solution methods and algorithms that have been primarily developed by CCS-2 staff 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 at Los Alamos, 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 & 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. The Los Alamos 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 or more, the T-5 group at Los Alamos has been developing methods for optimizing the quality of unstructured 2D and 3D meshes in multi-material domains. In the past few years, this technology is being deployed in Los Alamos 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 at Los Alamos 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 the EES-6 group 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 anyone in the geophysics community and offers a powerful alternative to purchasing multiple geological meshing software products at a huge cost.

Finally, a meshing infrastructure [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. This infrastructure, called MSTK (http://math.lanl.gov/~rao/Meshing-Projects/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 in the world that is available under an open-source license. The current efforts with MSTK 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 issues to all themes in the CPAM capabilities and, as a result, appear in Section 8.0. Here some specific challenges and issues for the PDE theme are discussed.

3.5.1 Applied Mathematics. Over the last decade Los Alamos has lost some of its most important applied mathematicians. In the 2009 report of the CNLS External Advisory Committee, comprised of internationally recognized scientists from academia, this concern was prominently noted:

> "...Among the internal challenges noted by the EAC, 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 the CNLS but it 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?

The 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 a 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: (i) cyber security, (ii) smartgrid dynamics, (iii) cell-signaling, (iv) interdiction of smuggling (v) 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 the CNLS have not been overly successful, largely because a new computer science PhD has very different goals, language and metrics for success compared to a postdoc in, say, statistical physics. 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 with 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 that there is little risk on the overall mission objective. It is essential, then, that funding for the basic research not always be tightly linked to applications. An open approach will provide the freedom and of research.

3.5.3 Solvers. There continues to be many challenges to a healthy solvers community at Los Alamos including fractured efforts and lack of support for direct research from large programs outside of specific programmatic application domains. Future direction for the solvers community at Los Alamos 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 work in three major areas: Efficient solution of a very complicated and coupled three-dimensional diffusion equation in time, Efficient canonical transformation between space-time variables (from satellite data) and canonical variables (needed for the diffusion coefficients in the diffusion equation), Efficient application of data-assimilation techniques to interpolate/extrapolate measurements of electromagnetic wave spectra from a few widely spaced satellites.

3.5.5 Computational Mechanics. At present we 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 at Los Alamos in the immediate post-World-War-II era by Ulam and von Neumann to treat numerically the complexity associated with the 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 1950's, 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 at the Laboratory, 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 in what 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 8 sub 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 National Laboratory 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/or 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 and 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 [Swinhoe2009, Evans2010, Fensin2009a, Fensin2009b, Peerani2009, Swinhoe2009, Lafleur2008, Swinhoe2007, Hendricks2003, Fensin2009c, 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 Los Alamos's 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 at Los Alamos 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 Los Alamos's 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 in Optimization 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, where the goal is to find the shortest route that meets a number of cities, and the protein folding problem, where the goal is to 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, in fact, of relevance in national security. For example, optimization provides more efficient ways to deal with large amounts of data. This is essential in scenarios where the data overtakes the amount of space for storage. Further, high-performance computing is necessary to enhance the security of nuclear weapons. MCMC techniques for optimization are thus key important in Los Alamos's goals and 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. This works supports the biosecurity mission of the laboratory. Influenza kills an average of 40,000 people every year in the United States 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 are 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 the 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. [Bhattacharya2007, Timm2007, Gnanakaran2007, Rousseau2007 Brumme2007, Rousseau2008] The laboratory has been on the forefront of developing theoretical biology as a field, and 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, and 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 such 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 at the laboratory and elsewhere. The problem with this approach is, of course, 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. The laboratory has a long history in carrying out these calculations, and is 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 some 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 [Yesilyurt2009, Solomon2009] and gamma ray transport
    - Codes: MCNP, MCATK
    - Applications: MCNP: criticality safety, radiography, nuclear oil well logging, fission and fusion nuclear reactor design, decontamination, decommissioning, waste transport and storage, medical: radiology (detector design and image reconstruction)
- Thermal X-ray transport [Kelley2010, Densmore2010a, McClarren2009, Densmore2009a, Hykes2009, Densmore2009b, Urbatsch2008, Densmore2008, Densmore2007a, Densmore2007b]
    - 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: 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. Los Alamos's KMC work has been in the early development of rate catalogs, the development of methods for accelerating KMC [e.g., Chatterjee2010]. 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 of this breadth include the current activities:

- 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,
- Statistical Physics (Nonequilibrium): Kinetics of colloids and granular materials,

The impact of this work varies with the application. Key components of the above effort 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 the 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.

The Statistical Sciences Group 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.

In addition, Monte Carlo theory has been applied to much project Los Alamos statistical work, as noted above. 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). (Krzakala2009)

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 [Das2005]. Apart from achieving unprecedented speed-ups, these Monte Carlo studies will likely be the foundation for future implementation of quantum annealing on quantum computers.

C.D. Batista and R.D. Somma, both researchers in 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 [Somma2007, Somma2008]. This result implies that quantum annealing, if implemented on a quantum computer, is at least as powerful as classical simulated annealing. In fact, [Somma2008] rigorously showed that some instances of quantum annealing always provide speed-ups with respect to the classical annealing method. The mapping in [Somma2007] 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. So far Phylogenetics has been used in biology for metagenomics, attribution, understanding pathogen evolution, and studying correlations relevant to vaccine development; and 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 lab 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 lab 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 [Bazavov2009] 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 the Lawrence Livermore National Laboratory (LLNL) and the United Kingdom's Atomic Weapons Establishment (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 don't have anyone developing parallel KMC methods, for example, as they do at Livermore or University of Toledo, but it is probably enough to import this technology, as we have. Los Alamos is known for some of the key development work in KMC, and Voter has written a well-known introductory article on KMC, for example 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 justifications, 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: The lab offers a wide number of resources to implement large-scale computational methods. From smaller clusters in the research groups to Roadrunner supercomputer, Los Alamos's researchers have access to execute their codes in high-performance computing centers. This unique environment at the lab 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, the laboratory is currently still in the forefront of this field.

4.3.8 QCD. These calculations are large and require huge collaborations. Previously Los Alamos was a lead of a small collaboration that was one of the leaders of the field, but recent move 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. The Jayenne Project's software is powerful, robust, and massively parallel; it is multi-dimensional, runs on Adaptive Mesh Refinement (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 Department of Energy's 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, the world's first computer with sustained petaFLOP/s performance. 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 mostly located in T and MST divisions, and it 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 Laboratory programs, such as weapons, surveillance, and other computational applications, should continue to sustain and advance existing capabilities.

4.4.5 Optimization. Los Alamos is now hosting a number of staff members with experience in Monte Carlo methods that simulate classical or quantum annealing processes for optimization. Some of these members 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, for example, H. Nishimori's research group in the Tokyo Institute of Technology, Japan. Another group is E. Tosatti's group in SISSA, Italy. Some of Los Alamos's recent contributions have put the lab 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: The lab offers a wide number of resources to implement large-scale computational methods. From smaller clusters in the research groups to Roadrunner supercomputer, Los Alamos's researchers have access to execute their codes in high-performance computing centers. This unique environment at the lab 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.

4.4.6 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 with whom we have contact. This work is part of an 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 part of the 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. While working in 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

There are many issues for the MC theme that are common to all themes. Those issues appear in Section 8.0. Here, some specific issues for MC are discussed.

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 that are now being worked on. Some modifications to the cross section capabilities will be required.

4.5.2 Kinetic MC. No issues that are not common ones, addressed 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 also 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 that are not common ones, addressed in Section 8.0.

5.0 Theme 4: Molecular Dynamics

(Theme Leader: Tim Germann, T Division)

Like its predecessor, the Monte Carlo (MC) 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 also 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 his 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 other 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 also how Navier-Stokes begins to become less accurate for stronger shocks. MD work at Los Alamos continued to growth 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, and so on. Here we will focus on five particularly active fields of research at Los Alamos, 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

- Advanced Algorithm Development, specifically AMD

Accelerated Molecular Dynamics (AMD) refers to a class of methods, developed beginning 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 1990's), 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: (1) 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 (2) 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, and 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 Grant Smith at Utah and Don 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 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 that are 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. These also require an enhanced fundamental understanding of these materials. Finally, the DHS and DoD must deal with a wide-range of unusual HE formulations (Improvised Explosive Devices, IED's) whose properties are not well understood. Improved means for assessing the performance characteristics, sensitivity and disposal issues, and methods for detection would again 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 – mission for Los Alamos' center for biosecurity center. Our MD simulation based approaches to characterize biomass and its degradation for biofuels is closely tied to Los Alamos'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 LANLs current civilian nuclear energy programs and will continue to be so as the importance of nuclear energy is anticipated to remain significant for the nations 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 the simulation predictions, but it will also assist interpretation of these experiments.

5.2.2 Material Dynamics. The areas of importance for dynamic materials modeling which have particular relevance to science campaigns, the ASC program and the DPE program are (1) the physics of plastic flow and melting in shocked materials [Holian, 1998], (2) the physics and kinetics of phase transformations in metals [Kadau, 2002, 2007a], (3) the physics of correlations and phase transformations in strongly coupled plasmas, (4) the physics of damage nucleation and growth in metals [Germann, 2005], (5) the physics of interfacial friction [Hammerberg, 2004], (6) the physics of Richtmyer-Meshkov and Rayleigh-Taylor [Kadau, 2007b, 2010] instabilities, (7) the physics of particulate ejection at shocked interfaces [Swaminarayan, 2008], (8) the 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 of these areas of non-energetic and energetic materials have been addressed in the past three decades at Los Alamos by T-Division 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 at Los Alamos as well as the first massively parallel Connection Machine simulations of shock-wave and interfacial phenomena, and 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 in the scientific community have been in the characterization of the development of substructure in shock loading and release in metals, the kinetics of phase transformations, the 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, for example, 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; Brad Holian was elected President of the SCCM Topical Group, a position normally held by experimental shock physicists, and Tim 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 HE's 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 especially, there are a large number 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 complex scenarios. Development of improved models for these conditions has been one of the major challenges for the current NNSA ASC program, and has attracted growing interest from the DoD community 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, and 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 for a successful evaluation. This would require very large scale three-dimensional simulations with an accurate description of phenomena at interfaces. Most 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 for this, where we have limited data available because of the inherent instability of the materials.

Atomistic simulations can, in principle, 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 Equation of State (EOS) of both the reactants and the primary products. However, clusters of solid products (soot, metal oxides) are likely much larger than this and cannot be included in the analysis. Similarly, reactive molecular dynamics simulations can now be performed on many millions of atoms. This gives us a base understanding of the

chemical reactions, but is not sufficient to understand propagation or coupling to gradients in stress or composition. Finally, 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 but highly active group of two members of T-1 and one member of MST-8, funded from various DOE Office of Science and LDRD sources. Impact on the scientific community has been substantial. This can be seen in the large number invitations to give talks or teach courses on these methods at international venues, to collaborate on outside proposals, and to collaborate. 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., see [Bai, 2010]) and evolution of post-shock plasticity. Neither of these processes can be easily treated with molecular dynamics nor existing kinetic modeling methods.

5.3 Comparison with Peers

5.3.1 Nuclear Energy. Compared to other institutions the present Los Alamos 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. LANL has 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 on this work were given by Holian in 1999 and 2001. Since that time, national labs 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 their flagship supercomputer platforms for such 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. The primary competition for the Los Alamos HE MD program is the LLNL effort, which is primarily funded through their ASC and DoD (JMP-MOU)

program. Their work often highly complements the Los Alamos 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 HE's would not normally generate, but which are important for NIF applications. SNL has a similar program to Los Alamos, but it is much smaller since 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. Carter White at NRL), but do not address the subject in a general way. There are several university professors 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 leading groups in the world on implementing all-atom molecular dynamics to study immunological and biofuel related problems. With respect to immunological problems, we 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 the AMD methods were invented at Los Alamos, and Los Alamos remains the undisputed world leader in the development and application of these methods. The most substantial AMD development efforts outside of Los Alamos are probably those of Kristen Fichthorn at Penn State, who develops hyperdynamics methodologies, and Andrew McCammon at UCSD, who develops an adaptation of hyperdynamics for biomolecular systems. The closely related adaptive kinetic Monte Carlo (AKMC) approach, discussed above, is most strongly represented in the groups of Graeme Henkelman at University of Texas and Normand 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 front is on how one extends some MD based methodologies that have sucussfully 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. We have made significant advancements in carbohydrates so far. In the second front concerns with 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 (for a recent review, see [Perez, 2009]). Time scales of microseconds are now routine, and time scales beyond seconds are possible in favorable cases. The 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 kind of 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 an LDRD-DR project on "Spatio-temporal frontiers of atomistic simulations in the petaflop computational world" (T. C. Germann, PI). All three AMD methods will continue to improve in their range and power as they are developed further and as more experience is gained with them. 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

Some challenges and issues are common to all themes in CPAM, and are covered in Section 8.0. Here some specific MD challenges and issues are discussed.

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. For example, 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 in by now standard algorithmic implementations of NEMD. Over the period of the next ten years, one can reasonably expect an order of magnitude increase in both due to platform enhancement. However, the 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 Los Alamos 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, which already show promise in the area of damage nucleation and localization, will be frontier areas in NEMD research and dynamic materials modeling in the future driven by Los Alamos NEMD research efforts. A key challenge has been retaining a critical mass of staff in this area, a problem exacerbated by retirements (Holian, Lomdahl) and departures (or extended leaves) of early and mid-career staff (Kadau, Strachan, Sewell) who were active in both 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 to limited-term staff of MD postdocs such as Marc Cawkwell, Ben Liu, Danny Perez, Chris Taylor, and Jian Wang, and recruitment of several new postdocs.

5.5.3 Energetic Materials. The core technical challenge presented 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 much of the information that cannot be obtained from experiment. This requires well-validated models that can be linked across length and timescales. Atomistic simulations can provide strong guidance on these issues, 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 the chemistry and microstructure of these materials is critical for the development of predictive models.

Current reactive molecular dynamics simulations are limited to either 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 the detonation propagation characteristics that are 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). Simulations at those scales 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 that are 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, and this has been the major focus of the Los Alamos program. Future emphasis should be placed on improving the accuracy (and complexity) of the non-reactive atomic potential functions (adding polarization functions, allowing adjustable charges), on understanding the sensitivity of the results to the input potential functions and input geometries, and on quantifying the uncertainties of the results of the models and their 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 probably 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 the folding of small proteins and individual secondary structural motifs such as short helices, β-hairpins and β-turns. One of the major challenges is to 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 facing the AMD methods 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, for example. Thus, a substantial part of the AMD development effort at Los Alamos is currently directed at

making progress on this low-barrier problem. Various attacks on the problem are being pursued, but one of the main themes is the 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 is a simulation technique that – as the name suggests – uses discrete events as a main driving force to simulate the evolution of a complex system. The notion of discrete event simulation and most of the theoretical underpinnings have been established in the 1970s and 1980s. Discrete event simulation is used predominantly for engineered systems that follow a set of prescribed rules, such as the Internet and communication networks in general, 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 discrete event simulation, 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 in 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 will focus mainly on concrete application codes in this section. For a general introduction to discrete event simulation, we refer the reader to [Banks et al, 2004].

DDES at Los Alamos has a tradition that dates back at least decades. Perhaps the best-known early example of a discrete event simulation project 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 at Los Alamos. They can be grouped into (i) Technical Domain Applications, (ii) Agent-based applications, and (iii) Simulation and Design Frameworks. In the following subsections we present a few example codes for each of these groups.

Under technical domains, the FastTrans project grew out of the legacy of the TRANSIMS transportation simulation code. FastTrans simulates vehicular traffic on a nationwide level. Our second example, the telecommunications simulation code MIITS (Multi-scale Integrated Information and Telecommunications System) has been used to simulate the nation's communication fabric. The third technical domain code, 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). Our final example in technical domain codes is CyberSim, which simulates the spread of malware through technical and online social networks.

Agent-based simulation codes focus on simulating the actions and thought processes of agents, such as humans. Our first example is the well-known EpiSims code, which simulates the spread of an epidemic, such as H1N1 through a population of millions of human agents

who go about their daily activities. Our second agent-based tool AFS (Agent Framework for Simulation) simulates the complex processes of an intelligent agent, such as a dam operator. Our third example, ActivitySim, generates activities for a population of millions of humans (which can be used by EpiSims) based on optimizing an objective function.

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

Discrete event simulation (DES) is a key technology component in the predictive science objective of Los Alamos's IS&T thrust. A goal of the Laboratory 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. At Los Alamos, FastTrans is one of the key modules in a suite of simulators that have been used to provide detailed analysis to the Department of Homeland Security for quick turn-around "what-if" scenario simulations.

6.1.2 MIITS: Multi-scale Integrated Information and Telecommunications System. MIITS is a SimCore-based discrete event simulation 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 to 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. In this project, 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 on each other: we are 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. One of Los Alamos's overarching goals is to remain the nation's premier national security laboratory of choice. This places it in a 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. The CyberSim simulation tool 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 missions of Los Alamos 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 United States' Department of Homeland Security 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, or alternatively speaking: there is a demand for the service that the network supplies. This demand is largely generated by people as part of their daily activities, such as driving to work, using energy to cook or to heat the house, using water and sewage systems, making phone calls, etc. Thus, an accurate model for the 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 Information Science and Technology 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 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.

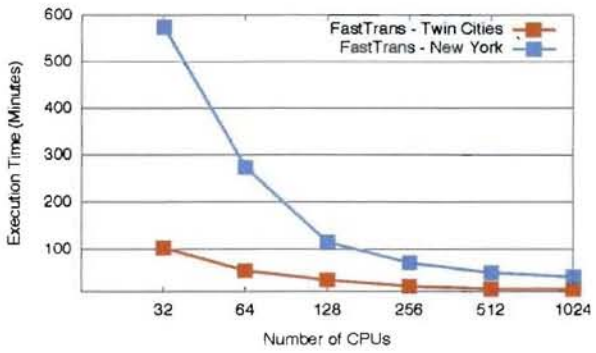
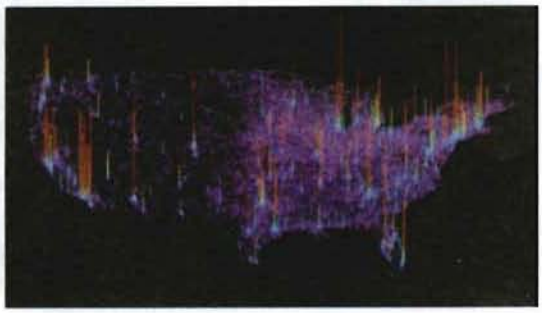


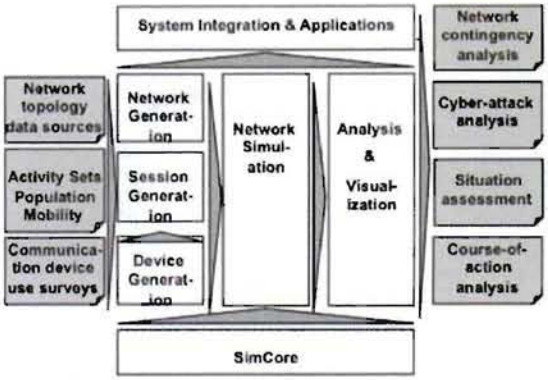
Figure 2.

Performance scaling with increasing cluster sizes (shown in the figure above) has been encouraging. 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 [Thulasidasan2010]. 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: Multi-scale Integrated Information and Telecommunications System. 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 of the spectrum, 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 (1) methods for design, analysis, and development of current and future large-scale communication networks and (2) 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 to 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 [Waupotitsch2006]. The left panel of the figure above shows an example simulation result for a Public Switched Telephone Network (PSTN) model (CONUS stands for 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' modular design provides the following advantages:

- Directly interoperable with other infrastructure simulations that are built on SimCore technology (such as ActivitySim, FastTrans, DemandSim) as well as through Hydra web services with other NISAC tools (such as 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: Malware Propagation on Online Social Networks. 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. The figure below shows an example of the geographic spread of an malware propagated through online social networks after a few days.

Figure 4.

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 which are routinely published by reliable sources such as the National Vulnerability Database (online at 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 which shows the time evolution of the malware spread, its severity, the businesses likely to be affected the most etc to the analyst.

The CyberSim suite has been used to model real world social networks such as email contact networks and online social networks such as Twitter and Facebook. 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. The suite 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 at Los Alamos 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 our research using the CyberSim tool has been very encouraging and we have been invited to present our results as a technical paper in the Telecom, Web, Networks Track of the WinterSim 2010 (WSC 2010) conference [Santhi2010].

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 [Eubank2004; Barret2005; Stroud2007; DelValle2007; Mniszewski2008a; Mniszewski2008b].

The synthetic population consisting of 265,796,301 individuals residing in households in the contiguous United States and District of Columbia 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, the type, and the location of each assigned activity. There are seven types of activity: home, work, shopping, visiting, social recreation, school, and college; plus a ninth 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 (synthetic population based on census data, business locations based on business directory data, and activity schedules based on the National household Transportation Survey data), 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

---

[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).

6.2.6 The Agent Framework for Simulation (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 Agent Framework for Simulation 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 [Muller1996]). 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. The graphic on the below depicts an example of the Hydro Operator responding to a flood control scenario.

casual contacts. EpiSimS has been used to analyze the impact of disease spread for different diseases 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 [Eubank2004; Barret2005]. 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 U.S. population [Stroud2007, Mniszewski2008; Mniszewski2008]. 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 the figure below.

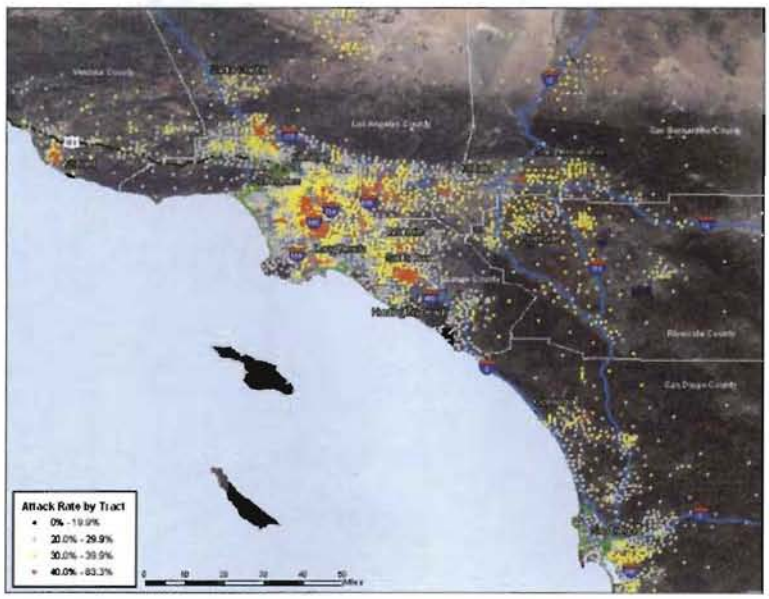


Figure 5.

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 United States population [DelValle2009; DelValle2010]. 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.

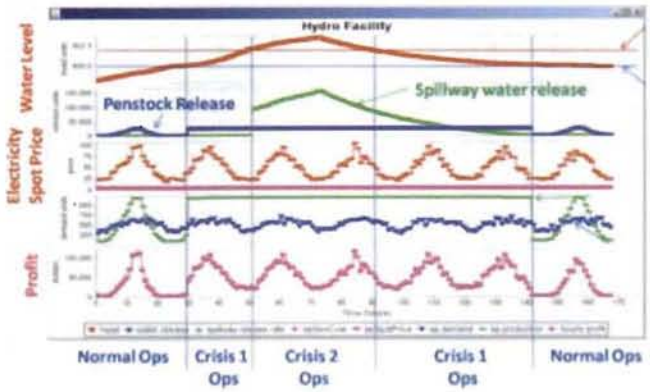


Figure 6.

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. The image below depicts the modeled spread of pandemic influenza.

Figure 7.

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 U.S. healthcare system, HCSim, for the Department of Homeland Security.

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, discrete event simulations (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, Services and Infos. An Entity is an object or component in the system that we want to model. A Service represents the functionality or behavior of an Entity. An Info is 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 (i.e., a family). 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 (ex. age, gender). Each activity has an associated utility function (ex. sigmoid) that gives a certain amount of utility depending on how long the activity is being executed. An activity also has a priority function (ex. 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 (ex. attending work/school on weekdays, shopping once per 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 (ex. local improvement, gradient method) that assembles and modifies scheduled activities based on priorities and constraints; 2) an objective function (ex. a weighted sum of utility, priority, and travel contributions) used to evaluate a suggested schedule for replacement; and 3) an exit condition (ex. 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 (ex. 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 2.6M individuals, with about one million households and more that 480 thousand different locations. The simulation was executed on the Los Alamos Institutional Computing Coyote cluster and was run for 10 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 Simulation Framework: SimCore. SimCore is a generic discrete event simulation 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 nation-wide socio-technical infrastructure
- 100s 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 e.g. overloaded network.

In a short, 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 a new functionality is very easy and does not require changing much of the existing code (changes are localized). E.g. 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, event if it does not fit well into the SimCore design. Unknown approximation techniques may require unforeseen implementation steps.
- Conceptual simplicity: so that as it grows, it doesn't become an impenetrable jungle. The places where the different components interact (like different MIITS protocols)

should be well defined. This is important so that the simulations can grow without anybody having to know details about all parts of it.

- 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 discrete-event simulation 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 discrete event simulation 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 therefore largely determined by the simulation engine used, and 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 [Smith1995], developed at the Los Alamos National Laboratory, 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 [Prevedouros1999], VISSIM [Concepts2001] and PARAMICS [Cameron1996]. An alternative approach to traffic simulation, where road links are modeled as queues, was described in [Eissfeldt2006]. A time-stepped, parallel implementation of this approach is described in [Cetin2002]. [Charypar2006] first proposed a discrete-event queue-based model for a sequential, single-processor environment. A parallel discrete-event approach to microsimulations was described in [Perumalla2006], 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 upto 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: Multi-scale Integrated Information and Telecommunications System. 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, which 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; it is a stand-alone tool that does not integrate well with other simulator tools. OPNET is a very successful tool used by industry players to assess their small- to mid-size networks; it 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 short-comings of network simulators, including GTNetS (good scalability), SwIM (good wireless channel models), pdns (parallel computing), OMNet++ (good shared-memory scalability).

6.3.3 BotSim. For the moment, we have not seen any other work that attempts to model and simulate P2P botnets at such a high resolution as we did in BotSim. Our work has been published at the **IEEE/IFIP International Conference on Dependable Systems and Networks** (DSN'09). Another paper is currently under review.

6.3.4 CyberSim: Malware Propagation on Online Social Networks. 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 the Los Alamos CyberSim tool makes it extremely flexible while at the same time providing comprehensive and realistic analysis capabilities.

For example, using the CyberSim tool, 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, the CyberSim tool is unique in providing this kind of capability.

6.3.5 EpiSims. There are several research teams including [German2006], [Ferguson2005], [Longini2004], [Lee2008]. However, most of these 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 The Agent Framework for Simulation (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 [Barrett2004]. ActivitySim builds and extends the utility-driven approach to activity scheduling by [Joh2001] 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 [Charypar2005]. Bhat et. al. (University of Texas) employs econometric models for activity patterns of adults only at the household and individual level in CEMDAP [Baht2004]. 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 [Feil2009]. 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 Simulation Framework: 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 [Thulasidasan2009a], [Thulasidasan2009b], and [Thulasidasan2010].

6.4.2 MIITS: Multi-scale Integrated Information and Telecommunications System. MIITS has been used in the Tier asset ranking studies as part of the National Infrastructure Simulation and Analysis Center (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 [Ramaswamy2007] and the Internet ranking methodology [Yan2009]. 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 the figure below.

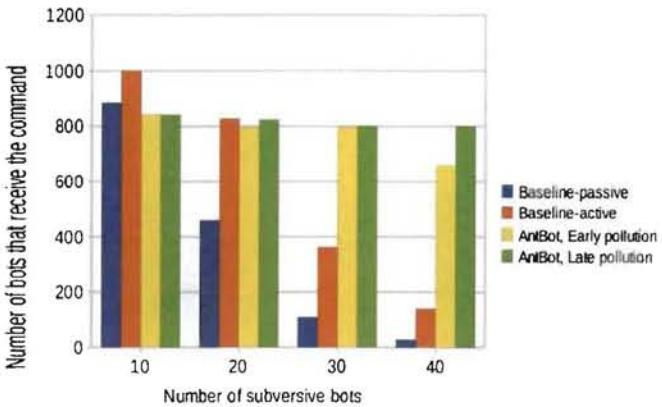


Figure 8.

6.4.4 CyberSim: Malware Propagation on Online Social Networks. 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 therefore 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 and continued funding is required to maintain and enhance our cyber analysis capabilities.

6.4.5 EpiSims. Currently, 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 their surrounding environment (e.g., disease). We have been trying to extend EpiSimS for a while but due to lack of funding we have not be able to do so.

6.4.6 The Agent Framework for Simulation (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. User 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 [Galli2009]. 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 Simulation Framework: SimCore. The library is a relatively mature code, with half a dozen simulators running on top of it. Nevertheless, there are various improvements that we are working on, or planning to. 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

Discrete event simulation (DES) is a key technology component in the predictive science objective of Los Alamos's IS&T thrust. A goal of the Laboratory 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 these cases, an engineered system enables the natural or human attackers to amplify damage. Discrete event simulation 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 topic 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 under utilized.

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 work- for-others sources resulting in spotty, inconstant 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.

Some challenges and issues are common to all themes in CPAM, and are covered in Section 8.0. Here some specific DES challenges and issues are discussed.

6.5.1 FastTrans. No issues except those that common to all themes and therefore covered in Section 8.0.

6.5.2 MIITS: Multi-scale Integrated Information and Telecommunications System. 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 Los Alamos LDRD and DOE National SCADA Testbed (NSTB) in addition to the NISAC program, but of course guaranteeing a steady funding stream remains a challenge.

6.5.3 BotSim. One challenge of BotSim 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 of BotSim is to model the activities and geographic distribution of both normal peers and bot machines in a realistic manner. In the future, we will continue to improve BotSim along these two lines.

6.5.4 CyberSim: Malware Propagation on Online Social Networks. 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 friends 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. One of our greatest non-technical challenges is funding. Some of our 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 The Agent Framework for Simulation (AFS). No issues except those that common to all themes and therefore 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 Simulation Framework: SimCore. No issues except those that common to all themes and therefore 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 that 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.

Table 1.

Approximate Code Category	Approximate Number of Codes
CFD	25
PDE	15
MC	10
MD	8
DES	11
Other (either do not fit in any of the above categories or fit in too many simultaneously)	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 7-1 below.

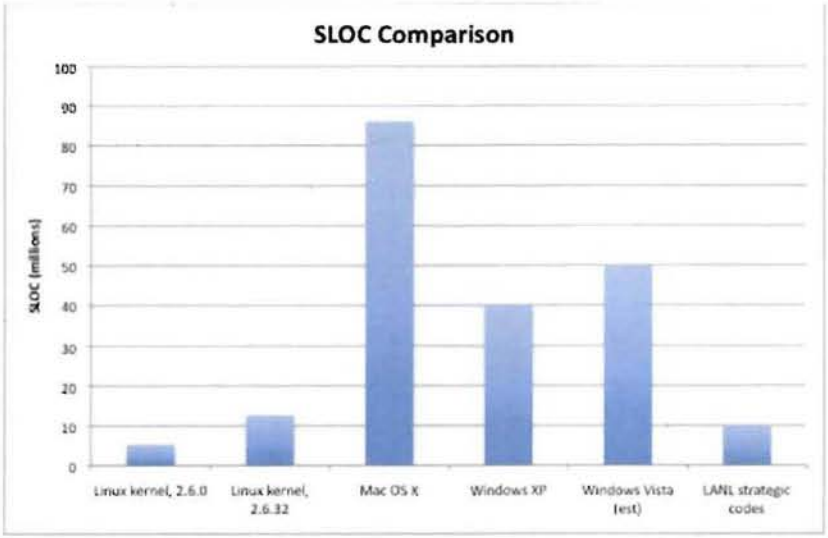


Figure 9. SLOC at Los Alamos versus other well-known software projects. Note the growth in SLOC between Linux versions, which is common.

In this figure, 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.

Figure 7-2 shows a relative breakdown of SLOC by Los Alamos technical division.

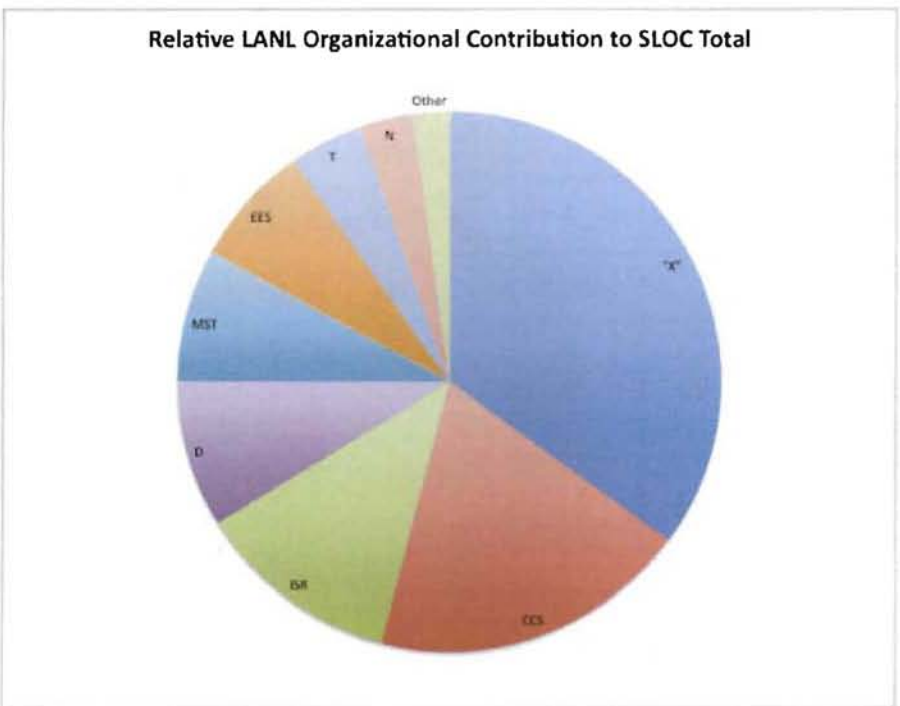


Figure 10. Relative SLOC comparisons by Los Alamos technical Division ("X" refers to a combination of the recently bifurcated X Division: XCP, X Computational Physics, and XTD, X Theoretical Design).

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 Los Alamos 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 the 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 LANS 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:
    - 6 integrated codes with both commercial and non-commercial licenses from CCS, T, and XCP Divisions. The codes have multiple users, form 10's to 1,000's.
    - 9 integrated codes licensed for open source distribution (GPL, LGPL, and/or BSD licenses) from CCS, EES, HPC, MST, and T Divisions.
- MC:
    - 3 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 at Los Alamos to date (e.g. MCNP).
    - 5 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.
    - 5 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 into too many simultaneously):
    - 6 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). This information is a clear indicator of the reputation and strength of Los Alamos in this area.

During this review, two classes of integrated codes were assessed:

- Climate, Ocean, and Sea Ice Applications
- 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 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 at LANL 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, is 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. Los Alamos has 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 the effort, the technical scope, and the approach are different in this case. 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 (and it does work), 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 it works, it is unique to the Los Alamos 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 many 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 US 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 Los Alamos 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. These are serious issues that must be resolved.

9.0 References

Ahn, H.T. and M. Shashkov, "Multi-material interface reconstruction on generalized polyhedral meshes." Journal of Computational Physics 226, 2096-2132 (2007).

Bo, W., H. Jin, et al., "Comparison and validation of multi phase closure models." Computers & Mathematics with Applications 56(5), 1291-1302 (2008).

Campbell, J.C. and M.J. Shashkov, "A tensor artificial viscosity using a mimetic finite difference algorithm." Journal of Computational Physics 172(2), 739-765 (2001).

Caramana, E.J., D.E. Burton, et al., "The construction of compatible hydrodynamics algorithms utilizing conservation of total energy." Journal of Computational Physics 146, 227-262 (1998).

Cummins, S.J., M.M. Francois, et al., "Estimating curvature from volume fractions." Computers & Structures 83(6-7), 425-434 (2005).

Densmore, J.D., J.S. Warsa, et al., "Stability analysis and time-step limits for a Monte Carlo Compton-scattering method." Journal of Computational Physics 229(10), 3691-3705 (2010).

Dijkstra H.A. and W. Weijer, "Stability of the Global Ocean Circulation: Basic Bifurcation Diagrams," Journal of Physical Oceanography, 32 933-948 (2005).

Dukowicz, J.K., and J.R. Baumgardner, "Incremental remapping as a transport/advection algorithm." J. Comput. Phys., 160, 318–335 (2000).

Dyadechko, V. and M. Shashkov, "Reconstruction of multi-material interfaces from moment data." Journal of Computational Physics 227(11), 5361-5384 (2008).

Evans, K.J., D.W.I. Rouson, A.G. Salinger, M.A. Taylor, W. Weijer and J.B. White III, "A scalable and adaptable solution framework with the components of the Community Climate System Model," Lecture Notes in Computer Science 5545, 332-341 (2009).

Francois, M.M. and B.K. Swartz, "Interface curvature via volume fractions, heights, and mean values on nonuniform rectangular grids." Journal of Computational Physics 229(3), 527-540 (2010).

Francois, M.M., R.B. Lowrie, et al., "A Material Interface Transition Algorithm for Multiphase Flow." Proceedings of the Asme Fluids Engineering Division Summer Conference -2008, Vol 1, Pt a and B: 173-180 (2009).

Glimm, J., J.W. Grove, et al., "Robust Computational Algorithms for Dynamic Interface Tracking in Three Dimensions." SIAM J. Sci. Comp. 21, 2240-2256 (2000).

Glimm, J., J.W. Grove, et al., "Interface Tracking for Axisymmetric Flows." SIAM J. SciComp 24, 208-236 (2002).

Grove, J.W., "Pressure-Velocity Equilibrium Hydrodynamic Models." Acta Mathematica Scientia 30B(1) (2010).

Hecht, M.W, D.D. Holm, M.R. Petersen and B.A. Wingate, "Implementation of the LANS-α turbulence model in a primitive equation ocean model," J. Comput. Phys. 227, 5691–5716 (2008a).

Holm, D.D., "Fluctuation effects on 3D Lagrangian mean and Eulerian mean fluid motion." Physica D 133, 215–269 (1999).

Knoll, D.A. and Keyes, D.E., "Jacobian-free Newton-Krylov methods: a survey of approaches and applications." J. Comput. Phys. 193:2, 357-397 (2004).

Knupp, P., L.G. Margolin, et al., "Reference Jacobian optimization-based rezone strategies for arbitrary Lagrangian Eulerian methods." Journal of Computational Physics 176(1), 93-128 (2002).

Lipscomb,W.H. and T.D. Ringler, "An incremental remapping transport scheme on a spherical geodesic grid." Mon. Wea. Rev. 133, 2335–2350 (2005).

Livescu, D. and J.R. Ristorcelli, "Buoyancy-driven, variable density turbulence," J. Fluid. Mech. 591, 43-71, (2007).

Livescu, D. and J.R. Ristorcelli, "Variable-density mixing in buoyancy-driven turbulence," J. Fluid Mech. 605, 145-180 (2008).

Livescu, D., J. Mohd-Yusof, and T. Kelley, "Direct Numerical Simulations of Compressible Reacting Turbulence with type Ia supernovae microphysics," Invited paper at the 14th SIAM Conference on Parallel Processing for Scientific Computing (PP10), Seattle, WA, February 24-26, 2010.

Livescu, D., J.R., Ristorcelli, R.A., Gore, S.H., Dean, W.H. Cabot, and A.W. Cook, "High-Reynolds number Rayleigh-Taylor turbulence," J. Turbul. 10(13), 1-32 (2009).

Livescu, D., J.R. Ristorcelli, M.R. Petersen, and R.A. Gore, "Variable-density Ray-leigh-Taylor turbulence at moderate Atwood numbers," to appear in Phys. Scr. (2010).

Loubere, R. and M.J. Shashkov, "A subcell remapping method on staggered polygonal grids for arbitrary-Lagrangian-Eulerian methods." Journal of Computational Physics 209(1), 105-138 (2005).

Loubère, R., P.-H. Maire, et al., "ReALE: A reconnection-based arbitrary-Lagrangian-Eulerian method." Journal of Computational Physics 229(12), 4724-4761 (2010).

Lowrie, R.B. "Tracer Advection using Characteristic Discontinuous Galerkin," Proceedings of Partial Differential Equations on the Sphere, Santa Fe, NM, 2009.

Lowrie, R.B. and J.D. Edwards, "Radiative shock solutions with grey nonequilibrium diffusion." Shock Waves 18(2), 129-143 (2008).

Lowrie, R.B. and R.M. Rauenzahn, "Radiative shock solutions in the equilibrium diffusion limit." Shock Waves 16(6), 445-453 (2007).

Margolin, L.G. and M. Shashkov, "Second-order sign-preserving conservative interpolation (remapping) on general grids." Journal of Computational Physics 184(1), 266-298 (2003).

Mohd-Yusof, J. and D. Livescu, "Adapting the CFDNS compressible Navier-Stokes solver to the Roadrunner architecture," Invited paper at the 21st International Conference on Parallel Computational Fluid Dynamics (Parallel CFD 2009), Moffett Field, CA, May 18-22, 2009.

Nadiga, B.T., M.A. Taylor and J. Lorenz, "Ocean modelling for climate studies: Eliminating short time scales in long-term, high-resolution studies of ocean circulation." Mathematical and Computer Modelling, 44(9-10), 870-86 (2006).

Petersen, M.R. and D. Livescu, "Forcing for statistically stationary compressible isotropic turbulence," to appear in Phys. Fluids (2010).

Petersen, M.R., M.W. Hecht and B.A. Wingate, "Efficient form of the LANS-α turbulence model in a primitive-equation ocean model," J. Comp. Phys. 227, 5717–5735 (2008).

Reckinger, S., D. Livescu, and O. Vasilyev, "Compressibility effects on single mode Rayleigh-Taylor instability using an adaptive wavelet-based method," to appear in Phys. Scr. (2010).

Reisner, J., A. Wyszogrodzki, V. Mousseau, and D. Knoll, "An efficient physics-based preconditioner for the fully implicit solution of small-scale thermally driven atmospheric flows." J. Comput. Phys. 189, 30-44 (2003).

Ringler, T., J. Thuburn, J. Klemp and W. Skamarock, "A unified approach to energy conservation and potential vorticity dynamics on arbitrarily structured C-grids," Journal of Computational Physics, 229, 3065-3090 (2010).

Ringler, T., L. Ju and M. Gunzburger, "A multiresolution method for climate system modeling: application of spherical centroidal Voronoi tessellations," Ocean Dynamics 58(5-6), 475-498 (2008).

Schofield, S.P., R.V. Garimella, et al., "A second-order accurate material-order-independent interface reconstruction technique for multi-material flow simulations." Journal of Computational Physics 228(3), 731-745 (2009).

Shashkov, M., "Closure models for multimaterial cells in arbitrary Lagrangian-Eulerian hydrocodes." International Journal for Numerical Methods in Fluids 56(8), 1497-1504 (2008).

Thuburn, J., T. Ringler, J. Klemp and W. Skamarock, 2009: Numerical representation of geostrophic modes on arbitrarily structured C-grids, Journal of Computational Physics, 2009: 228 (22), 8321-8335.

Vachal, P., R. V. Garimella, et al. (2004). "Untangling of 2D meshes in ALE simulations." Journal of Computational Physics 196(2): 627-644.

Zhang, D. Z., X. Ma, et al. (2006). "Interspecies stress in momentum equations for dense binary particulate systems." Physical Review Letters 97(4): 048301/048301-048304.

Almgren, et al., "CASTRO: A New Compressible Astrophysical Sovler. I. Hydrodynamics and Self-Gravity." accepted by *Ap J S* (2010).

Bennett, et al., "The effect of 12C+12C rate uncertainties on s-process yields." *Journal of Physics, Conference Series* **202**, 012023 (2010).

Budge, K.G., Fryer, C.L., Hungerford, A.L., "Supernova theory, Simulation and neutrino fluxes." *JPhCS* **136**, 2040 (2008).

Clayton, G., T.R. Geballe, F. Herwig, C. Fryer, and M. Asplund, "Very Large Excesses of 18O in Hydrogen-deficient Carbon and R Coronae Borealis Stars: Evidence for White Dwarf Mergers." *Ap J* **662**, 1220-1230 (2007).

Diehl, et al., "NuGrid, Nuclear Burning in 3-D Double Degenerate Merger Simulations." *Proceedings of the 10th Symposium on Nuclei in the Cosmos*, Mackinac Island, MI, 2008.

Ellinger, C., P. Young, and C.L. Fryer, "Nucleosynthetic Constraints on the Progenitor of Cassiopeia A", *Proceedings of the 10th Symposium on Nuclei in the Cosmos*, Mackinac Island, MI, 2008.

Fryer et al., "Nucleosynthesis from Supernovae as a Function of Explosion Energy from NuGrid." *Proceedings of the 10th Symposium on Nuclei in the Cosmos*, Mackinac Island, MI, 2008.

Fryer, C.L, "Neutrinos from Fallback onto Newly Formed Neutron Stars." *Ap J* **699**, 409 (2009).

Fryer, C.L. and P.A. Young, "Late-Time Convection in the Collapse of a 23 Msun Star." *Ap J* **659**, 1438 (2007).

Fryer, C.L., A.L. Hungerford, and G. Rockefeller, "Supernova Explosions:. Understanding Mixing." *IJMPD* **16**, 941, (2007).

Fryer, C.L., A.L. Hungerford, and P.A. Young, "Light-Curve Calculations of Supernovae from Fallback Gamma-Ray Bursts." *Ap J* **662**, L55 (2007).

Herwig, et al., "Convective-reactive proton-C12 combustion in Sakurai's object (V4334 Sagittarii) and implications for the evolution and yields from the first generations of stars." accepted by *Ap J* (2010).

Herwig, et al., "Nucleosynthesis simulations for a wide range of nuclear production sites from NuGrid." *Proceedings of the 10th Symposium on Nuclei in the Cosmos*, Mackinac Island, MI, 2008.

Hirschi, et al., "NuGrid: s process in massive stars." *Proceedings of the 10th Symposium on Nuclei in the Cosmos*, Mackinac Island, MI, 2008.

Hungerford, et al., "Trends in 56Ni and 44Ti Synthesis in Core-Collapse Supernovae from NuGrid." *Proceedings of the 10th Symposium on Nuclei in the Cosmos*, Mackinac Island, MI, 2008.

Joggerst, C.C., A. Heger, and S.E. Woosley, "Mixing in Zero- and Solar-Metallicity SNe." *Ap J* **693**, 1780 (2009).

Joggerst, C.C., A. Heger, S.E. Woosley, "Multidimensional Simulations of Mixing in Zero- and Solar-Metallicity SNe." *AIPC* **990**, 257 (2008).

Joggerst, C.C., et al., "The Nucleosynthetic Imprint of 15-40 Msun Primordial Supernovae on Metal-Poor Stars." *Ap J* **709**, 11 (2010).

Livescu, D., J. Mohd-Yusof, and T. Kelley, "Direct Numerical Simulations of Compressible Reacting Turbulence with type Ia supernovae microphysics," Invited paper at the *14th SIAM Conference on Parallel Processing for Scientific Computing* (PP10), Seattle, WA, February 24-26, 2010.

Magkotsios, G., "Ti44 and Ni56 in core-collapse supernovae." Proceedings of the 10th Symposium on Nuclei in the Cosmos, Mackinac Island, MI, 2008

Motl, et al., "Numerical Simulations of Double White Dwarf Mergers." HEAD meeting, Nov. 19, 2007.

Pignatari, et al., "Complete nucleosynthesis calculations for low-mass stars from NuGrid." *Proceedings of the 10th Symposium on Nuclei in the Cosmos*, Mackinac Island, MI, 2008.

Raskin, C., et al., "On Type Ia supernovae from the collisions of two white dwarfs." *MNRAS* **399**, L156 (2009).

Rockefeller, et al.,"Nucleosynthetic Yields from Gamma-Ray Bursts." *Proceedings of the 10th Symposium on Nuclei in the Cosmos*, Mackinac Island, MI, 2008.

Young, P., C. Ellinger, D. Arnett, C. Fryer, and G. Rockefeller, "Spatial Distribution of Nucleosynthesis Products in Cassiopeia A: Comparison Between Observations and 3D Explosion Models." *Proceedings of the 10th Symposium on Nuclei in the Cosmos*, Mackinac Island, MI, 2008.

Young, P.A. et al., "Finding Tracers for Supernova Produced 26Al." *Ap J* **699**, 938 (2009).

Young, P.A., and C.L. Fryer, "Uncertainties in Supernova Yields. I. one-dimensional Explosions." *Ap J* **664**, 1033 (2007).

[Garimella, 2004]: R.V. Garimella, ``MSTK: A Flexible Infrastructure

[Garimella, 2008]: R.V. Garimella, K. Lipnikov, ``Solution of the

[Vachal, 2004]: P. Vachal, R.V. Garimella, M.J. Shashkov, ``Untangling

Ahn, H.T., and M.Shashkov, "Adaptive Moment-of-Fluid Method." *J. Comput. Phys.* **228**, 2792-2821 (2009).

Beirao da Veiga, L., and K. Lipnikov, "A mimetic discretization of the Stokes problem with selected edge bubbles." *SIAM J Sci. Comp.* **32**, (2010).

Bowers, K.J., B.J. Albright, B. Bergen, L. Yin, K.J. Barker, and D.J. Kerbyson, "0.374 Pflop/s Trillion-Particle Kinetic Modeling of Laser Plasma Interaction on Roadrunner." *Proc. 2008 ACM/IEEE Conf. Supercomputing*, Gordon Bell Prize Finalist Paper (2008b).

Bowers, K.J., B.J. Albright, L. Yin, B. Bergen, and T.J.T. Kwan, "Ultra high performance three-dimensional electromagnetic relativistic particle-in-cell simulation." *Phys. Plasmas* **15,** 055703 (2008a).

Brezzi, F., A. Buffa, and K. Lipnikov, "Mimetic finite differences for elliptic problems." *M2AN* **43**, 277-295 (2009).

Brezzi, F., K. Lipnikov, and M. Shashkov, "Convergence of mimetic finite difference method for diffusion problems on polyhedral meshes with curved faces." *M3AS* **16**, 275-297 (2006).

Brezzi, F., K. Lipnikov, M. Shashkov, and V. Simoncini, "A new discretization methodology for diffusion problems on generalized polyhedral meshes." *Comput. Meth. Appl. Mech. Engr.* **196**, 3682-3692 (2007).

Brown, D., J. Bell, D. Estep, W. Gropp, B. Hendrickson, S. Keller-McNulty, D. Keyes, J.T. Oden, L. Petzold, and M. Wright, "Applied Mathematics at the U.S. Department of Energy: Past, Present and a View to the Future." (2008).

Delzanno, G.L., L. Chacon, Y. Chung, G. Lapenta, ``An

Dendy, J.E., "Black-box multigrid." *J. Comp. Phys.* **48**, 366-386 (1982).

Dyadechko, V., and M. Shashkov, "Reconstruction of mutli-material Interfaces from moment data." *J. Comput. Phys.* **227**, 5361-5384 (2008).

Fichtl , E.D., J.S. Warsa, and J.D. Densmore, "The Newton-Krylov Method Applied to Negative-Flux Fixup in SN Transport Calculations." *Nucl. Sci. Engr.* (accepted for publication) (2010).

Garimella, R., and K. Lipnikov, "Solution of the diffusion equation in multi-material domains by subdivision of elements along reconstructed interfaces." *Int. J. Numer. Meth. Fluids,* in press (2010).

Gill D.F., Y.Y. Azmy, J.S. Warsa, and J.D. Densmore, "Newton's Method for the Computation of k-Eigenvalues in SN Transport Applications." *Nucl. Sci. Engr*, submitted (2010).

Hecht, M., D.D. Holm, M. Petersen and B.A. Wingate, "Implementation of the LANS-alpha turbulence model in a primitive equation ocean model." *J. Comp. Phys* (2008).

Hecht, M., D.D. Holm, M. Petersen, and B.A. Wingate, "The LANS-alpha and Leray turbulence parameterizations in primitive equation ocean modeling." *J. Phys. A.* (2008).

Hecht, M., E Hunke, M. Maltrud, M. Petersen, and B.A. Wingate, "Lateral Mixing in the Eddying Regime and a new Broad-Ranging Formulation," *Eddy Resolving Ocean Modeling*, AGU, Hecht and Hasumi eds. (2008).

Holm, D.D. and B. A .Wingate, "Baroclinic instabilities of the two-layer quasigeostrophic alpha model." *J. Phys. Oceanograph*,(2005).

Holm, D.D. and B. Nadiga, "Modeling mesoscale turbulence in the barotropic double-gyre circulation." *J. Phys Ocean* (2003).

Holm, D.D., J. Marsden, and T. Ratiu, "The Euler-Poincaré Equations and Semidirect Products with Applications to Continuum Theories." *Advances in Mathematics* (1998).

Joubert, W. and J. Cullum, "Scalable algebraic multigrid on 3500 processors." *ETNA* **23**, 105-128 (2006).

K.Lipnikov and M.Shashkov, "A mimetic tensor artificial viscosity for Lagrangian hydrocodes on arbitrary polygonal meshes." Los Alamos Report LAUR 10-00006 (2010).

Knoll, D.A. and D.E. Keyes, "Jacobian-free Newton-Krylov methods: a survey of approaches and applications." *J. Comput. Phys.* **193**, 357-397 (2004).

Kuzmin, D., M.Shashkov, and D.Svyatskiy, "A Constrained finite element method satisfying the discrete maximum principle for anisotropic diffusion problems," *J. Comput. Phys.* **228**, 3448-3463 (2009).

Lipnikov, K., D. Moulton, and D. Svyatskiy, "A Multilevel Multiscale Mimetic (M3) method for two-phase flows in porous media." *J. Comput. Phys.* **227**, 6727-6753 (2008).

Lipnikov, K., D. Moulton, and D. Svyatskiy, "A multilevel multiscale mimetic (M3) method for an anisotropic infiltration problem." *Lecture Notes in Computer Science* **5544**, 685-694 (2009).

Lipnikov, K., D. Svyatskiy, and Yu.Vassilevski, "Interpolation-free monotone finite volume method for diffusion equations on polygonal meshes." *J. Comput. Phys.* **228**, 703-716 (2009).

Lipnikov, K., J.D. Moulton, and D. Svyatskly, "A multilevel, multiscale mimetic (M-3) method for two-phase flows in porous media." *J. Comp. Phys.* **227**, 6727-6753 (2008).

Lipnikov, K., M. Shashkov and I. Yotov, "Local flux mimetic finite difference methods." *Numer. Math.* **112,** 115-152 (2009).

Liska, R. and M. Shashkov, "Enforcing the discrete maximum principle for linear finite element solutions of second-order elliptic problems," *Commun. Comput. Phys.* **3**, 852-877 (2008).

Morel, J.E., T.-Y.B. Yan, and J.S. Warsa, "Linear Multifrequency-Grey Acceleration Recast for Preconditioned Krylov Iterations." *J. Comp. Phys.* **227**, 244-263 (2007).

Petersen, M., M. Hecht, and B.A. Wingate, "Efficient form of the LANS-alpha primitive equation ocean model." *J. Comp. Phys.* (2008).

R. Camassa and D.D. Holm, "An integrable shallow water equation with peaked solitons." *Phys. Rev. Let.*(1993).

Rosa, M., J.S. Warsa, and T.M. Kelley, "Fourier Analysis of Cell-Wise Block-Jacobi Splitting in Two-Dimensional Geometry." *Proceedings of the Joint International Topical Meeting on Mathematics & Computation*, Saratoga Springs, NY, May 3-7, 2009.

Rosa, M., J.S. Warsa, J.H. Chang, "Fourier Analysis of Inexact Parallel Block-Jacobi Splitting with Transport Synthetic Acceleration," *Nucl. Sci. Engr.* **164**, 248-263, (2010).

Shashkov, M., "Closure models for multimaterial cells in arbitrary Lagrangian-Eulerian hydrocodes." *Int. J. Numer. Meth. in Fluids* **56**, 1497-1504 (2007).

Svyatskiy, D., Yu. Vassielvski, and K. Lipnikov "A monotone finite volume scheme for advection-diffusion equations on unstructured polygonal meshes." *J. Comp. Phys.* **229** (2010).

Timmermans, M.-L., L. Rainville, L. Thomas, and A. Proshutinsky, "Moored observations of bottom-intensified motions in the deep Canada Basin, Arctic Ocean," *J. Marine Research,* in press (2010).

Vrugt, J.A., B.A. Robinson, and J.M. Hyman, "Self-adaptive multimethod search for global optimization in real parameter spaces." *IEEE Transactions on Evolutionary Computation*, 1-17, doi:10.1109/TEVC.2008.924428 (2009).

Vrugt, J.A., C.J.F. ter Braak, M.P. Clark, J.M. Hyman, and B.A. Robinson, "Treatment of input uncertainty in hydrologic modeling: Doing hydrology backward with Markov chain Monte Carlo simulation," *Water Resour. Res.* **44**, W00B09 (2008).

Warsa, J.S., "A Continuous Finite Element-Based Discontinuous Finite Element Method for S_N Transport." *Nucl. Sci. Engr.* **160**, 385-400 (2008).

Warsa, J.S., J.D. Densmore, A.K. Prinja, and J.E. Morel, "Manufactured Solutions in the Thick Diffusion Limit." *Nucl. Sci. Engr.*. accepted for publication, (2010).

Wingate, B. A., "The maximum allowable time step for the shallow water α model and its relation to time-implicit differencing," *Monthly Weather Review* (2004).

Wingate, B.A., P. Embid, M. Holmes-Cerfon, and M. Taylor, "Low Rossby Number Limiting Dynamics with Finite Froude number." *J. Fluid Mech*, in review (2010).

Wohlberg, B. and D.M. Tartakovsky, "Delineation of geological facies from poorly differentiated data," *Adv. Water Resour.*, doi:10.1016/j.advwatres.2008.10.014 (2008).

Woodgate, R.A., K. Aagaard, R.D. Muench, J.Gunn, G. Bjork, B. Rudels, A.T. Roach, and U. Schauer, "The Arctic Ocean Boundary Current along the Eurasian slope and the adjacent Lomonosov Ridge: Water mass properties, transports and transformations from moored instruments.," *Deep-Sea Research* (2001).

Zhang, D.Z., W.B. VanderHeyden, Q. Zou, and N.T. Padial-Collins, "Pressure calculation in disperse and continuous multiphase flows." *International Journal of Multiphase Flow* **33**, 86-100 (2007).

Zhang, D.Z., Q. Zou, W.B. VanderHeyden, and X. Ma, "Material point method applied to multiphase flows." *Journal of computational physics* **227**,3159-3173 (2008).

Adaptation based on Monge-Kantorovich Optimization," J. Comp. Phys.,

Bhat, C.R., et. al., "A Comprehensive Micro-simulator for Daily Activity-travel Patterns (CEMDAP)," *Transportation Research Record* (2004).

Bai, X.M., A.F. Voter, R.G. Hoagland, M. Nastasi, and B.P. Uberuaga, "Efficient annealing of radiation damage near grain boundaries via interstitial emission." *Science* **327**, 1631 (2010).

Barrett, C.L., S.G. Eubank, and J. P. Smith, If Smallpox Strikes Portland." *Scientific Amer*ican **292**(3), 54-61 (2005).

Baskes, M.I., S.G. Srinivasan, S.M. Valone, and R.G. Hoagland, "Multi-state Modified Embedded Atom Method." *Phys. Rev. B* **75**, 94113 (2007).

Bazavov, A. et al., "Equation of state and QCD transition at finite temperatu." *Phys Rev D* **80**, 014504 (2009).

Bhattacharya, T., M. Daniels, D. Heckerman, B. Foley, N. Frahm, C. Kadie, J. Carlson, K. Yusim, B. McMahon, B. Gaschen, S. Mallal, J.I. Mullins, D.C. Nickle, J.Herbeck, C.Rousseau, G.H. Learn, T. Miura, C. Brander, B. Walker, and B. Korber, "Founder effects in population based assessment of HIV polymorphisms and HLA allele associations or Founder effects contribute to perceived associations between HIV sequence polymorphisms and HLA class I alleles," 1583-1586 ori:doi:10.1126/science.1131528. Los Alamos report LA-UR-06-3312, May 2006; *Science* **315,** 5818 (2007).

Booth, T.E. et al., "Exact regional Monte Carlo weight cancellation for second Eigenfunction calculations." LA-UR 09-05872. *Nuclear Science and Engineering*, accepted (2010).

Booth, T.E., "Comments on Monte Carlo probability of initiation estimates for neutron fission chains," LA-UR-09-08080, *Nuclear Science and Engineerin*, accepted (2010).

Booth, T.E., "Monte Carlo probability of initiation estimates in MCNP," LA-UR-09-05874 (2009).

Booth, T.E. and J.E. Gubernatis, "Monte Carlo Determination of Multiple Extremal Eigenpairs," *Phys. Rev. E* **80**:4 (2009).

Booth, T.E. and J.E. Gubernatis, "Improved Criticality Convergence Via a Modified Monte Carlo Power Iteration," (invited paper) *International Conference on Mathematics, Computational Methods & Reactor Physics* (M&C 2009), Saratoga Springs, New York, May 3-7, 2009, on CD-ROM. LA-UR-08-06461.

Brumme, Z.L., C.J. Brumme, D. Heckerman, B.T. Korber, M. Daniels, J. Carlson, C. Kadie, T. Bhattacharya, C. Chui, J. Szinger, T. Mo, R.S. Hogg, J.S.G. Montaner, N. Frahm, C. Brander, B.D. Walker, and P.R. Harrigan, "Evidence of Differential HLA Class I-Mediated Viral Evolution in Functional and Accessory/Regulatory Genes of HIV-1," *Public Library of Science Pathogens* **3**:7 (2007)
e94. ori:doi:10.1371/journal.ppat.0030094. Published online 6 July 2007 Los Alamos report LA-UR-07-0410, Jan 2007.'

Cameron, G., and G. Duncan, "Paramics: Parallel microscopic simulation of road traffic." *Journal of SuperComputing* (1996).

Cawkwell, M.J., T.D. Sewell, L. Zheng, and D.L. Thompson, "Shock-induced shear bands in an energetic molecular crystal: Application of shock-front absorbing boundary conditions to molecular dynamics simulations." *Phys. Rev. B* **78**, 014107 (2008).

Cetin, N., A. Burri, and K. Nagel, "Parallel queue model approach to traffic microsimulations." 2002.

Charypar, D., K. Axhausen, and K. Nagel, "An event-driven queue-based microsimulation of traffic flow." *Transport Systems Planning and Transport Telematics* (2006).

Charypar, D. et. al, "Generating Complete All-Day Schedule Plans with Genetic Algorithms," *Transportation* **32**:4, 369-397 (2005).

Chen, T., P. Langan, A.D. French, G.P. Johnson, and S. Gnanakaran, "Conformational Flexibility of Soluble Cellulose Oligomers: Chain Length and Temperature Dependence." *J. Am. Chem. Soc.* **131**, 14786-14794 (2009).

Coe, J.D., T.D. Sewell, and M.S. Shaw, "Nested Markov chain Monte Carlo sampling of a density functional theory potential: Equilibrium thermodynamics of dense fluid nitrogen." *J. Chem. Phys.* **131**, 074105 (2009).

Concepts, I.T., "Vissim simulation tool." In http://www.itc-world.com/VISSIMinfo.htm. (2001).

Eissfeldt, N., D. Krajzewicz, K. Nagel, and P. Wagner. "Simulating traffic flow with queues." (2006).

Perumalla, K., "A systems approach to scalable transportation network modeling." *2006 Winter Simulation Conference* (2006).

Prevedouros, P.D., and Y. Wang. "Simulation of a large freeway/ arterial network with integration, tsis/corsim and watsim." *Transportation Research Record* **1678**, 197–207 (1999).

Smith, L., R. Beckman, D. Anson, K. Nagel, and M. E. Williams, "Transims: Transportation analysis and simulation system." *Proceedings of the Fifth National Conference on Transportation Planning Methods*, Seattle,Washington. Transportation Research Board 2000. Highway capacity manual. Transportation Research Board (1995).

Yan, G., P. Datta, S. Eidenbenz, S. Thulasidasan, V. Ramaswamy, "Criticality Analysis and Assessment of National Internet Infrastructure," *Computer Networks* (2010).

CVE, National Vulnerability Database maintained by NIST maintained online at: http://nvd.nist.gov/ (2010).

Das, A. and B.K. Chakrabarti, "Quantum Annealing and Related Optimization Methods," *Lecture Note in Physics* **679** (2005).

Das, A. and B.K. Chakrabarti, "Reaching the ground state of a spin glass using a zero-temperature quantum Monte Carlo method," *Phys. Rev. E* **78**, 061121 (2008).

627-644 (2004).

Chatterjee, A. and A.F. Voter *Journal of Chemical Physics* (2010).

Barrett, C.L. et. al, "Activity Generator," *TRANSIMS 3.1*, Chapter 3, LA-UR-00-1725 (2004).

Baskes, M.I., "Atomistic model of plutonium." *Phys. Rev. B* **62**, 15532 (2000).

2010

de Supinski, B.R. et al., BlueGene/L Applications: Parallelism on a Massive Scale. Int. J. High Performance Computing Applications 22, 33–51. 2008:

Del Valle SY, Hyman JM, Hethcote HW, Eubank SG. Mixing Patterns Between Age Groups in Social Networks. Social Networks 29: 539-554 (2007).

DelValle2006: Del Valle, Ambrosiano J, Cash L, Doyle J, Edwards B, et al. National population and healthcare sector impacts of 2009 Influenza A (H1N1). Los Alamos Unlimited Release 10-00186 (2010).

DelValle2009: Del Valle S, Ambrosiano J, Bent R, Daniel B, Dauelsberg L, et al. National Population and Economic Impacts of 2009 Influenza A (H1N1). Los Alamos Unlimited Release 09-06335 (2009).

Dendy,2010]: J. E. Dendy and J. D. Moulton, ``Black Box Multigrid with Coarsening by a Factor of Three,'' J. Numer. Lin. Alg. App., vol. 17, 577-598 (2010)

Densmore2007a: T.M. Evans and J.D. Densmore, "Methods for Coupling Radiation, Ion, and Electron Energies in Grey Implicit Monte Carlo," J. Comp. Phys. 225, 1695-1720 (2007).

Densmore2007b: 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).

Densmore2008: 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).

Densmore2009a: J.D. Densmore, "Asymptotic Analysis of Spatial Discretizations in Implicit Monte Carlo: Extension to a Courant Time-Step Limit," Trans. Am. Nucl. Soc. 101, 437-440 (2009).

Densmore2009b: J.D. Densmore, "Asymptotic Analysis of Spatial Discretizations in Implicit Monte Carlo," Proc. International Conference on Mathematics, Computational Methods & Reactor Physics, Saratoga Springs, New York, May 3-7, 2009.

Densmore2010a: J.D. Densmore, J.S. Warsa, and R.B. Lowrie, "Stability Analysis and Time-Step Limits for a Monte Carlo Compton-Scattering Method," J. Comp. Phys. 229, 3691-3705 (2010).

Diffusion Equation in Multi-Material Domains by Sub-division of

Elements along Reconstructed Interfaces," Intl. J. of Num. Meth. in

Evans2010: Louise Evans, Stephen Tobin, Howard Menlove, M.A. Schear, S.Y. Lee, M.T. Swinhoe, "Nondestructive Determination of Plutonium Mass in Spent Fuel: Preliminary Modeling Results Using the Passive Neutron Albedo Reactivity Technique," Waste Management 2010, Phoenix AZ.

Favorite2009a: Jeffrey A. Favorite, "Eigenvalue Sensitivity Analysis Using the MCNP5 Perturbation Capability," Proceedings of the 2009 Nuclear Criticality Safety Division (of the American Nuclear Society) Topical Meeting on Realism, Robustness, and the Nuclear Renaissance, Richland, Washington, September 13-17, CD-ROM (2009).

Favorite2009b: Jeffrey A. Favorite, "On the Accuracy of the Differential Operator Monte Carlo Perturbation Method for Eigenvalue Problems," Transactions of the American Nuclear Society, 101,

460-462 (2009).

Favorite2009c: Jeffrey A. Favorite, Keith C. Bledsoe, and David I. Ketcheson, "Surface and Volume Integrals of Uncollided Adjoint Fluxes and Forward-Adjoint Flux Products," Nuclear Science and Engineering, 163, 1, 73-84 (2009).

Favorite2009d: Jeffrey A. Favorite, "Surface and Volume Integrals of Uncollided Adjoint Fluxes and Forward-Adjoint Flux Products in Arbitrary Three-Dimensional Geometries Using MCNP," Transactions of the American Nuclear Society, 101, 633-635 (2009).

Feil2009: M. Feil et. al, 2009, "New Approaches to Generating Comprehensive All-day Activity-travel Schedules," Transport and Spatial Planning.

Fensin2009a: Michael L. Fensin, Stephen J. Tobin, Howard O. Menlove, Martyn T. Swinhoe, "Quantifying the Passive Gamma Signal from Spent Nuclear Fuel in Support of Determining the Plutonium Content In Spent Nuclear Fuel With Non-destructive Assay," 50th INMM annual meeting 2009 Tucson AZ.

Fensin2009b: M. L. Fensin, S. J. Tobin, M. T. Swinhoe, H. O. Menlove, N. P. Sandoval, "A Monte Carlo Based Spent Fuel Analysis Safeguards Strategy Assessment," GLOBAL 2009, Paris, France.

Fensin2009c: Michael L. Fensin, Steven J. Tobin, Nathan P. Sandoval, Martyn T. Swinhoe, Scott J. Thompson, "A Monte Carlo Linked Depletion Spent Fuel Library for Assessing Varied Non-destructive Assay Techniques for Nuclear Safeguards," Advances in Nuclear Fuel Management IV (ANFM 2009), Hilton Head Island, South Carolina 4/12/2009.

Ferguson2004: Ferguson NM, Cummings DAT, Fraser C, Cajka JC, Cooley PC, Burke DS. Strategies for mitigating an influenza pandemic. Nature 442: 448-452 (2006).

Fluids (to appear 2010).

Galli2009: E. Galli et al., 2009, "ActivitySim: Large-scale Agent-based Activity Generation for Infrastructure Simulation," Agent Directed Simulation Symposium, Spring Simulation Multiconference.

Germann, T.C. and K. Kadau, 2008: Trillion-Atom Molecular Dynamics Becomes a Reality. Int. J. Modern Phys. C. 19, 1315-1319.

Germann, T.C., K. Kadau, and P. S. Lomdahl, 2005: 25 Tflop/s Multibillion-atom Molecular Dynamics Simulations and Visualization/Analysis on BlueGene/L, Proc. 2005 ACM/IEEE Conf. Supercomputing, Gordon Bell Prize Finalist Paper.

Germann, T.C., K. Kadau, and S. Swaminarayan, 2009: 369 Tflop/s molecular dynamics simulations on the petaflop hybrid supercomputer 'Roadrunner'. Concurrency Computat.: Pract. Exper. 21, 2143-2159.

Germann2006: Germann TC, Kadau K, Longini IM, Macken CM. Mitigation strategies for pandemic influenza in the United States, Proc. Natl. Acad. Sci. U.S.A. 103:5935-5940 (2006).

Gnanakaran2007: "Clade Specific Differences between Human Immunodeficiency Virus Type 1 Clades B and C: Diversity and Correlations in C3--V4 Regions of gp120'," S. Gnanakaran, Dorothy Lang, Marcus Daniels, Tanmoy Bhattacharya,Cynthia Derdyn, and Bette Korber. Journal of Virology 81:9 (2007) 4886--4891. ori:doi:10.1128/JVI.01954-06. Published ahead of print 13 December 2006 Los Alamos report LA-UR-06-1255.

Hammerberg, J.E., B.L. Holian, T.C. Germann, and R. Ravelo, 2004: Nonequilibrium Molecular Dynamics Simulations of Metallic Friction at Ta/Al and Cu/Ag Interfaces. Metal. and Mater. Trans. A 35, 2741-2745.

Hammond, G.E. and P.C. Lichtner (2010) Field-Scale Modeling for the Natural Attenuation of Uranium at the Hanford 300 Area using High Performance Computing, Water Resources Research, accepted.

Hammond, G.E., P.C. Lichtner and M.L. Rockhold (2010) Stochastic Simulation of Uranium

Migration at the Hanford 300 Area, Journal of Contaminant Hydrology, doi:10.1016/j.jconhyd.2010.04.005.

Hammond, G.E., P.C. Lichtner, C. Lu and R.T. Mills (2010) PFLOTRAN: Reactive flow and transport code for use on laptops to leadership-class supercomputers, Bentham E-Book on Mathematical Modeling of Reactive Transport in Groundwater, accepted.

Hammond, G.E., P.C. Lichtner, R.T. Mills and C. Lu (2008) Toward petascale computing in geosciences: application to the Hanford 300 Area, Journal of Physics Conference Series, 125, 012051 doi:10.1088/1742-6596/125/1/012051.

Hayes2006: David K. Hayes, Rene G. Sanchez, A.C. (Skip) Kahler," Zeus: Fast-Spectrum Critical Assemblies with an Iron-HEU Core Surrounded by a Copper Reflector," PHYSOR-2006, ANS Topical Meeting on Reactor Physics, Organized and hosted by the Canadian Nuclear Society. Vancouver, BC, Canada. 2006 September 10-14.

Heim, A.J., N. Grønbech-Jensen, E. M. Kober, J. J. Erpenbeck, and T. C. Germann, 2008: Interaction Potential for Atomic Simulations of Conventional High Explosives. Phys. Rev. E 78, 046709.

Hendricks2003: J. Hendricks, M. Swinhoe, S. Tobin, W. Geist and D. Mayo, "Neutron Multiplicity Counting for Nuclear Safeguards with MCNPX," ANS annual meeting 2003 San Diego, CA.

Holian, B.L. and P. S. Lomdahl, 1998: Plasticity Induced by Shock Waves in Nonequilibrium Molecular-Dynamics Simulations. Science 280, 2085-2088.

Hutchinson2007: J. Hutchinson, D. Loaiza, B. Rooney, "Correcting for Room Return Neutrons Using an Empirical Relationship." ANS Transactions, Vol. 96, 2007

Hutcthinson2009a: J. Hutchinson, J. Bess, "Subcritical Noise Measurements with a Nickel-Reflected Plutonium Sphere," Nuc. Sci. & Eng., Vol. 163, 285-290, 2009.

Hutcthinson2009b: J. Hutchinson, T. Valentine, "Subcritical Measurements of a Plutonium Sphere Reflected by Polyethylene and Acrylic." Nuc. Sci. & Eng., Vol. 161, 357-362, 2009.

Hykes2009: J.M. Hykes and J.D. Densmore, "Non-Analog Monte Carlo Estimators for Radiation Momentum Deposition," J. Quant. Spectrosc. Radiat. Transfer 110, 1097-1110 (2009).

Joh2001: C. Joh et. al., 2001, "Understanding Activity Scheduling and Rescheduling Behaviour: Theory and Numerical Illustration," GeoJournal 53:359-371.

Kadau, K., C. Rosenblatt, J. L. Barber, T. C. Germann, Z. Huang, P. Carlès, and B. J. Alder, 2007b: The importance of fluctuations in fluid mixing. Proc. Natl. Acad. Sci. USA 104, 7741-7745.

Kadau, K., J. L. Barber, T. C. Germann, B. L. Holian, and B. J. Alder, 2010: Atomistic methods in fluid simulation. Phil. Trans. Roy. Soc. A 368, 1547-1560.

Kadau, K., T. C. Germann, and P. S. Lomdahl, 2006: Molecular Dynamics Comes of Age: 320 Billion Atom Simulation on BlueGene/L. Int. J. Mod. Phys. C 17, 1755-1761.

Kadau, K., T. C. Germann, P. S. Lomdahl, and B. L. Holian, 2002: Microscopic view of structural phase transitions due to shock waves. Science 296, 1681-1684.

Kadau, K., T. C. Germann, P. S. Lomdahl, R. C. Albers, J. S. Wark, A. Higginbotham, and B. L. Holian, 2007a: Shock waves in polycrystalline iron, Phys. Rev. Lett. 98, 135701.

Kelley2010: Timothy M. Kelley, Todd Urbatsch, Aimee Hungerford, Gabriel Rockefeller, Chris L. Fryer, Paul J. Henning, Jeff Densmore, and Barbara DeVolder; "Using Roadrunner to Model Shock Breakout in Supernovae and NIF Experiments," ADTSC Highlights submission, January 11, 2010.

KiedrowskiBrown2008: Kiedrowski, B.C. ; Brown, F.B.; "Using Wielandt's method to eliminate confidence interval underprediction bias in MCNP5 criticality calculations," Transactions of the American Nuclear Society (2008) vol.99, p.338-40.

KiedrowskiBrown2009a: Kiedrowski, B. C. Brown, F.B; "An information theory based analysis of fission source correlation in Monte Carlo k-eigenvalue calculations," American Nuclear Society - International Conference on Mathematics, Computational Methods and Reactor Physics 2009, M and

C 2009 (2009) Vol.4, p.2417-2428.

KiedrowskiBrown2009b: Brian Kiedrowski and Forrest Brown, "Estimating Reactivity Changes from Material Substitutions with Continuous Energy Monte Carlo," Transactions of the American Nuclear Society, 101, 427-429 (November 2009).

KiedrowskiBrown2009c: Brian Kiedrowski and Forrest Brown, "Adjoint-Weighted Kinetics Parameters with Continuous Energy Monte Carlo," Transactions of the American Nuclear Society, 100, 297-299 (June 2009).

Krzakala2009: F. Krzakala and L. Zdeborova, Following Gibbs States Adiabatically – The Energy Landscape of Mean Field Glassy Systems, arXiv:0909.3820 (2009).

Kum, O., B.M. Dickson, S.J. Stuart, B.P. Uberuaga, and A.F. Voter, 2004: Parallel Replica Dynamics with a Heterogeneous Distribution of Barriers: Application to n-Hexadecane Pyrolysis. J. Chem. Phys. 121, 9808.

Kwan2009: Thomas J.T. Kwan, Tai-Sen Wang, Michael Berninger, Charles Snell, Lin Yin, "Simulation of the Cygnus Rod-Pinch Diode Using the Radiographic Chain Model", IEEE Trans. Plas. Sci. 37, Special Issue ICPS 2008 (April 2009).

Lafleur2008: A. Lafleur, W. Charlton, H. O. Menlove and M. T. Swinhoe, "Non-destructive Measurements of Fissile Material Using Self Indication Neutron Resonance Absorption," 8th Int. Conference on Facility Operations Interface Portland, OR, 3/30/2008.

Langner2006: D. Langner, K. Kroncke, J. Marlow, H. Menlove and M. T. Swinhoe, "A Configurable Epithermal Neutron Multiplicity Counter," INMM 47th annual meeting Nashville, TN 7/17/2006.

LA-UR-09-01727

Lee2008: Lee BY, Bedrord VL, Roberts MS, Carley KM. Virtual Epidemic in a Virtual City: Simulating the Spread of Influenza in a US Metropolitan Area. Translational Research 151: 275-287 (2008).

Library for Developing Mesh Based Applications," in Proceedings of

Lopgini2004: Longini IM, Halloran ME, Nizam A, Yang Y. Containing Pandemic Influenza with Antiviral Agents. Am. J. of Epidemiology 159: 623-633 (2004).

Lu, C. and P.C. Lichtner (2007) High resolution numerical investigation on the effect of convective instability on long term CO2 storage in saline aquifers, Journal of Physics: Conference Series, 78 (2007) 012042 doi:10.1088/1742-6596/78/1/012042.

McClarren2009: Ryan G. McClarren, Todd J. Urbatsch, "A modified implicit Monte Carlo method for time-dependent radiative transfer with adaptive material coupling," Journal of Computational Physics 228 (2009) 5669-5686.

Menikoff, R. and T.D. Sewell, 2002: Constituent properties of HMX needed for mesoscale simulations. Combust. Theor. Modell. 6, 103-125.

Mills, R.T., G.E. Hammond, P.C. Lichtner, V. Sripathi, G. Mahinthakumar and B.F. Smith (2009) Modeling subsurface reactive flows using leadership-class computing, Journal of Physics Conference Series, 180, 012062doi:10.1088/1742-6596/180/1/012062.

Mniszewski2008a: Mniszewski S, Del Valle S, Stroud P, Riese J, Sydoriak S. EpiSimS simulation of a multi-component strategy for pandemic influenza. In Proceedings of the 2008 Spring Simulation Multiconference (2008).

Mniszewski2008b: Mniszewski S, Del Valle S, Stroud P, Riese J, Sydoriak S. Pandemic simulation of antivirals + school closures: buying time until strain-specific vaccine is available. Computational & Mathematical Organization Theory 14: 209-221 (2008).

Mniszewski2009: S. Mniszewski et. al., 2009, "Infrastructure Modeling Accelerated," Institutional Computing Cerrillos Proposal.

of 2D Meshes in ALE Simulations," J. Comp. Phys., vol 196, n 2,

Optimal Robust Equidistribution Method for Two-Dimensional Grid

Paternoster2009: R. Paternoster, J. Hutchinson, D. Gardner, "Guidelines for Criticality Safe Transport of Fissile Materials under Field-Expedient Conditions," LA-UR-09-03642, 2009.

Peerani2009: P. Peerani, M. T. Swinhoe, A-L Weber and L. G. Evans, "ESARDA Multiplicity Benchmark Exercise Phases III and IV," ESARDA Bulletin No 42 11/1/2009.

Perez, D., B.P. Uberuaga, Y. Shim, J.G. Amar, and A.F. Voter, 2009: Accelerated Molecular Dynamics Methods: Introduction and Recent Developments. Annual Reports in Comp. Chem. 5, 79.

Ramaswamy2007: V. Ramaswamy, S. Thulasidasan, P. Romero, S. Eidenbenz, L. Cuellar, Simulating the National Telephone Network: A Socio-technical Approach to Assessing Infrastructure Criticality, Proceedings of 2007 IEEE Military Communications Conference, 2007

Rousseau2007: "Extensive Intra-subtype Recombination in South African Human Immunodeficiency Virus Type 1 Subtype C Infections," Christine M. Rousseau, Gerald H. Learn, Tanmoy Bhattacharya, David C. Nickle, David Heckerman,Senica Chetty, Christian Brander, Philip J.R. Goulder, Bruce D. Walker, Photini Kiepiela, Bette T. Korber, and James I. Mullins. Journal of Virology 81:9 (2007) 4492--4500. ori:doi:10.1128/JVI.02050-06. Published ahead of print 21 February 2007.

Rousseau2008: "HLA Class-I Driven Evolution of Human Immunodeficiency Virus Type 1 Subtype C Proteome: Immune Escape and Viral Load," Christine M. Rousseau, Marcus G. Daniels, Jonathan M. Carlson, Carl Kadie, Hayley Crawford,Andrew Prendergast, Philippa Matthews, Rebecca Payne, Morgane Rolland, Dana N. Raugi, Brandon S. Maust, Gerald H. Learn, David C. Nickle, Hoosen Coovadia, Thumbi Ndung'u, Nicole Frahm, Christian Brander, Bruce D.Walker, Philip J. R. Goulder, Tanmoy Bhattacharya, David E. Heckerman, Bette T. Korber, and James I. Mullins) Journal of Virology 82:13 (2008) 6434--6446. ori:doi.

Sanbonmatsu, K.Y. and C.-S. Tung, 2007: High performance computing in biology: Multimillion atom simulations of nanoscale systems. J. Struct. Biol. 157, 470-480.

Sanbonmatsu, K.Y., S. Joseph, and C.-S. Tung, 2005: Simulating movement of tRNA into the ribosome during decoding. Proc. Natl. Acad. Sci. USA 102, 15854-15859.

Sanchex2008: Rene Sanchez, David Loaiza, Robert Kimpland, David Hayes, Charlene Cappiello, and Mark Chadwick, "Criticality of a Np-237 Sphere," Nuc. Sci. & Eng., Vol. 158, 1-14, 2008.

Sanchez2004: Rene Sanchez, David Loaiza, Glenn Brunson, and Robert Kimpland, "Critical Experiments with Highly Enriched Uranium and Matrix Elements (Si, Mg, Al, Gd, and Fe)," Nuc. Sci. & Eng., Vol. 147, 307-318, 2004.

Santhi2010: CyberSim: Geographic, Temporal, and Organizational Dynamics of Malware Propagation, Nandakishore Santhi, Guanhua Yan, and Stephan Eidenbenz, invited paper at the WinterSim 2010 (WSC 2010) conference.
Eubank2005: Eubank S, Goclu H, Kumar A, Marathe M, Srinivasan A, Totoczkal Z, Wang N. Modelling disease outbreaks in realistic urban social networks. Nature 429: 180-184 (2004).

Santoro2007:G.E. Santoro and E. Tosatti, Computing: Quantum to Classican and Back, Nature Physics 3, 593 (2007).

Shim, Y., J.G. Amar, B.P. Uberuaga, and A.F. Voter, 2007: Reaching extended length scales and time scales in atomistic simulations via spatially parallel temperature-accelerated dynamics. Phys. Rev. B 76, 205439.

Solomon2009: Clell Solomon, Avneet Sood, Thomas Booth, "A Weighted Adjoint Source for Weight-Window Generation by Means of a Linear Tally Combination", 2009 International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics, May 3-7, 2009, Saratoga Springs, New York, USA.

Somma2007: R. D. Somma, C. D. Batista, and G. Ortiz, A Quantum Approach to Classical Statistical Mechanics , Phys. Rev. Lett. 99, 030603 (2007).

Somma2008: R.D.Somma, S. Boixo, H. Barnum, and E. Knill, Quantum Simulations of Classical

Annealing Processes, Phys. Rev. Lett. 101, 130504 (2008).

Sorensen, M.R. and A.F. Voter, 2000: Temperature Accelerated Dynamics for Simulation of Infrequent Events. J. Chem. Phys. 112, 9599.

Stroud2007: Stroud P, Del Valle S, Sydoriak S, Riese J, Mniszewski S. Spatial Dynamics of PandemicInfluenza in a Massive Artificial Society. Journal of Artificial Societies and Social Simulation 10(9) (2007).

Swaminarayan, S, T. C. Germann, K. Kadau, and G. C. Fossum, 2008: 369 Tflop/s Molecular Dynamics Simulations on the Roadrunner General-Purpose Heterogeneous Supercomputer. Proc. 2008 ACM/IEEE Conf. Supercomputing, Gordon Bell Prize Finalist Paper.

Swinhoe2007: M. T. Swinhoe and H. O. Menlove, "Research Reactor Fuel Counter Performance," ESARDA Conference 2007, Aix-en-Provence 4/15/2007.

Swinhoe2009: M. T. Swinhoe, S. J. Tobin, M. L. Fensin and H. O. Menlove, "An Integrated Approach for Determining Plutonium Mass in Spent Fuel Assemblies with Nondestructive Assay," ANIMMA conference France 6/7/2009.

Swinhoe2009: M.T. Swinhoe, J. B. Marlow, and H. O. Menlove, "High Precision Non-destructive Assay of Small Samples for Pu Bulk Handling Facilities," 6th ANS International Topical Meeting, NPIC & HMIT Knoxville, TN 4/5/2009.

Taylor, C.D., 2009: Connections between the energy functional and interaction potentials for materials simulation. Phys. Rev. B 80, 024104.

the 12th International Meshing Roundtable, Williamsburg, VA (2004).

Thulasidasan2009a: S. Thulasidasan, S. Eidenbenz: Accelerating Traffic Microsimulations: A Parallel Discrete-Event Queue-based Approach for Speed and Scale. In Proceedings of the ACM/SIGSIM Winter Simulation Conference, December 2009

Thulasidasan2009b: S. Thulasidasan et al: Designing Systems for Large-Scale, Discrete-Event Simulations: Experiences with the FastTrans Parallel Microsimulator. In the Proceedings of the International Conference on High Performance Computing (HiPC), December 2009

Thulasidasan2010: S. Thulasidasan, S. Kasiviswanathan, S. Eidenbenz, P. Romero: Explicit Spatial Scattering for Load Balancing in Distributed Discrete Event Simulations with Conservative Time Synchronization: In Proceedings of the ACM/IEEE/SCS Workshop on Principles of Advanced and Distributed Simulation, 2010

Timm2007: "Human Leukocyte Antigen-Associated Sequence Polymorphisms in Hepatitis C Virus Reveal Reproducible Immune Responses and Constraints on Viral Evolution," Joerg Timm, Bin Li, Marcus, G. Daniels, TanmoyBhattacharya, Laura L. Reyor, Rachel Allgaier, Thomas Kuntzen, Will Fischer, Brian E. Nolan, Jared Duncan, Julian Schulze zur Wiesch, Arthur Y. Kim, Nicole Frahm, Christian Brander, Raymond T. Chung, George M. Lauer, BetteT. Korber, and Todd M. Allen. Hepatology, 46:2 (2007) 339—349 ori:doi:10.1002/hep.21712. Published online 8 June 2007 Los Alamos report LA-UR-06-8196, November 2006.

Urbatsch2008: Todd Urbatsch and Scott Mosher, "An Improved Algorithm for Calculating the Number of IMC Source Particles," Transactions of the American Nuclear Society (2008), Vol 98, p.633-5.

Valone, S.M., M. I. Baskes, and R. L. Martin, 2006: Atomistic Model of Helium Bubbles in Gallium-Stabilized Plutonium Alloys, Phys. Rev. B 73, 214209.

vol 227, n 23, 9841-9864 (2008).

Voter, A.F., 1997: Hyperdynamics: Accelerated Molecular Dynamics of Infrequent Events. Phys. Rev. Lett. 78, 3908.

Voter, A.F., 1998: Parallel Replica Method for Dynamics of Infrequent Events. Phys. Rev. B 57, R13985.

Voter, A.F., F. Montalenti and T.C. Germann, 2002: Extending the Time Scale in Atomistic Simulation of Materials. Annu. Rev. Mater. Res. 32, 321.

Waupotitsch2006: R. Waupotitsch, S. Eidenbenz, L. Kroc, J.P. Smith, Multi-Scale Integrated Information and Telecommunications System (MIITS): First Results from A Large-Scale End-to-End Network Simulator, Proceedings of Winter Simulation Conference 2006

Yesilyurt2009: Yesilyurt, G.; Martin, W.R.; Brown, F.B.; "On-the-fly doppler broadening for Monte Carlo codes," American Nuclear Society - International Conference on Mathematics, Computational Methods and Reactor Physics (2009) Vol.3, p.1674-1685.

Zhang, L., S.V. Zybin, A.C.T. van Duin, S. Dasgupta, W.A. Goddard III, and E.M. Kober, 2009: Carbon Cluster Formation during Thermal Decomposition of Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine and 1,3,5-Triamino-2,4,6-trinitrobenzene High Explosives from ReaxFF Reactive Molecular Dynamics Simulations. J. Phys. Chem. A 113, 10619–10640.

Zhou, S.J., D.L. Preston, P.S. Lomdahl, and D.M. Beazley, 1998: Large-Scale Molecular Dynamics Simulations of Dislocation Intersection in Copper. Science 279, 1525-1527.

Appendix A: Selected CPAM Statistics

Computational Physics and Applied Mathematics Capability Review

June 8-10, 2010

APPENDIX A: SELECTED STATISTICS

CY2009-2010

Table of Contents

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 xxx 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, Univerisity 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, 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*, Invited Speaker, Minisymposium on Cancer Modeling, SIAM Computational Sciences and Engineering, Miami, FL, March 2009.
Jiang, J., *Multiscale Model of Tumor Growth and Angiogenesis*, Plenary Speaker, 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 xxx 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.

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.
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. Tiemey, 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.
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.

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.

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.

Delzanno, G.L. and J.M. Finn, *Transport and Linear Stability Studies for PPCD Optimization in RFPs*, International Sherwood Fusion Theory Conference, April 2010.

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.

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 36th International Conference on Plasma Science (ICOPS), 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.

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.

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.

Hickmott, D.D., H. Xu, Y. Zhao, J. Luo, K. Lokshin, and W. Mao, *Applications of Neutron Diffraction Studies at LANSCE to Environment and Energy Problems*, 2009 Goldschmidt Conference, Davos, Switzerland, June 21-26, 2009.

Huang, L., and H. Denli, *How to Design A Sparse Array for Seismic Monitoring?*, 2009 SEG Summer Research Workshop, Banff, Canada, August 23-27, 2009.

Hush, D.R., M.T. Bement, and T.K. Wong, *Inferring Hardness from High-Speed Video of the Machining Process,* ASME International Manufacturing Science and Engineering Conference, Evanston, IL, October 7-10 2008, 20081007-20081010; MSEC 2008: Proceedings of the Asme International Manufacturing Science and Engineering Conference 2008, Vol 2, 29-36, 2009.

Jordanova, V.K., R.M. Thorne, W. Li, and Y. Miyoshi, *Storm-time Excitation of Whistler-mode Chorus Obtained from Global Ring Current Simulations*, Fall Meeting American Geophysical Union, December 14-18, 2009.

Jordanova, V.K., S. Zaharia, and G. Toth, *Storm-time Dynamics of the Coupled Inner Magnetosphere*, Conference on The Non-linear Magnetosphere, Vina del Mar, Chile, January 19-23, 2009.

Kaul, A.M. and C.L. Rousculp, *Current Pulse Effects on Cylindrical Damage Experiments,* 2009 17th IEEE International Pulsed Power Conference (PPC 2009), Washington, DC, June 28-July 2 2009; 2009 17th IEEE International Pulsed Power Conference (PPC 2009) 956-961, 2009.

Keating, G., and D. Pasqualini, *Integrated System Dynamics Model to Assess Options for Emissions Reductions Related to Energy-Water Sustainability in Sonoma County*, 2nd Forum on Energy and Water Sustainability, Santa Barbara, CA, April 10, 2009.

Kern, K., *Modeling Human Resource Development for Nuclear Power Programs*, International Conference on Human Resource Development for Introducing and Nuclear Power Programmes ; Abu Dhabi, United Arab Emirates, March 14, 2010.

Kiedrowski, B.C., and F.B. Brown, *An Information Theory Based Analysis of Fission Source Correlation in Monte Carlo k-eigenvalue Calculations,* 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, 2417-2428, 2009.

Kim, Y., H.W. Herrmann, J.R. Langenbrunner, C.S. Young, S.C. Evans, T.J. Sedillo, A.M. McEvoy, W. Stoeffl, C. Horsfield, and M. Rubery, *Simultaneous Measurements of DT Fusion Gamma-ray and Neutron-induced Secondary Gamma-ray Using Gas Cherenkov Detector,* 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.

LeClaire, R., and D. Powell, *Advanced Techniques Using Conductor*, 27th International Conference of the System Dynamics Society, Albuquerque, NM, July 26-30, 2009.

LeClaire, R., D. Powell, and A. Zagonel, *Tools and Techniques for Modular Programming in Vensim*," 27th International Conference of the System Dynamics Society, Albuquerque, NM, July 26-30, 2009.

LeClaire, R.J. and R.W. Bent, *Interoperable Architecture Development for Critical Infrastructure Protection Modeling and Simulation*, LA-UR-09-02197, Risk Analysis of Complex Systems for National Security Applications, Santa Fe, NM, April, 2009.

LeClaire, R.J., *Consequences, Uncertainty and Risk to Critical Infrastructures from a Dam Disruption*, LA-UR-09-02182, presented at the 2009 LANL Risk Conference, Santa Fe, NM, April, 2009.

LeClaire, R.J., D.R. Powell, and A. Zagonel, *Tools and Techniques for Modular Programming in Vensim*, LA-UR-09-04760, workshop presented at the 27th International Conference of the System Dynamics Society, Albuquerque, NM, July, 2009.

LeClaire, R.J., G.B. Hirsch, and A. Bandlow, *Learning Environment Simulator (LES): A Tool for Local Decision Makers and First Responders*, LA-UR-09-01792, presented at the 27th International Conference of the System Dynamics Society, Albuquerque, NM, July, 2009.

LeClaire, R.J., G.B. Hirsch, and A. Bandlow, *Leveraging DHS Modeling and Simulation Investments to Support State and Local Decision Makers*, presented at the Workshop on Grand Challenges in Modeling, Simulation, and Analysis for Homeland Security, Arlington, VA, March 17-18, 2010.

Leggett, S.K., B. Burningham, M.C. Cushing, M.S. Marley, D.J. Pinfield, D. Saumon, R.L. Smart, and S.J. Warren, *The 600 K T9 Dwarfs: Analysis of the Spectral Energy Distributions,* Cool Stars, Stellar Systems and the Sun. 15th Cambridge Workshop on Cool Stars, Stellar Systems and the Sun, July 21-25 2008, St. Andrews, Scotland, UK; AIP Conference Proceedings vol.1094, 541-544, 2009.

Letellier, B.C., R.J. Pawar, and D. Sanzo, *Statistical Abstraction of High-Fidelity CO2 Pressure Histories in 2-D, Uniform, Cylindrical Domains*, 9th Annual Carbon Capture and Sequestration Conference, Pittsburgh, PA, May 10-13, 2010.

Lichtner, P.C., *Field-Scale Model for the Natural Attenuation of Uranium at the Hanford 300 Area Using High Performance Computing*, LBNL, Berkeley, CA, November 6, 2009.

Lindemuth, I.R., R.E. Siemon, B.S. Bauer, M.A. Angelova, W.L. Atchison, S.F. Garanin, and V. Makhin, *Numerical Simulation of Metallic Surface Plasma Formation by Megagauss Magnetic Fields,* 2009 17th IEEE International Pulsed Power Conference (PPC 2009), Washington, DC, June28-July 2 2009; 2009 17th IEEE International Pulsed Power Conference (PPC 2009) 193-199, 2009.

Lipnikov, K. *A Multiscale Multilevel Mimetic (M3) Method for Well-driven Flows in Porous Media*, Amsterdam, The Netherlands, May 31-June 2, 2010.

Lipnikov, K. *Anisotropic Mesh Adaptation for Solution of Finite Element Problems using Edge-based Error Estimates*, 18th international Meshing Roundtable, Salt Lake City, UT, October 2009.

Lipnikov, K. *Mimetic Finite Difference (MFD) Methods: Theory and Applications,* 2010 DOE Applied Mathematics Program Meeting, Berkeley, CA, May 4, 2010.

Lipnikov, K. *Solving the Diffusion and Stokes Problems on Polygonal and Polyhedral Meshes*, International Converence on Finite Element Methods in Engineering and Science (FEMTEC 2009), Granlibakken Conference Center, Lake Tahoe, CA, January 2009.

Lipnikov, K., *Local Flux Mimetic Finite Difference Method for Diffusion Problems*, International Converence on The Mathematics of Finite Elements and Applicatios (MAFELAP), Brunel University, London, UK, June 2009.

Livescu, D. and J.R. Ristorcelli, *Mixing Asymmetry in Variable-density Turbulence*, 12th European Turbulence Conference, Marburg, Germany, September 7-10, 2009.

Livescu, D. J.R. Ristorcelli, and R.A. Gore, *Mixing Asymmetry in Variable-density Turbulence*," 62th annual Meeting of the American Physical Society, Division of Fluid Dynamics, Minneapolis, MN, November 22-24, 2009.

Lowrie, R.B., *Discontinuous Galerkin for P1-Euler Radiation Hydrodynamics*, Numerical Methods for Multi-material Fluids and Structures, Pavia, Italy, September 21-25 2009.

Mniszewski, S., E. Galli, S. Eidenbenz, C. Teuscher, L. Cuellar, and M. Ewers, *ActivitySim: Large-Scale Agent-Based Activity Generation for Infrastructure Simulation*, Agent-Directed Simulation Symposium (ADS 2009), Spring Simulation Multiconference(SpringSim 2009), San Diego, CA, March, 2009.

Mniszewski, S., E. Galli, S. Eidenbenz, C.Teuscher, L. Cuellar, and M. Ewers, *ActivitySim: Large-Scale Agent-Based Activity Generation for Infrastructure Simulation*, Risk Symposium 2009, Santa Fe, NM, April, 2009.

Mniszewski, S., P. Fasel, E. Vivoni, A. White, and E. Springer, *Increased Efficiency for High-Resolution Baron Fork Simulations Using Basin Structure Characteristics*, 9th SAHRA Annual Meeting, Tucson, AZ, September, 2009.

Mniszewski, S.,R. Bent, S. Eidenbenz, and S.Thulasidasan, *Large-Scale Telephone Network Simulation: Discrete Event vs. Steady State*, 12th Communications and Networking Simulation Symposium (CNS 2009), Spring Simulation Multiconference (SpringSim 2009) San Diego, CA, March, 2009.

Moulton, J.D., *Challenges for Multilevel Sampling in Statistical Inference,* Copper Mountain Conference on Multigrid Methods, Copper Mountain, CO, March 22-27, 2009.

Moulton, J.D., *Multilevel Modeling in Highly Heterogeneous Media,* SIAM Conference on Computational Science and Engineering, Miami, FL, March 2-6, 2009.

Moulton, J.D., *The Multi-process High Performance Computing Simulator Thrust,* Advanced Subsurface Capability for Environmental Management (ASCEM) Kickoff Meeting, Lawrence Berkeley National Laboratory, Berkeley, CA, January 20-21, 2010.

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.

Nease, B.R., T. Ueki, T.M. Sutton, and F.B. Brown, *Instructive Concepts about the Monte Carlo Fission Source Distribution,* 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, 2407-2416, 2009.

Nelson, E.M., J.J. Petillo, and B. Levush, *Improved Symmetries in the Finite-element Gun Code MICHELLE,* 2009 IEEE International Vacuum Electronics Conference (IVEC), Rome, Italy, April 28-30 2009; 2009 IEEE International Vacuum Electronics Conference (IVEC) 507-508, 2009.

Pawar, R.J., *CO2-PENS: A Systems Level Approach For Evaluating Geologic CO2 Storage Systems Presentation at University Of Wyoming*, Laramie, WY, January 13, 2009.

Petersen, M.R., D. Livescu, J. Mohd-Yusof, and S. Dean, *High Resolution Numerical Simulations of Compressible Isotropic Turbulence*, 62th annual Meeting of the American Physical Society, Division of Fluid Dynamics, Minneapolis, MN, November 22-24, 2009.

Petersen, M.R., D. Livescu, R.A. Gore, and K. Stalsberg-Zarling, *High Atwood Number Rayleigh-Taylor Instability with Gravity Reversal*, JOWOG 32MIX, Los Alamos, NM, April 19-22, 2010.

Petillo, J., D. Panagos, S. Ovtchinnikov, B. Held, J. Deford, E. Nelson, K. Nguyen, E. Wright, K. Jensen, and B. Levush, *Applications and Current Status of the Finite-element MICHELLE Gun Collector Simulation Code,* 2009 IEEE International Vacuum Electronics Conference (IVEC), Rome, Italy, April 28-30 2009, 20090428-20090430; 2009 IEEE International Vacuum Electronics Conference (IVEC) 463-464, 2009.

Phillips, W.S., *Ground-Based Nuclear Explosion Monitoring R&D*, AFTAC Seismic Review Panel, Los Alamos, NM, March 4, 2009.

Pineda-Porras, O., *New Perspectives on the Damage Estimation for Buried Pipeline Systems due to Seismic Wave Propagation*, 7th International Conference on Lifeline Earthquake Engineering, American Society of Civil Engineering, Oakland, CA, June 28–July 1, 2009.

Powell, D., *Optimal Pandemic Influenza Strategies for Nations*, Risk Analysis of Complex Systems for National Security Applications, Santa Fe, NM, 2009.

Powell, D.R., R. Haffenden, and R.J. LeClaire, *Selected Survey of Infrastructure Disruption Events and Consequences*, presented at the Workshop on Grand Challenges in Modeling, Simulation, and Analysis for Homeland Security, Arlington, VA, March 17-18, 2010.

Ralchenko, Y., J. Abdallah, A. Bar-Shalom, J. Bauche, C. Bauche-Arnoult, C. Bowen, H.-K. Chung, J. Colgan, G. Faussurier, C.J. Fontes, M. Foster, F. de Gaufridy de Dortan, I. Golovkin, S.B. Hansen, R.W. Lee, V. Novikov, J. Oreg, O. Peyrusse, M. Poirier, A. Sasaki, H. Scott, and H.L. Zhang, *Multi-code ab initio Calculation of Ionization Distributions and Radiation Losses for Tungsten in Tokamak Plasmas,* Atomic Processes in Plasmas. 16th International Conference on Atomic Processes in Plasmas, Monterey, CA, March 22-26 2009; AIP Conference Proceedings vol.1161, 242-250, 2009.

Reckinger, A.J., D. Livescu, and O.V. Vasilyev, *Wavelet-based Simulations of Single-mode Rayleigh-Taylor Instability*, 62th annual Meeting of the American Physical Society, Division of Fluid Dynamics, Minneapolis, MN, November 22-24, 2009.

Reckinger, S., D. Livescu, and O. Vasilyev, *Compressibility Effects on the Single Mode Rayleigh-Taylor Instability*, 2nd International Conference Turbulent Mixing and Beyond, Trieste, Italy, July 26-August 7, 2009.

Rousculp, C.L., P.J. Turchi, W.A. Reass, D.M. Oro, F.E. Merrill, J.R. Griego, and R.E. Reinovsky, *PHELIX,* 2009 17th IEEE International Pulsed Power Conference (PPC 2009), Washington, DC, June28-July 2 2009; 2009 17th IEEE International Pulsed Power Conference (PPC 2009)368-371, 2009.

Rubinstein, R., W.R.T. Bos, D. Livescu, and W. Woodruff, *Closure Models for Inhomogeneous Turbulence,* 12th European Turbulence Conference, Marburg, Germany, September 7-10, 2009.

Scannapieco, A.J, N.T. Padial-Collins, and F.L. Cochran, *A Study of Radiation Flow*, Proc. NEDPC, Lawrence Livermore National Laboratory, Livermore, CA, October 26-30, 2009.

Schmitt, M.J., J.F. Benage, F.J. Wysocki, T.J.T. Kwan, C.A. Ekdahl, W.S. Daughton, and M.S. Murillo, *Equation of State of Warm Dense Matter at DARHT-2 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.

Schofield, S.P., *Interface Tracking Methods for Multi-material Flows,* SIAM Conference on Computational Science and Engineering, Miami, FL, March 2-6, 2009.

Schofield, S.P., *Multi-material Incompressible Flow Simulations Using the Moment-of-Fluid (MOF) Method,* USNCCM X, Columbus, OH, July 2009.

Sherrill, M.E., J. Abdallah, C.J. Fontes, H.L. Zhang, and D.P. Kilcrease, *NLTE Opacities of Mid- and High-Z Cocktails,* Atomic Processes in Plasmas. 16th International Conference on Atomic Processes in Plasmas, Monterey, CA, March 22-26 2009; AIP Conference Proceedings vol.1161,10-16, 2009.

Solomon, C.J., A. Sood, and T.E. Booth, *A Weighted Adjoint Source for Weight-window Generation by Means of a Linear Tally Combination,* 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, 1686-1702, 2009.

Stephens, D.C., S.K. Leggett, M.S. Marley, D. Saumon, M.C. Cushing, T.R. Geballe, D.A. Golimowski, X. Fan, and K.S. Noll, *The 0.8 to 14.5 μm Spectral Energy Distributions of Mid-L to Mid-T Dwarfs,* Cool Stars, Stellar Systems and the Sun. 15th Cambridge Workshop on Cool Stars, Stellar Systems and the Sun, St. Andrews, Scotland, UK, July 21-25 2008; AIP Conference Proceedings vol.1094, 172-177, 2009.

Theiler, J., N.R. Harvey, R. Porter, and B. Wohlberg, *Simulation Framework for Spatio-spectral Anomalous Change Detection*, SPIE: Algorithms and Technologies for Multispectral, Hyperspectral, and Ultraspectral Imagery XV, Orlando, FL, April 2009.

Toole G.L, *Energy Transmission Research: New Mexico Renewables,* Science and Technology Committee, New Mexico State Legislature, 2009.

Toole G.L, et al., *Electric Power Transmission Network Design for Wind Generation in the Western United States: Algorithms, Methodology, and Analysis*, 2010 IEEE Power Engineering Society Transmission and Distribution Conference and Exposition, New Orleans, LA, 2010.

Toole G.L, et al., *Windpower-Water Equivalency for the Western US Region*, GWPC Water/Energy Sustainability Forum, Salt Lake City UT, 2009.

Toole G.L.,*WinDS Transmission Path Validation/RES Portfolio Validation*, DOE-EERE Annual Windpower and Hydropower program review, Washington, DC, 2010.

Turchi, P.J., W.A. Reass, C.L. Rousculp, D.M. Oro, F.E. Merrill, J.R. Griego, and R.E. Reinovsky, *Evaluation of Conductor Stresses in a Pulsed High-current Toroidal Transformer,* 2009 17th IEEE International Pulsed Power Conference (PPC 2009), Washington, DC, USA, June 28-July 2 2009; 2009 17th IEEE International Pulsed Power Conference (PPC 2009), 372-377, 2009.

Welling, D.T., V. Jordanova, and S. Zaharia, *Virtual Satellites in the RAM-SCB Inner Magnetosphere Model*, 38th COSPAR Scientific Assembly, Bremen, Germany, July 18-25, 2010.

Welling, D.T., V. Jordanova, S. Zaharia, and G. Toth, *Coupling RAM-SCB to a Magnetospheric GCM and Polar Wind Outflow Model*, Fall Meeting American Geophysical Union, December 14-18, 2009.

Welling, D.T., V. Jordanova, S. Zaharia, and G. Toth, *Exploring the Effects of Ionospheric Outflow on the Inner Magnetosphere using RAM-SC*B, 38th COSPAR Scientific Assembly, Bremen, Germany, July18-25, 2010.

Wohlberg, B. and J. Theiler, *Improved Change Detection with Local Co-registration Adjustments*, First Workshop on Hyperspectral Imaging and Signal Processing: Evolution in Remote Sensing (WHISPERS), Grenoble, France, August 2009.

Wohlberg, B. and J. Theiler, J., *Symmetrized Local Co-registration Optimization for Anomalous Change Detection*, SPIE Computational Imaging VIII, San Jose, CA, January 2010.

Wohlberg, B. and P. Rodríguez, *An l1-TV Algorithm for Deconvolution with Salt and Pepper Noise*, IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP), Taipei, Taiwan, April 2009.

Wohlberg, B., *Block Estimation Methods in Exemplar-based Image Restoration*, SIAM Conference on Imaging Science (IS10), Chicago, IL, April 2010.

Wohlberg, B., *Inpainting with Sparse Linear Combinations of Exemplars*, IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP), Taipei, Taiwan, April 2009.

Wu, Y., J. Jiang, D. Kaiser, D., and M. Alber, *Cell Order in Bacterial Swarms Arises from Reversals of Moving Directions*, American Physical Society March Meeting, Portland, OR, March 15-19, 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.

Yesilyurt, G., W.R. Martin, and F.B. Brown, *On-the-fly Doppler Broadening for Monte Carlo Codes.* 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, 1674-1685, 2009.

Zaharia, S., V.K. Jordanova, and D. Welling, *RAM-SCB Simulations of the Near-Earth Magnetosphere: Effect of Plasma Sheet Conditions and Magnetic Coupling on Ring Current/Region-2 Field-aligned Currents*, IAGA, Sopron, Hungary, August 23-30, 2009.

Zellner, M.B., M. Byers, G. Dimonte, J.E. Hammerberg,T.C. Germann, P.A. Rigg, and W.T. Buttler, *Influence of Shockwave Profile on Ejection of Micron-scale Material from Shocked Sn Surfaces: An Experimental Study,* 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, Vol 1/2, 2009.

Zhou, R. L. Huang, H. Denli, and J. Rutledge, *Double-Difference Tomography Using Microearthquake Data for Monitoring CO2 Injection at Aneth, Utah*, Annual Conf. On Carbon Capture and Sequestration, Pittsburgh, PA, May 4-7, 2009.

Abdel-Fattah A, Tarimala S, Garcia E, Martinez B, Ware D, Lichtner P, Reimus P, Roback R, Los Alamos National Laboratory SFA Progress Report: II Plutonium transport by calcite colloids, Environmental Remediation Sciences Program Science focus area Annual Meeting, Lansdowne VA, April 20-24,-2009, LA-UR-09-01226
Abdel-Fattah AI, Reimus P, Ware S, Colloid facilitated transport of plutonium in saturated porous media, AIChE Annual Meeting Philadelphia PA Nov 18, 2008, LA-UR-08-07388
Abdel-Fattah AI, Transport of Pu(VI) in natural alluvium by natural calcite colloids, Migration 09, Kennewick WA, September 21, 2009, LA-UR-09-06088
Arrowsmith SJ, Hazardous release: acoustic sensing of urban winds, External Proposal Call/Quad Chart, LA-UR-09-05943
Arrowsmith SJ, Whitaker R, Inframonitor: methodology & application to the Utah network, Infrasound technology workshop 2008, Bermuda, November 3, 2008, LA-UR-08-06888
Beckham RE, Tarimala S, Roberts P, Abdel-Fattah AI, Enhanced micromixing in porous media Lattice-Boltzmann modeling and microfluidic experimental results, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08087
Birdsell KH, Diaconu D, Overview of the collaboration between LANL and Romanian Institute for Nuclear Research(ICN) on radioactive waste management, Gulf Cooperation Countries Technical Training Visit, Los Alamos NM, July 2009, LA-UR-09-04802
Broxton DE, Birdsell KH, Vesselinov VV, Katzman D, Conceptual models for chromium contamination in the vicinity of Sandia canyon, Citizens advisory board meeting, Pojoaque, February 27, 2008, LA-UR-08-01177
Carey JW, Wellbore integrity and CO2-brine flow along the casing-cement microannulus, 9th Intl Conf on Greenhouse Gas Control Technologies Washington DC Nov 16-20, 2008, LA-UR-08-07140
Chrystal AE, Heikoop JM, Longmire P, Dale M, Larson TE, Perkins GB, Fabryka-Martin JT, Simmons AM, Fessenden-Rahn J, Using Isotopes to Define Background Groundwater Nitrate at the Los Alamos National Laboratory in North Central New Mexico USA, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08027
Cisneros-Dozal L M, Heikoop J, Fessenden J, Fawcett P, Kawka O, et al., Glacial-Interglacial Climatic Shifts during the mid-Pleistocene in Northern New Mexico USA : insights from C/N ratios d13C and alkane abundance, European geosciences union general assembly 2008, Vienna Austria, April 13, 2008, LA-UR-08-01775
Cisneros-Dozal LM, Fessenden J, Block C, Feddema R, Engel R, Miller P, Wallander R, Evaluating the carbon sequestration potential of agricultural fields, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7, 2009, LA-UR-09-02796
Cisneros-Dozal LM, Heikoop J, Fessenden J, Fawcett P, Kawka O, et al., Glacial-interglacial climatic shifts during the mid-Pleistocene in northern New Mexico USA: inferences from 13c and d analyses of lacustrine organic matter, European geosciences union general assembly 2008, Vienna Austria, April 13, 2008, LA-UR-08-00924
Cisneros-Dozal LM, Heikoop JM, Fessenden-Rahn J, Fawcett P, Kawka O, et al., Mid-Pleistocene lacustrine records of carbon and nitrogen elemental and isotopic data from Valles Caldera New Mexico USA, 2007 American Geophysical Union Fall Meeting, San Francisco CA, December 2007, LA-UR-07-7994
Dai Z, Deng H, Wolfsberg AV, Lu Z, Reimus P, Upscaling of Reactive Mass Transport in Fractured Rocks with Multimodal Reactive Mineral Facies, 2009 American Geophysical Union Fall Meeting, San

Francisco CA, December 14-18, 2009, LA-UR-10-00051
Dai Z, Wolfsberg A, Lu Z, Zyvoloski G, Reimus P, Upscaling flow and transport parameters for fracture network systems, 2007 American Geophysical Union Fall Meeting, San Francisco CA, December 2007, LA-UR-07-6280
Dean CA, Reimus PW, Effective Kd values for radionuclides in Yucca Mountain saturated alluvium, 2008 International High-Level Radioactive Waste Management, Las Vegas NV, September 7, 2008, LA-UR-08-03122
Denli H, Huang L, Double-difference elastic waveform tomography in the time domain, Society of Exploration Geophysicists Annual Meeting 2009, Houston TX, October 26, 2009, LA-UR-09-07083
Denli H, Huang L, Elastic-wave reverse-time migration with a Wavefield-separation imaging condition, Society of Exploration Geophysicists (SEG) Annual Meeting, Las Vegas NV, November 9, 2008, LA-UR-08-07248
Denli H, Huang L, Elastic-wave sensitivity analysis for seismic monitoring, Society of Exploration Geophysicists (SEG) Annual Meeting, Las Vegas NV, November 9, 2008, LA-UR-08-07247
Denli H, Huang L, Quantitative Monitoring for Geologic Carbon Sequestration Using Double-Di, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08084
Dixon PR, Program Development Efforts in Advancing DOE-EM Subsurface Simulation and Performance Assessment Capability: The SAFEMAP Project, SDCLES Briefing, LA-UR-09-03778
Dixon PR, 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, LA-UR-09-04308
Dubey MK, Airborne photoacoustic observations of aerosol optical properties aloft Alaska: quantifying Arctic radiative forcing, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-19, 2008, LA-UR-08-07824
Dubey MK, Costigan K, Wunch D, Wennberg P, Simulations of Los Angeles Region carbon-dioxide emissions: comparisons with observations, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08035
Dubey MK, Coupled climate model simulations to bracket the impacts of increasing Asian aerosols emissions and aggressive future clean air policies, 2007 American Geophysical Union Fall Meeting, San Francisco CA, December 2007, LA-UR-07-8200
Dubey MK, Feasibility of greenhouse gas monitoring from space, LDRD Day Meeting, Santa Fe NM, September 14, 2009, LA-UR-09-05614
Fabryka-Martin JT, Simmons AM, Longmire P, Data reliability for groundwater monitoring wells at Los Alamos National Laboratory, 8th Annual Espanola Basin Workshop, Santa Fe NM, March 3–4 2009, LA-UR-09-01281
Fessenden JE, CO2 monitoring mitigation and verification, Jet Propulsion Laboratory Meeting, Los Alamos NM, May 29, 2008, LA-UR-08-04078
Fessenden-Rahn J, Standoff Detection of O2-Locating Tunnels, Quad Chart for potential sponsors, LA-UR-09-05596
Flowers BA, Dubey MK, Observations of aerosol long-range transport for Asia using a new 3-laser photoacoustic spectrometer, Gordon Research Conf on Atmospheric Chemistry, Waterville Valley NH, August 23-28, 2009, LA-UR-09-07202
Han J, Carey JW, Zhang J, A Water Chemistry Model Applied to CO2 Corrosion under Geologic Conditions, NACE 2010, San Antonio TX, March 14-18, 2010, LA-UR-10-00780
Harp DR, Vesselinov VV, Birdsell KH, Hydrogeologic property inference using spatially-dependent

aquifer parameters, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08028

Harp DR, Vesselinov VV, Identification of hydrostratigraphy: Optimization of Markov-chain geostatistical model by adjusting facies conductivity mean facies lengths and mean transition lengths, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08029

Hartse HE, Denli H, Huang L, Zou R, Time-Reversal Location of Small Mining Explosions and Earthquakes, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08066

Heikoop JM, Longmire P, Dale M, Chrystal AE, Climate Effects on Oxygen Isotope Recharge Elevation Calculations from the Sierra de Los Valles and the Pajarito Plateau, EBTAG 2010, Santa Fe NM, March 4, 2010, LA-UR-10-01209

Huang L, Cheng Arthur, Rutledge J, Time-Lapse VSP Data Processing for Monitoring CO2 Injection, 2009 SEG Annual Meeting, Houston TX, October 25-30, 2009, LA-UR-09-07335

Huang L, Denli H, Double-Difference Elastic Waveform Tomography Using Time-Lapse Seismic Data for Monitoring CO2 Migration, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7, 2009, LA-UR-09-02831

Huang L, Denli H, How to Design a Sparse Array for Seismic Monitoring?, 2009 SEG Summer Research Workshop, Banff Canada, August 23-27, 2009, LA-UR-09-05425

Huang L, Denli H, Imaging faults in the cap rock and monitoring and estimating reservoir changes, DOE/NETL Pittsburgh PA October 2008, LA-UR-08-06782

Huang L, High-resolution wave-equation migration imaging, Talk to Japanese visitors, LA-UR-09-03689

Huang L, Huthwaite P, Simonetti F, Multi-scale Ultrasound Breast Tomography, 2010 SPIE Medical Imaging, San Diego CA, February 13-18, 2010, LA-UR-10-00916

Huang L, Huthwaite P, Simonetti F, The Different Structural Scales of the Breast and Their Impact on Time-of-Flight and Diffraction Tomography, 2010 SPIE Medical Imaging, San Diego CA, February 13-18, 2010, LA-UR-10-00783

Huang L, Li C, Duric N, Breast ultrasound tomography with total-variation regularization, 2009 SPIE Medical Imaging, Orlando FL, February 7-12, 2009, LA-UR-09-00713

Huang L, Li C, Duric N, Breast ultrasound tomography with total-variation regularization, 2009 SPIE Medical Imaging, Orlando FL, February 7-12, 2009, LA-UR-09-00407

Huang L, Rutledge J, Zhou R, Denli H, Cheng Arthur, Peron Janusz, VSP Monitoring of CO2 Injection at the Aneth Oil Field in Utah, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-19, 2008, LA-UR-09-00409

Huang L, Rutledge J, Zhou R, Denli H, Peron J, Zhao M, Cheng A, Time-Lapse VSP Surveys for Monitoring CO2 Migration at the Aneth Oil Field in Utah, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7, 2009, LA-UR-09-02797

Huang L, Seismic imaging and monitoring for geologic carbon sequestration, 2009 Seismological Society of America Annual Meeting Monterey CA, April 8-10, 2009, LA-UR-09-02052

Huang L, Seismic monitoring verification and accounting, Project Review Southwest Partnership on Carbon Sequestration, LA-UR-08-07022

Huang L, Simonetti F, A Novel Synthetic Aperture Technique for Breast Tomography with Toroidal Arrays, 2009 SPIE Medical Imaging, Orlando FL, February 7-12, 2009, LA-UR-09-00712

Huang L, Simonetti F, A Novel Synthetic Aperture Technique for Breast Tomography with Toroidal Arrays, 2009 SPIE Medical Imaging, Orlando FL, February 7-12, 2009, LA-UR-09-00406

Huang L, Simonetti F, Huthwaite P, Rosenberg R, Detecting breast microcalcifications using super-resolution and wave-equation ultrasound imaging: A numerical phantom study, 2010 SPIE Medical Imaging, San Diego CA, February 13-18 2010, LA-UR-10-00917

Huang L, Simonetti F, Huthwaite P, Rosenbert R, Detecting breast microcalcifications using super-resolution and wave-equation ultrasound imaging: A numerical phantom study, 2010 SPIE Medical Imaging, San Diego CA, February 13-18, 2010, LA-UR-10-00782

Huang L, Super-resolution seismic imaging for tunnel detection and monitoring, LANL DHS Program Office, LA-UR-09-05923

Huang L, Zhou R, Rutledge J, Denli H, Double-Difference Tomography of Microseismic Data for Monitoring Carbon Sequestration, 2009 SEG Annual Meeting, Houston TX, October 25-30, 2009, LA-UR-09-07023

J Han, Carey JW, Zhang J, A Water Chemistry Model Applied to Corrosion under Geologic Conditions, Corrosion Center JIP board meeting Ohio University, Athens OH, October 19, 2009, LA-UR-09-06674

Johnson P, LeBas PY et al., Effects of Acoustic Waves on Stick—Slip Behavior in Sheared Granular Media, Intnl School on Complexity 11th Course Grains Friction and Faults, Erice Sicily, July 20, 2009, LA-UR-09-05249

Johnson PA, Time Reversal Mirrors, LDRD Day Meeting, Santa Fe NM, September 14, 2009, LA-UR-09-05461

Keating E, Kang Q, Dash Z, Kwicklis E, Particle tracking-based strategies for simulating transport in a transient groundwater flow field at Yucca Flat Nevada test site USA, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08248

Kelkar SM, Ding M, Chu S, Robinson B, Arnold B, et al., An Updated Site Scale Saturated Zone Ground Water Transport Model for Yucca Mountain, 2007 American Geophysical Union Fall Meeting, San Francisco CA, December 2007, LA-UR-07-7505

Kwicklis, Keating E, Gable C, Integrated models for the vadose and saturated volcanics/alluvium groundwater systems at Yucca Flat, UGTA kick-off meeting, Las Vegas NV, November 7, 2007, LA-UR-07-07761

L. Prasad, J. Theiler, A structural framework for anomalous change detection and characterization, paper # 7341-24, Proceedings of SPIE Defense, Security, and

Sensing Symposium, Orlando FL. April 2009

Le Bas PY, Carey JW, Johnson PA, Probing rock for chemical-induced mechanical-change due to exposure to super critical C02 applying NEWS, ICU, Santiago Chile, January 11th-18th 2009, LA-UR-09-00081

Levitt D, Eddebbarh A, Wilson C, Wolfsberg A, Herr J, Assessing surface water resource availability for oil shale development using the WARMF Model, 29th Oil Shale Symposium, Golden CO, October 19-23, 2009, LA-UR-09-04852

Lichtner PC, Field-Scale Model for the Natural Attenuation of Uranium at the Hanford 300 Area using High Performance Computing, LBNL, Berkeley CA, November 6, 2009, LA-UR-09-07249

Lichtner PC, Hammond GE, Massively Parallel Simulation of Uranium Migration at the Hanford 300 Area, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08024

Lichtner PC, Modeling multiscale-multiphase-multicomponent subsurface reactive flows using advanced computing, Intl workshop on modeling reactive transport in porous media, Strasbourg France, January 21, 2008, LA-UR-08-00259

Lichtner PC, Moulton D, Philip B, Lu C, Hammond G, et al., The next generation massively parallel reactive flow and transport code PFLOTRAN: application to CO2 storage in saline aquifers, ERSP 3rd annual PI meeting, Lansdowne VA, April 7, 2008, LA-UR-08-01600
Lichtner PC, PFLOTRAN: Application to Uranium Migration at the Hanford 300 Area, ERSP PI Meeting, Lansdowne VA, April 23, 2009, LA-UR-09-03062
Lichtner PC, PFLOTRAN: Next-generation model for simulating reactive flow and transport at the petascale, ERSP PI Meeting, Lansdowne VA, April 23 2009, LA-UR-09-03061
Longmire P, Heikoop J M, Ding Mei, Rearick M S, Katzmann D, Geochemical
CA, December 14-18, 2009, LA-UR-09-08033
processes controlling chromium fixation within the Sandia Canyon Wetland Los Alamos New Mexico, American Geophysical Union Fall Meeting, San Francisco
Miller TA, Vesselinov VV, Integrated approach for 3D geology rendering numerical meshing and modeling for flow and transport studies Pajarito plateau New Mexico, Espanola Basin Advisory Group Meeting, Santa Fe NM, March 3, 2009, LA-UR-09-01306
Modrak, RT, Maceira M, Van Wijk J, Pasyanos M, Joint inversion of surface wave and gravity observations: Application to East Africa, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08177
Pawar RJ, CO2-PENS: a systems level approach for evaluating geologic CO2 storage systems, Presentation at University of Wyoming, Laramie WY, January 13, 2009, LA-UR-09-00750
Perkins GB, Larson TE, Longmire P, Heikoop JM, Differentiation among Multiple Sources of Anthropogenic Nitrate in a Complex Groundwater System using Dual Isotope Systematics: A case study from Mortandad Canyon New Mexico, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08031
Reimus P, Schafer T, Hauser W, Walther C, Geckels H, Degueldre C, Trick T, The CFM (colloid formation and migration) project at the Grimsel test site (GTS Switzerland): model interpretations of first field experiments, Migration 09, 12th Intl Conf on the Chemistry and Migration Behaviour of Actinides and Fission Products in the Geosphere, Kennewick WA, September 20-25, 2009, LA-UR-09-06011
Robinson BA, Earth & Environmental Sciences Division Overview, General Presentation for meetings where EES overview needed, LA-UR-09-03861
Robinson BA, Next steps in spent fuel disposition, general meeting use, LA-UR-09-04469
Rowland JC, Wilson CJ, Brumby S, Pope P, River mobility in a permafrost dominated floodplain, 216th European Geophysical Union meeting, Vienna Austria, April 2009, LA-UR-09-02447
Rowland JC, Wilson CJ, Brumby SP, Pope PA, Arctic River Mobility: A baseline assessment, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-08030
S. Dillard, L. Prasad, and S. Swaminarayan, Rapid Image Segmentation and Exploitation, 2009 GEOINT symposium, Oct 18-21, San Antonio, TX (2009)-Poster and Software Demonstration
Ulrich T J, Van Den Abeele K, Le Bas PY, Anderson BE, Griffa M, Guyer RA, Three Component Time Reversal Imaging using Nonlinear Elasticity, ICU, Santiago Chile, January 11th-18th 2009, LA-UR-09-00079
Zhou R, Huang L, Denli H, Rutledge J, Double-difference tomography using microearthquake data for monitoring CO2 injection at Aneth UT, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7, 2009, LA-UR-09-02742
Zhou R, Huang L, Rutledge J, Denli H, Zhang H, Double-difference tomography of microseismic data for monitoring carbon sequestration, Society of Exploration Geophysicists Annual Meeting, Houston TX,

October 25-30, 2009, LA-UR-09-02290

Zhou R, Huang L, Rutledge J, Denli H, Zhang H, Double-difference tomography using microearthquake data for monitoring CO2 injection at Aneth UT, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7, 2009, LA-UR-09-02743

Ziock H, Boncella J, Maurer S, Monnard PA, Coupling of Genetics and Metabolism and the Origin of Life, LDRD Project review, LA-UR-09-00726

Ziock HJ, Colgate SA, Is information possible without Life?, Decade of the Mind IV, Santa Ana Pueblo NM, January 14-15, 2009, LA-UR-09-00152

Peer-Reviewed Articles

The following list includes xxx peer-reviewed articles by CPAM capability area staff. The list was compiled via submissions by staff in this capability area.

Abdallah, J.; M.E. Sherrill, D.P. Kilcrease, C.J. Fontes, H.L. Zhang, and J. Oelgoetz, *The Reduced Detailed Configuration Accounting (RDCA) Model for NLTE Plasma Spectral Calculations*, High Energy Density Physics vol.5, no.3, 204-207, 2009.
Agouzal, A., K. Lipnikov, and Yu. Vassilevski, *Hessian-free Metric-based Mesh Adaptation via Geometry of Interpolation Error*, Comput. Math. Math. Phys. 50, 131-145, 2010.
Agouzal, A., L. Lipnikov, and Yu. Vassilevski, *Error Estimates for a Finite Element Solution of the Diffusion Equation Based on Composite Norms*, J. Numer. Math. 17, 77-95, 2009.
Ahn, H.T., and M. Shashkov, *Adaptive Moment-of-Fluid Method*, J. Comput. Phys. Vol.228, iss.8, 2792-2821, 2009.
Ahn, H.T., M. Shashkov, and M.A. Christon, *The Moment-of-Fluid Method in Action*, Comm. Numer. Meth. Eng. Vol.25, iss.10, 1009-1018, 2009.
Aluie, H. and G.L. Eyink, *Localness of Energy Cascade in Hydrodynamic Turbulence. II. Sharp Spectral Filter,* Physics of Fluids, Volume 21, Issue 11, 115108, 2009.
Aluie, H. and G.L. Eyink, *Scale Locality of Magnetohydrodynamic Turbulence*, Phys.Rev. Lett. vol. 104, Issue 8, id. 081101, 2010.
Anderson B.E., R.A. Guyer, T.J. Ulrich, and P.A. Johnson, *Time Reversal of Continuous-wave Monochromatic Signals in Elastic Media*, Appl. Phys. Lett. **94**(11), 111908, 2009.
Anderson B.E., R.A. Guyer, T.J. Ulrich, P.-Y. Le Bas, C. Larmat, M. Griffa, and P.A. Johnson, *Energy Current Imaging Method for Time Reversal in Elastic Media*, Appl. Phys. Lett. **95**(2), 021907, 2009.
Anderson D.N., *Rediscovering Signal Complexity as a Teleseismic Discriminant*, PAGEOPH **66:**3, doi 101007/S00024-008-0449-Y, 2009.
Arcudi, F., G.L. Delzanno, and J.M. Finn, *The Effect of Plasma Flow on Line-tied Magnetohydrodynamic Modes*, Phys. Plasmas (in press) 2010.
Arrowsmith S., R. Burlacu, R. Whitaker, and G. Randall, *A Repeating Source of Infrasound from the Wells Nevada Earthquake Sequence*, Geophys. Res. Lett. **36**, L11817, 2009.
Azhgirey, I.L., V.I. Belyakov-Bodin, I.I. Degtyarev, S.G. Mashnik, F.X. Gallmeier, and W. Lu, *CTOF Measurements and Monte Carlo Analyses of Neutron Spectra for the Backward Direction from an Iron Target Irradiated with 400-1200 MeV Protons*, Nucl. Instrum. Methods Phys. Res., Sect. B Vol.267, iss.23-24, 3601-3605, 2009.
Bailey, D., M. Berndt, M. Kucharik, and M. Shashkov, *Reduced-dissipation Remapping of Velocity in Staggered Arbitrary Lagrangian-Eulerian Method*, J. Comput. Applied Math. Vol.233, iss.12, 3148-3156, 20100415, 2010.
Bakosi, J., P. Franzese, and Z. Boybeyi, *Joint PDF Modelling of Turbulent Flow and Dispersion in an Urban Street Canyon*, Boundary Layer Meteorol. Vol.131, iss.2,245-261, 2009.
Bauer, A.L., T.L. Jackson, and Y. Jiang., *Topography of Extracellular Matrix Mediates Vascular Morphogenesis and Migration Speeds in Angiogenesis*, PLoS Comput Biol. 5, e1000445, 2009.
Bauer, A.L., T.L. Jackson, Y. Jiang, and T. Rohlf, *Receptor Cross-talk in Angiogenesis: Mapping Environmental Cues to Cell Phenotype Using a Stochastic, Boolean Signaling Network Model*, J Theor Biol. 264, 838-46, 2010.

Beirao da Veiga, L. and L. Lipnikov, *A Mimetic Discretization of the Stokes Problem with Selected Edge Bubbles*, SIAM J Sci. Comp. 32, 875-893, 2010.

Beirao da Veiga, L., L. Lipnikov, and G. Manzini, *Convergence Analysis of the High-order Mimetic Finite Difference Method*, Numer. Math. 113, 325-356, 2009.

Beirao da Veiga, L., V. Gyrya, L. Lipnikov, and G. Manzini, *Mimetic Finite Difference Method for the Stokes Problem on Polygonal Meshes*, J. Comp. Phys. 228, 7215-7232, 2009.

Bement, M.T. and T.R. Bewley, *Excitation Design for Damage Detection Using Iterative Adjoint-based Optimization-Part 1: Method Development*, Mech. Syst. Signal Process. Vol.23, iss.3, 783-793, 2009.

Bement, M.T.and T.R. Bewley, *Excitation Design for Damage Detection Using Iterative Adjoint-based Optimization-Part 2: Experimental Demonstration*, Mech. Syst. Signal Process. Vol.23, iss.3, 794-803, 2009.

Bent, R., A. Berscheid, and G.L. Toole, *Transmission Network Expansion Planning with Simulation Optimization,* Proc. 24th AAAI Conference on Artificial Intelligence, Atlanta, GA, July 2010.

Bent, R., S. Eidenbenz, and S. Thulasidasan, *Large-Scale Telephone Network Simulation: Discrete Event vs. Steady State,* Proc. 12th Communications and Network Symposium, Spring Simulation Multi Conference, San Diego, CA, March 1-8, 2009.

Bent, R., T. Djidjeva, B. Hayes, J. Holland, H. Khalsa, S. Linger, M. Mathis, S. Mniszewski, and B. Bush, *Hydra: A Service-Oriented Architecture for Scientific Simulation Integration,* Proc.42nd Annual Simulation Symposium, Spring Simulation Multi Conference, San Diego, CA, March 1-8, 2009.

Bettencourt, L.A.M., D.I. Kaiser, and J. Kaur, *Scientific Discovery and Topological Transitions in Collaboration Networks*, Journal of Informetrics 3, 210-221 (2009).

Bettencourt, L.A.M., J. Lobo, and G.B. West, *The Self Similarity of Human Social Organization and Dynamics in Cities*, in Complexity Perspectives on Innovation and Social Change, D. Lane, D. Pumain, S. Van der Leeuw and G.B. West (eds.) Springer, Heidelberg, Germany, 2009. ISBN 978-1-4020-9662-4

Bettencourt, L.A.M., *The Rules of Information Aggregation and Emergence of Collective Intelligent Behavior*, Top. Cognitive Sci. 1, 598-620, 2009.

Blair M.W., L.G. Jacobsohn, S.C. Tornga, and O. Ugurlu, *Luminescence Response of Nanophosphor Aluminum Oxide Dosimeters as Compared to Commercial A12O3:C*, J. Lumin. **130**(5), 825-831, 2010.

Bledsoe, K.C., J.A. Favorite, and T. Aldemir, *Using the Schwinger Inverse Method for Solutions of Inverse Transport Problems in Two-dimensional Cylindrical Geometries,* Ann. Nucl. Energ. Vol.36, iss.7, 966-973, 2009.

Bollen, H.V., A. De Sompel, L. Hagberg, and R. Chute, *A Principal Component Analysis of 39 Scientific Impact Measures,* PLoS ONE, 4:e6022, 2009.

Bollen, H.V., A. De Sompel, L. Hagberg, L. Bettencourt, R. Chute, M.A. Rodriguez, and L. Balakireva, *Clickstream Data Yields High-resolution Maps of Science,* Plos One, 4:E4803, 2009.

Bollt, E.M. et al.,*Graduated, Adaptive Image Denoising: Local Compromise between Total Variation and Isotropic Diffusion,* Adv. Comp. Math vol. 31, 61-85, 2009.

Booth, T.E. and J.E. Gubernatis, *Monte Carlo Determination of Multiple Extremal Eigenpairs*, Phys. Rev. E Vol.80, iss.4, pt.2, 046704, 2009.

Booth, T.E. and J.E. Gubernatis, *Sewing Algorithm*, Comput. Phys. Comm, Vol.180, iss.4, 509-511, 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.: Conf. Ser. 180 012055, 2009.

Brezzi, F., A. Buffa, and K. Lipnikov, *Mimetic Finite Differences for Elliptic Problems*, M2AN: Math. Model. Numer. Anal. 43, 277-295, 2009.

Brown, L.S. and R.L. Singleton, *Temperature Equilibration in a Fully Ionized Plasma: Electron-ion Mass Ratio Effects*, Phys. Rev. E Vol.79, iss.6, pt.2, 066407, 2009.

Brown, M., M. Nelson, M. Williams, A. Gowardhan, and E. Pardyjak, *A Non-CFD Modeling System for Computing 3D Wind and Concentration Fields in Urban Environments*, 5th Int. Symp. Comp. Wind Eng., Chapel Hill, NC, 2010.

Carey J.W., R. Svec, R. Grigg, J. Zhang, and W. Crow, *Experimental Investigation of Wellbore Integrity and CO2-brine Flow along the Casing-cement Microannulus*, Int. J. Greenhouse Gas Control **4**(2), 272-282, 2010.

Chacón, L., G.L. Delzanno, and J.M. Finn, *Robust, Multidimensional Mesh Motion Based on Monge-Kantorovich Wquidistribution*," J. Comput. Phys. (in press) 2010.

Chadwick, M.B., R.C. Little, T. Kawano, P. Talou, D. Viera, M. Jandel, T.A. Bredeweg, M.C. White, A.P. Tonchev, and J.A. Becker, *Actinide ENDF/B-VII Cross-section Evaluations and Validation Testing*, Ann. Nucl. Energ. Vol.36, iss.3, 258-262, 2009.

Chartrand, R. and B. Wohlberg, *Total-Variation Regularization with Bound Constraints*, Proc. 35th Int. Conf. Acoustics, Speech, Signal Processing (ICASSP), 2010.

Chartrand, R. and B. Wohlberg, *Total-variation Regularization with Bound Constraints*, Proc. IEEE Int. Conf. Acoustics, Speech, Signal Process. (ICASSP), 2010.

Chartrand, R., *Fast Algorithms for Nonconvex Compressive Sensing: MRI Reconstruction from Very Few Data*, Proc. IEEE Int. Symp. Biomed. Imaging, 262-265, 2009.

Chartrand, R., K.R. Vixie, B. Wohlberg, and E.M. Bollt, *A Gradient Descent Solution to the Monge-Kantorovich Problem*, Applied Math. Sci. 3:22, 1071-1080, 2009.

Chartrand, R., K.R. Vixie, B., Wohlberg, and E.M. Bollt, *A Gradient Descent Solution to the Monge-Kantorovich Problem*, Appl. Math. Sci. vol. 3, 1071-1080, 2009.

Chen, L., J. Bortnik, R.M. Thorne, R.B. Horne, and V.K. Jordanova, *Three-dimensional Ray Tracing of VLF Waves in a Magnetospheric Environment Containing a Plasmaspheric Plume*, Geophys. Res. Lett. 36, L22101, doi:10.1029/2009GL040451, 2009.

Chen, L., R.M. Thorne, V.K. Jordanova, C.-P. Wang, M. Gkioulidou, L. Lyons, and R.B. Horne, *Global Simulation of EMIC Wave Excitation during the 2001 April 21st Storm from Coupled RCM-RAM-HOTRAY Modeling*, J. Geophys. Res., in press, 2010.

Ching, J., M. Brown, S. Burian, F. Chen, R. Cionco, S. Hanna, A. Hultgren, T. McPherson, D. Sailor, H. Taha, and D. Williams, *National Urban Database and Portal Access Tool*, Bull. Amer. Met. Soc. 90(8), 1157-1168, 2009.

Connington, K., Q. Kang, H. Viswanathan, S. Chen, and A. Abdel-Fattah, *Peristaltic Particle Transport Using the Lattice-Boltzmann Method*, Phys. Fluids **21**(5), 053301, 2009.

Cowee, M.M., D. Winske, and S.P. Gary, *Two-dimensional Hybrid Simulations of Superdiffusion at the Magnetopause Driven by Kelvin-Helmholtz Instability*, J. Geophys. Res. Space Phys. Vol.114, A10209, 2009.

Cushing, M.C., T.L. Roellig, M.S. Marley, D. Saumon, S.K. Leggett, J.D. Kirkpatrick, J.C. Wilson, G.C. Sloan, A.K. Mainzer, J.E. Van Cleve, and J.R. Houck, *A Spitzer Infrared Spectrograph Spectral Sequence of M, L, and T Dwarfs*, Astrophys. J. Vol.706, iss.1, 923-923, 2009.

Daligault, J. and G. Dimonte, *Correlation Effects on the Temperature-relaxation Rates in Dense Plasmas*, Phys. Rev. E Vol.79, iss.5, pt.2, 056403, 2009.

Daughton W., V. Roytershteyn, H. Karimabadi, et al., *Secondary Island Formation in Collisional and Collisionless Kinetic Simulations of Magnetic Reconnection*, Modern Challenges in Nonlinear Plasma Physics (accepted), 2010.

Daughton, W., V. Roytershteyn, B.J. Albright, H. Karimabadi, L. Yin, and K.J. Bowers, *Transition from Collisional to Kinetic Regimes in Large-scale Reconnection Layers*, Phys. Rev. Lett. Vol.103, iss.6, 065004, 2009.

Daughton, W., V. Roytershteyn, B.J. Albright, H. Karimabadi, L. Yin, and K.J. Bowers, *Influence of Coulomb Collisions on the Structure of Reconnection Layers*, Phys. Plasm. Vol.16, iss.7, 072117, 2009.

Daughton, W., V. Roytershteyn, B.J. Albright, H. Karimabadi, L. Yin, and K.J. Bowers, *Transition to Fast Magnetic Reconnection in Large-Scale Semi-Collisional Plasmas*, PRL 103, 065004, 2009.

Daughton, W., V. Roytershteyn, B.J. Albright, H. Karimabadi, L. Yin, and K.J. Bowers, *Influence of Coulomb Collisions on the Structure of Reconnection Layers*, Phys. Plasma 16, 072117-072117-16, 2009.

Delzanno, G.L. and J.M. Finn, *The Fluid-dynamic Approach to Equidistribution Methods for Grid Generation and Adaptation*, Comput. Phys. Commun. (submitted) 2010.

Dendy, J.E. and J.D. Moulton, *Black Box Multigrid with Coarsening by a Factor of Three,* J. Numer. Lin. Alg. App. 17, 577-598, doi:10.1002/nla.705, 2010.

Deshpande A., J. Gans, S.W. Graves, L. Green, L. Taylor, H.B. Kim, Y.A. Kunde, P.M. Leonard, Po-E Li, J. Mark, J. Song, M. Vuyisich, and P.S. White, *A Rapid Multiplex Assay for Nucleic Acid-Based Diagnostics*, J. Microbiol. Meth. 80,155-163, 2010.

Dimonte, G. and P. Ramaprabhu, *Simulations and Model of the Nonlinear Richtmyer-Meshkov Instability*, Phys. Fluids Vol.22, iss.1, 014104, 2010.

Dremov, V.V., A.V. Karavaev, S.I. Samarin, F.A. Sapozhnikov, M.A. Zocher, and D.L. Preston, *Molecular Dynamics Characterization of Thermodynamic and Mechanical Properties of Pu as Dependent upon Alloying Additions and Defects Concentration. Part I,* J. Nucl. Mater. Vol.385, iss.1, 79-82, 20090315, 2009.

Egedal, J., W. Daughton, J.F. Drake, N. Katz, and A. Le, *Formation of a Localized Acceleration Potential During Magnetic Reconnection with a Guide Field*, Phys. Plasma. Vol.16, iss.5, 050701, 2009.

Elliott, S., *Dependence of DMS Global Sea-air Flux Distribution on Transfer Velocity and Concentration Field Type,* J. Geophys. Res. Biogeosci. 114, G02001, 2009.

Evans, K.J., D.W.I. Rouson, A. Salinger, M.A. Taylor, W. Weijer, and J.B. White, *A Scalable and Adaptable Solution Framework within Components of the Community Climate System Model,* Lect. Notes Comput. Sci. 5545, 332-341, 2009.

Eyink G.L. and H. Aluie, *Localness of Energy Cascade in Hydrodynamic Turbulence. I. Smooth Coarse Graining,* Phys. Fluids, Volume 21 Issue 11, 115107, 2009.

Favorite, J.A., K.C. Bledsoe, and D.I. Ketcheson, *Surface and Volume Integrals of Uncollided Adjoint Fluxes and Forward-Adjoint Flux Product* , Nucl. Sci. Eng. Vol.163, iss.1, 73-84, 2009.

Fernandez, J.C., J.J. Honrubia, B.J. Albright, K.A Flippo, D.C. Gautier, B.M. Hegelich, M.J. Schmitt, M. Temporal, and L. Yin, *Progress and Prospects of Ion-driven Fast Ignition*, Nucl. Fusion Vol.49, iss.6, 065004, 2009.

Finn, J.M. and G.L. Delzanno, *Generalized Monge-Kantorovich Optimization for Grid Generation and Adaptation in Lp*, SIAM J. Sci. Comput. (submitted) 2009.

Fontes, C.J., J. Abdallah, C. Bowen, R.W. Lee, and Yu. Ralchenko, *Review of the NLTE-5 Kinetics Workshop*, High Energy Density Physics vol.5, no.1-2, 15-22, 2009.

Fortney, J.J., S.H. Glenzer, M. Koenig, B. Militzer, D. Saumon, and D. Valencia, *Frontiers of the Physics of Dense Plasmas and Planetary Interiors: Experiments, Theory, and Applications*, Phys. Plasma. vol.16, no.4, 041003, 2009.

Foster Jr., J.T., A.A. Barhorst, C.N.S. Wong, and M.T. Bement, *Modeling Loose Joints in Elastic Structures—Experimental Results and Validation,* J. Vib. Contr. Vol.15, iss.4, 549-565, 2009.

Fotiades, N., R.O. Nelson, M. Devlin, S. Holloway, T. Kawano, P. Talou, M.B. Chadwick, J.A. Becker, and P.E. Garrett, *Feeding of the 11/2(-) Isomers in Stable Ir and Au Isotopes*, Phys. Rev. C Vol.80, iss.4, 044612, 2009.

Francois, M.M. and B.K. Swartz, *Interface Curvature via Volume Fractions, Heights, and Mean Values on Nonuniform Rectangular Grids*, J.Comput. Phys. Vol. 229, 527-540, 2010.

Fryer, C.L., P.J. Brown, F. Bufano, J.A. Dahl, C.J. Fontes, L.H. Frey, S.T. Holland, A.L. Hungerford, S. Immler, P. Mazzali, P.A. Milne, E. Scannapieco, N. Weinberg, and P.A. Young, *Spectra and Light Curves of Failed Supernovae*, Astrophys. J. Vol.707, iss.1, 193-207, 2009.

Galli, E., S. Eidenbenz, S. Mniszewski, C. Teuscher, L. Cuellar, and M. Ewers, *ActivitySim: Large-Scale Agent-Based Activity Generation for Infrastructure Simulation*, Proc. 2009 Spring Simulation Multiconference, 2009.

Gardner, R.P., and A. Sood, *On the Future of Monte Carlo Simulation for Nuclear Logs,* Appl. Radiat. Isot. Vol.68, iss.4-5, 932-935, 2010.

Garimella R. and K. Lipnikov, *Solution of the Diffusion Equation Multi-material Domains by Subdivision of Elements Along Reconstructed Interfaces,* Int. J. Numer. Meth. Fluids (in press) 2010.

Garimella R.V., *Conformal Refinement of Unstructured Quadrilateral Meshes*, Proc. 18th Int. Meshing Roundtable, Salt Lake City, UT, 2009.

Garimella R.V., S. Schofield, M.M. Francois, and R. Loubere, *A Second-order Accurate Material Order-independent Interface Reconstruction for Multi-material Flow Simulations,* J. Comput. Phys. 228:3, 745, 2009.

Gary, S.P., H. Karimabadi, and V. Roytershteyn, *Turbulence in Electron-positron Plasmas: Dissipation Wavenumbers*, Astrophys. J. 701 1695-1700, 2009.

Geballe, T.R., D. Saumon, D.A. Golimowski, S.K. Leggett, M.S. Marley, and K.S. Noll, *Spectroscopic Detection of Carbon Monoxide in Two Late-type T Dwarfs*, Astrophys. J. Vol.695, iss.2, 844-854, 2009.

Gintautas, V. and A.Hübler, *A Simple, Low-cost, Data-logging Pendulum Built from a Computer Mouse,* Phys. Educ. 44, 488, 2009.

Gintautas, V., A. Hagberg, and L.M.A. Bettencourt, *When is Social Computation Better than the Sum of its Parts?,* In Social Computing and Behavioral Modeling, 93–101, New York, NY, 2009.

Gnanakaran, S., M.G. Daniels, T. Bhattacharya, A.S. Lapedes, A. Sethi, M. Li, H. Tang, K. Greene, H. Gao, B.F. Haynes, M.S. Cohen, G.M. Shaw, M. Seaman, A. Kumar, F. Gao, D.C. Montefiori, and B. Korber, *Genetic Signatures in the Envelope Glycoproteins of HIV-1 that Associate with Broadly Neutralizing Antibodies*, PLOS Comp. Biol. (submitted).

Göddeke, D., H. Wobker, R. Strzodka, J. Mohd-Yusof, P. McCormick, and S. Turek, *Co-Processor Acceleration of an Unmodified Parallel Solid Mechanics Code with FeastGPU,* Int. J. Comput. Sci. Engineer. Vol.4, iss.4, 254-269, 2009.

Gowardhan, A., E. Pardyjak, I. Senocak, and M. Brown, *A CFD-based Wind Solver for a Fast Response Transport and Dispersion Model*, 5th Int. Symp. Comp. Wind Eng., Chapel Hill, NC, 2010.

Gowardhan, A.A., M.J. Brown, and E.R. Pardyjak, *Evaluation of a Fast Response Pressure Solver for Flow around an Isolated Cube*, Environ. Fluid. Mech., DOI 10.1007/s10652-009-9152-5, 2009.

Griesel, A., S.T. Gille, J. Sprintall, J.L. McClean, and M.E. Maltrud, *Assessing Eddy Heat Flux and its Parameterization: A Wavenumber Perspective from a 1/10 Degrees Ocean Simulation,* Ocean Modelling Vol.29, iss.4, p.248-260, 2009.

Griesel, A., S.T. Gille, J. Sprintall, J.L. McClean, J.H. LaCasce, and M.E. Maltrud, *Isopycnal Diffusivities in the Antarctic Circumpolar Current Inferred from Lagrangian Floats in an Eddying Model*, J. Geophys. Res., doi:10.1029/2009JC005821 (in press) 2010.

Grinstein, F.F., *On Integrating Large Eddy Simulation and Laboratory Turbulent Flow Experiments*, Philos. Trans. R. Soc. London, Ser. A Vol.367, iss.1899, 2931-2945, 2009.

Grove, J.W., *Pressure-Velocity Equilibrium Hydrodynamic Models*, Acta Math. Sci. 30B(1), 2010.

Gutfraind, A., A. Hagberg, and F. Pan,*Optimal Interdiction of Unreactive Markovian Evaders*, in Integration of AI and OR Techniques in Constraint Programming for Combinatorial Optimization Problems, Springer Berlin / Heidelberg, 2009.

Gutfraind, A., *Terrorism as a Mathematical Problem*, SIAM News vol. 42, 12, 2009.

Gutfraind, A., *Understanding Terrorist Organizations with a Dynamic Model,* in Mathematical Methods in Counterterrorism, Springer-Verlag, 2009.

Gutfraind, A., *Understanding Terrorist Organizations with a Dynamic Model*, Studies in Conflict and Terrorism vol. 32, 45–59, 2009.

Habib, S., A. Pope, Z. Lukic, D. Daniel, P. Fasel, N. Desai, K. Heitmann, C.-H. Hsu, L. Ankeny, G. Mark, S. Bhattacharya, and J. Ahrens, *Hybrid Petacomputing Meets Cosmology: The Roadrunner Universe Project*, J. Phys. Conf., Volume 180, Issue 1, pp. 012019, 2009.

Haffenden, R, contributing author to *Implications of Regulation on the Protection of Critical Infrastructures*, Wiley Handbook of Science and Technology for Homeland Security, 2010.

Hakel, P. R.C. Mancini, J. Abdallah, M.E. Sherrill, and H.L. Zhang, *X-ray Line Polarization Spectroscopy of Li-like Si Satellite Line* Spectra, J. Phys. B: At. Mol. Opt. Phys. Vol.42, iss.8, 085701, 2009.

Ham, M.I., V. Gintautas, M.A. Rodriguez, R.A. Bennett, C.L. Santa Maria, and L.M.A. Bettencourt, *Density-dependence of Functional Development in Spiking Cortical Networks Grown in vitro*, Biol. Cybern. 102, 71, 2010.

Hauck, C.D. and R.B. Lowrie, *Temporal Regularization of the PN Equations*, SIAM J. Multiscale Model. Simul. Volume 7, 1497-1524, 2009.

Hemez, F., H.S. Atamturktur, and C. Unal, *Defining Predictive Maturity for Validated Numerical Simulations*, Comput. Struct. Vol.88, iss.7-8, 497-505, 2010.

Henig, A., D. Kiefer, K. Markey, D.C. Gautier, K.A. Flippo, S. Letzring, R.P. Johnson, T. Shimada, L. Yin, B.J. Albright, K.J. Bowers, J.C. Fernandez, S.B. Rykovanov, H.C. Wu, M. Zepf, D. Jung, V.K. Liechtenstein, J. Schreiber, D. Habs, and B.M. Hegelich, *Enhanced Laser-Driven Ion Acceleration in the Relativistic Transparency Regime*, Phys. Rev. Lett. Vol.103, iss.4, 045002, 2009.

Henke H., P.A. Robinson, P.M. Drysdale, and P.N. Loxley, *Spatiotemporal Dynamics of Pattern Formation in the Primary Visual Cortex and Hallucinations*, Biol. Cybern. 101, 3, 2009.

Huang, L., and F. Simonetti, *Synthetic Aperture Diffraction Tomography for Three-Dimensional Imaging*, Proc. R. Soc. **465**(2109), 2877-2895, 2009.

Hunke, E.C. and C.M. Bitz, *Age Characteristics in a Multidecadal Arctic Sea Ice Simulation*, J. Geophys. Res. 114, C08013, doi:10.1029/2008JC005186, 2009.

Jayne, S.R., N.G. Hogg, S.N. Waterman, L. Rainville, K.A. Donohue, R.D. Watts, K.L. Tracey, J.L. McClean, M.E. Maltrud, B. Qiu, S. Chen, and P. Hacker, *The Kuroshio Extension and its Recirculation Gyres.* Deep Sea Res. Oceanogr. Res. Paper Vol.56, iss.12, p.2088-2099, 2009.

Jeffery, N. and B. Wingate, *The Effect of Tilted Rotation on Shear Instabilities at Low Stratifications,* J. Phys. Oceanogr. 31, 3147-3161, 2009.

Jordanova, V.K., H. Matsui, P.A. Puhl-Quinn, M.F. Thomsen, K. Mursula, and L. Holappa, *Ring Current Development during High Speed Streams*, J. Atm. Sol. Terr. Phys. 71, 1093, doi:10.1016/j.jastp.2008.09.043, 2009.

Jordanova, V.K., R.M. Thorne , W. Li , and Y. Miyoshi, *Excitation of Whistler-mode Chorus from Global Ring Current Simulations* J. Geophys. Res. (in press), 2010.

Kawano, T., P. Talou, J.E. Lynn, M.B. Chadwick, and D.G. Madland, *Calculation of Nuclear Reaction Cross Sections on Excited Nuclei with the Coupled-channels Method*, Phys. Rev. C Vol.80, iss.2, 024611, 2009.

Kirkwood, R.K., J. Milovich, D.K. Bradley, M. Schmitt, S.R. Goldman, D.H. Kalantar, D. Meeker, O.S. Jones, S.M. Pollaine, P.A. Amendt, E. Dewald, J. Edwards, O.L. Landen, and A. Nikroo, *Sensitivity of Ignition Scale Backlit Thin-shell Implosions to Hohlraum Symmetry in the Foot of the Drive Pulse*, Phys. Plasma. Vol.16, iss.1, 012702, 2009.

Kline, J.L., D.S. Montgomery, C. Rousseaux, S.D. Baton, V. Tassin, R.A. Hardin, K.A. Flippo, R.P. Johnson, T. Shimada, L. Yin, B.J. Albright, H.A. Rose, and F. Amiranoff, *Investigation of Stimulated Raman Scattering Using a Short-pulse Diffraction Limited Laser Beam Near the Instability Threshold*, Laser Part. Beams Vol.27, iss.1, 185-190, 2009.

Korber, B. and S. Gnanakaran, *The Implications of Patterns in HIV Diversity for Neutralizing Antibody Induction and Susceptibility,* Curr. Opin. HIV AIDS. 4, 408-417, 2009.

Krasheninnikova N., X. Tang and R. Roytershteyn, *Scaling of Plasma Sheath in Magnetic Field Parallel to the Wall*, Phys. Plasmas 17, 057103, 2010.

Kucharik M., R.V. Garimella, S. P. Schofield, and M.J. Shashkov, *A Comparative Study of Interface Reconstruction Methods for Multi-material ALE Simulations*, J. Comput. Phys. 229, 2432-2452, 2010.

Kucharik M., S.P. Schofield, R.V. Garimella, and M.J. Shashkov, *A Comparative Study of Interface Reconstruction Methods for Multi-material ALE Simulations*, J. Comput. Phys. 229:7, 2432-2452, 2009.

Kucharik, M., R.V. Garimella, S.P. Schofield, and M.J. Shashkov, *A Comparative Study of Interface Reconstruction Methods for Multi-material ALE Simulations*, J. Comput. Phys. Vol.229, iss.7, 2432-2452, 2010.

Kulkarni, S.S., A. Lapedes, H. Tang, S. Gnanakaran, M.G. Daniels, M. Zhang, T. Bhattacharya, M. Li, V.R. Polonis, F.E. McCutchan, L. Morris, D. Ellenberger, S.T. Butera, R.C. Bollinger, B.T. Korber, R.S. Paranjape, and D.C. Montefiori, *Highly Complex Neutralization Determinants on a Monophyletic Lineage of Newly Transmitted Subtype C HIV-1 Env Clones from India*, Virol. 385, 505-20, 2009.

Kuzmin, D., M.J. Shashkov, and D. Svyatskiy, *A Constrained Finite Element Method Satisfying the Discrete Maximum Principle for Anisotropic Diffusion Problems*, J. Comput. Phys. Vol.228, iss.9, 3448-3463, 2009.

Le, A., J. Egedal, W. Daughton, J.F. Drake, W. Fox, and N. Katz, *Magnitude of the Hall Fields During Magnetic Reconnection*, Geophys. Res. Lett. Vol.37, L03106, 2010.

Le, A., J. Egedal, W. Daughton, W. Fox, and N. Katz, *Equations of State for Collisionless Guide-Field Reconnection* , Phys. Rev. Lett. Vol.102, iss.8, 085001, 2009.

Leggett, S.K., B. Burningham, D. Saumon, M.S. Marley, S.J. Warren, R.L. Smart, RL; H.R.A. Jones, P.W. Lucas, D.J. Pinfield, and M. Tamura, *Mid-infrared Photometry of Cold Brown Dwarfs: Diversity in Age, Mass, and Metallicity*, Astrophys. J. Vol.710, iss.2, 1627-1640, 2010.

Leggett, S.K., M.C. Cushing, D. Saumon, M.S. Marley, T.L. Roellig, S.J. Warren, B. Burningham, H.R.A. Jones, J.D. Kirkpatrick, N. Lodieu, P.W. Lucas, A.K. Mainzer, E.L. Martin, M.J. McCaughrean, D.J. Pinfield, G.C. Sloan, R.L. Smart, M. Tamura, and J. Van Cleve, *The Physical Properties of Four Similar to 600 K T Dwarfs*, Astrophys. J. Vol.695, iss.2, 1517-1526, 2009.

Lemons, D.S., D. Winske, W. Daughton, and B. Albright, *Small-angle Coulomb Collision Model for Particle-in-cell Simulations*, J. Comput. Phys. Vol.228, iss.5, 1391-1403, 2009.

Lemons, D.S., K.J. Liu, D. Winske, and S.P. Gary, *Stochastic Analysis of Pitch Angle Scattering of Charged Particles by Transverse Magnetic Waves*, Phys. Plasma. Vol.16, iss.11, 112306, 2009.

Lestone, J.P. and S.G. McCalla, *Statistical Model of Heavy-ion Fusion-fission Reactions*, Phys. Rev. C Vol.79, no.4, 044611, 2009.

Lin, Y., B. Wohlberg, and H. Guo, *UPRE Method for Total Variation Parameter Selection*, Signal Processing 90:8, doi:10.1016/j.sigpro.2010.02.025, 2546-2551, 2010.

Lipnikov, K., D. Svyatskiy, and Yu. Vassilevski, *A Monotone Finite Volume Scheme for Advection-diffusion Equations on Unstructured Polygonal Meshes*, J. Comp. Phys. 229, 4017-4032, 2010.

Lipnikov, K., D. Svyatskiy, and Yu. Vassilevski, *Interpolation-free Monotone Finite Volume Method for Diffusion Equations on Polygonal Meshes*, J. Comp. Phys. 228, 703-716, 2009.

Lipnikov, K., J. Moulton, and D. Svyatskiy, *A Multilevel Multiscale Mimetic (M3) Method for an Anisotropic Infiltration Problem*, Lecture Notes in Computer Scienc, Vol.5544, 685-694, 2009.

Lipnikov, K., J.D. Moulton and D. Svyatskiy, *A multilevel multiscale mimetic (M^3) method for an anisotropic infiltration problem*, 8n G. Allen , J. Nabrzyksi, E. Seidel, G.D. Van Albada, J.J. Dongarra, and P.M.A. Sloot, editors, Computational Science-ICCS 2009, 9th International Conference Baton Rouge, LA, May 25-27 2009 Proc. Part I Lecture Notes in Computer Science, vol. 5544, 685-694, 2009.

Lipnikov, K., M. Shashkov, and I. Yotov, *Local Flux Mimetic Finite Difference Methods*, Numerische Mathematik Vol.112, iss.1, 115-152, 2009.

Lipnikov, K., M.J. Shashkov, and I. Yotov, *Local Flux Mimetic Finite Difference Methods*, Numerishe Mathematik 112, 115-152, 2009.

Liska, R., M. Shashkov, P. Vachal, and B. Wendroff, *Optimization-based Synchronized Flux-corrected Conservative Interpolation (Remapping) of Mass and Momentum for Arbitrary Lagrangian-Eulerian Methods*, J. Comput. Phys. Vol.229, iss.5, 1467-1497, 2010.

Livescu, D. and J.R. Ristorcelli, *Mixing Asymmetry in Variable-density Turbulence*, in Advances in Turbulence XII, Editor: B. Eckhardt, Springer Proceedings in Physics vol. 132, 545-548, 2010.

Livescu, D. J.R. Ristorcelli, R.A. Gore, S.H. Dean, W.H. Cabot, and A.W. Cook, *High-Reynolds Number Rayleigh-Taylor Turbulence*, J. Turbul. Vol.10, iss.13, 1-32, 2009.

Livescu, D., J.R. Ristorcelli, M.R. Petersen, and R.A Gore, *Variable-density Rayleigh-Taylor Turbulence at Moderate Atwood Numbers*, Phys. Scr. (in press) 2010.

Livescu, D., J.R. Ristorcelli, R.A. Gore, S.H. Dean, W. Cabot, and A.W. Cook, *High-Reynolds Number Rayleigh-Taylor Turbulence*, J. Turbul. 10(13), 1-32, 2009.

Loxley P.N. and P.A. Robinson *Soliton Model of Competitive Neural Dynamics during Binocular Rivalry*, Phys. Rev. Lett. 102, 258701, 2009.

Luo, S.N., T.C. Germann, and D.L. Tonks, *Spall Damage of Copper Under Supported and Decaying Shock Loading*, J. Applied Phys. Vol.106, iss.12, 123518, 2009.

Lynch, R.M., T. Shen, R. Rong, B. Li, W. Honnen, J. Mulenga, S. Allen, S. Zolla-Pazner, A. Pinter, S. Gnanakaran, and C.A. Derdeyn, *Subtype-specific Conservation of Isoleucine 309 in the Env V3 Domain is Linked to Immune Evasion in Subtype C HIV-1 Infection,* Virol. (in press).

Lynch, R.M., T. Shen, S. Gnanakaran, and C.A. Derdeyn, *Appreciating HIV-1 Diversity: Subtypic Differences in Env*, AIDS Res. Hum. Retrovir. 25, 237-248, 2009.

M. Bradonji´C, A. Hagberg, and A.G. Percus, *The Structure of Geographical Threshold Graphs*, Internet Math 5, 113–140, 2009.

Maltrud, M., F. Bryan, and S. Peacock, *Boundary Impulse Response Functions in a Century-long Eddying Global Ocean Simulation,* Environ. Fluid Dynam. Vol.10, iss.1-2, p.275-295, 2010.

Manga, M., and J. Rowland, *Response of Alum Rock Springs to the October 30 2007 Alum Rock Earthquake and Implications for the Origin of Increased Discharge after Earthquakes*, Geofluids **9**, 237-250, doi: 101111/J1468-8123200900250, 2009.

Manor, R., A. Hagberg, and E. Meron, *Wavenumber Locking and Pattern Formation in Spatially Forced Systems*, New J. Phys. 1:063016 (19pp), 2009.

Margolin, L.G., *Finite-scale Equations for Compressible Fluid Flow*, Philos. Trans. R. Soc. London, Ser. A Vol.367, iss.1899, 2861-2871, 2009.

Mau, Y., A. Hagberg, and E. Meron, *Dual-Mode Spiral Vortices,* Phys. Rev E. 80:065203(R), 2009.

McClarren, R.G. and T.J. Urbatsch, *A Modified Implicit Monte Carlo Method for Time-dependent Radiative Transfer with Adaptive Material Coupling*, J. Comput. Phys. 228, 5669-5686, 2009.

Mernild, S.H. and B. Hasholt, *Observed Runoff, Jökulhlaups, and Suspended Sediment Load from the Greenland Ice Sheet at Kangerlussuaq, West Greenland, for 2007 and 2008,* J. Glaciol. 55(193), 855–858, 2009.

Mernild, S.H. and G.E. Liston, *The influence of air temperature inversion on snow melt and Glacier Surface Mass-balance Simulations, SW Ammassalik Island, SE Greenland.* J. Clim. Appl. Meteorol. vol. 49(1), 47-67, 2010.

Mernild, S.H., G.E. Liston, C.A. Hiemstra, and J.H. Christensen, *Greenland Ice Sheet Surface Mass-balance Modeling in a 131-year Perspective 1950–2080,* J. Hydrometeorol. vol. 11(1), 3-25, 2010.

Mernild, S.H., G.E. Liston, C.A. Hiemstra, and K. Steffen, *Record 2007 Greenland Ice Sheet Surface Melt-extent and Runoff,* Eos Trans. AGU 90(2), 13-14, 2009.

Mernild, S.H., G.E. Liston, C.A. Hiemstra, K. Steffen, E. Hanna and J.H. Christensen, *Greenland Ice Sheet Surface Mass-balance Modeling and Freshwater Flux for 2007, and in a 1995-2007 Perspective,* Hydrolog. Process. DOI: 10.1002/hyp.7354, 2009.

Mernild, S.H., G.E. Liston, K. Steffen, and P. Chylek, *Meltwater Flux and Runoff Modeling in the Ablation Area of the Jakobshavn Isbræ, West Greenland,* J. Glaciol. 56(195), 20-32, 2010.

Moaveni, B., J.P. Conte, and F.M. Hemez, *Uncertainty and Sensitivity Analysis of Damage Identification Results Obtained Using Finite Element Model Updating*, Comput. Aided Civ. Infrastruct. Eng. Vol.24, iss.5, 320-334, 2009.

Molvig, K., M. Alme, R. Webster, and C. Galloway, *Photon Coupling Theory for Plasmas with Strong Compton Scattering: Four Temperature Theory*, Phys. Plasma. Vol.16, iss.2, 023301, 2009.

Mora, C.I., L.R. Riciputi, K.D. Walker, and D.R. Cole, *High Temperature Hydrothermal Alteration of the Boehls Butte Anorthosite: Origin of A Bimodal Plagioclase Assemblage*, Contrib. Mineral. Petrol. **157**(6), 781-795, 2009.

Nahar, S.N., J. Oelgoetz, and A.K. Pradhan, *Recombination Rate Coefficients for KLL Dielectronic Satellite Lines of Fe XXV and Ni XXVII*, Physica Scripta Vol.79, iss.5, 055301, 2009.

Nemenman, I., W. Hlavacek, Y. Jiang, and M. Wall, *Editorial: Selected papers from the Second q-bio Conference on Cellular Information Processing*, IET Systems Biology 3, 297-299, 2009.

Neophytou, M., M. Brown, and A. Gowardhan, *An Inter-comparison of Three Urban Wind Models using Oklahoma City Joint Urban 2003 Wind Field Measurements*, 5th Int. Symp. Comp. Wind Eng., Chapel Hill, NC, 2010.

Oelgoetz, J., C.J. Fontes, H.L. Zhang, S.N. Nahar, and A.K. Pradhan, *On the Importance of Satellite Lines to the Helium-like K Alpha Complex and the G Ratio for Calcium, Iron and Nickel*, Mon. Not. Roy. Astron. Soc. Vol.394, iss.2, 742-750, 2009.

Pei, S., Y. Cui, C.A. Rowe, X. Gao, J. Zhao, and H.S. Liu, *Wave Attenuation Structure of Upper Crust from Amplitude Tomography in Japan*, Bull. Seismol. Soc. Am. **99**(1), P428-434, 2009.

Petersen, M.R. and D. Livescu, *Forcing for Statistically Stationary Compressible Isotropic Turbulence* Phys. Fluids (in press) 2010.

Picard, R.R. and T.E. Booth, *Ensuring Finite Moments in Monte Carlo Simulations via Iterated ex post facto Sampling*, Math. Comput. Simulat. Vol.79, iss.7, 2106-2121, 2009.

Pindzola, M.S., J.A. Ludlow, F. Robicheaux, J. Colgan, and C.J. Fontes, *Fully Relativistic Time-dependent Close-coupling Method for Electron-impact Ionization of Atomic Ions*, Phys. Rev. A: At. Mol. Opt. Phys. Vol.80, iss.5, 052706, 20091113, 2009.

Pineda, O., and M. Najafi, *Seismic Damage Estimation for Buried Pipelines – Challenges after Three Decades of Progress*, J. Pipeline Syst. Eng. Pract. Vol. 1, No. 1, 19-24, 2010.

Pineda, O., and M. Ordaz, *Seismic Fragility Formulations for Segmented Buried Pipeline Systems Including the Impact of Differential Ground Subsidence*, , J. Pipeline Syst. Eng. Pract. (accepted) 2010.

Pope, A., S. Habib, Z. Lukic, D. Daniel, P. Fasel, N. Desai, and K. Heitmann, *Computing in Science and Engineering*, (in print) 2010.

Pradhan, A.K., S.N. Nahar, M. Montenegro, Y. Yu, H.L. Zhang, C. Sur, M. Mrozik, and R.M. Pitzer, *Resonant X-ray Enhancement of the Auger Effect in High-Z Atoms, Molecules, and Nanoparticles: Potential Biomedical Applications*, J. Phys. Chem. A Vol.113, iss.45, 12356-12363, 20091112, 2009.

Quest, K.B., H. Karimabadi, and W. Daughton, *Linear Theory of Anisotropy Driven Modes in a Harris Neutral Sheet*, Phys. Plasma. Vol.17, iss.2, 022107, 2010.

R. Bent, P. Van Hentenryck, and E. Upfal, *Online Stochastic Optimization under Time Constraints,* Ann. Oper. Res. (in press) 2010.

Reckinger, S., D. Livescu, and O. Vasilyev, *Compressibility Effects on Single Mode Rayleigh-Taylor Instability Using a Wavelet-based Method*, Phys. Scr. (in press) 2010.

Ringler, T., J. Thuburn, J. Klemp and W. Skamarock, *A Unified Approach to Energy Conservation and Potential Vorticity Dynamics on Arbitrarily Structured C-grids*, J. Comput. Phys. (accepted), 2009.

Ristorcelli, J.R. and D. Livescu, *Correcting the Anisotropic Gradient Transport of k*, Flow, Turbul. Comb. (in press) 2010.

Roberts, A., J. Cherry, R. Doscher, S. Elliott and L. Sushama, *Exploring the Potential for Arctic Systems Modeling,* Bull. Amer. Meteorol. Soc. (in press).

Roberts, P.M., and A.I. Abdel-Fattah, *Seismic Stress Stimulation Mobilizes Colloids Trapped in A Porous Rock*, Earth Planet. Sci. Lett. **284,** 538-543, 2009.

Rodríguez, P. and B. Wohlberg, *Efficient Minimization Method for a Generalized Total Variation Functional*, IEEE Trans. Image Process. 18:2, doi:10.1109/TIP.2008.2008420, 322-332, 2009.

Rong R., B. Li, R.M. Lynch, R.E. Haaland, M.K. Murphy, J. Mulenga, S.A. Allen, J.L. Blackwell, A. Pinter, G.M. Shaw, E. Hunter, J.E. Robinson, S. Gnanakaran, and C.A. Derdeyn, *Escape from Autologous Neutralizing Antibodies in Acute/Early Subtype C HIV-1 Infection Requires Multiple Pathways,* PLoS Pathogens, Epub September 18, 2009.

Rowland, J.C., M.T. Stacey, and W.E. Dietrich, *Turbulent Characteristics of A Shallow Wall-Bounded Plane Jet: Experimental Implications for River Mouth Hydrodynamics*, J. Fluid Mech. **627,** 423-449, 2009.

Rowland, J.C., W.E. Dietrich, G. Day, and G. Parker, *The Formation and Maintenance of Single-Thread Tie Channels Entering Floodplain Lakes, Observations from Three Diverse River Systems*, J. Geophys. Res. Earth Surface **114**, F02013, 2009.

Roytershteyn V., W. Daughton, S. Dorfman et al., *Magnetic Reconnection Near the Dreicer Limit*, Phys. Plasmas 17, 055706, 2010.

Rubinstein, R., W.R.T. Bos, D. Livescu, and W. Woodruff, *Closure Models for Inhomogeneous Turbulence,* in Advances in Turbulence XII, Editor: B. Eckhardt, Springer Proceedings in Physics vol. 132, 767-770, 2010.

Sampson, D.H., H.L. Zhang, and C.J. Fontes, *A Fully Relativistic Approach for Calculating Atomic Data for Highly Charged Ions*, Phys. Rep. Vol.477, iss.4-6, 111-214, 2009.

Schofield S, M.A. Christon, R.V. Garimella, R.B. Lowrie, B.K. Swartz and V. Dyadechko *Multimaterial Incompressible Flow Simulation Using the Moment-of-Fluid Method*, Int. J. Numer. Meth. Fluids, 2009. DOI:10.1002/fld.2108.

Schofield S. P. and J.M. Restrepo, *Stability of Planar Buoyant Jets in Stratified Fluids*, Phys. Fluids 22, 053602, 2010.

Schofield S.P., M.A. Christon, V. Dyadechko, R. V. Garimella, R. B. Lowrie, and B.K. Swartz, *Multi-material Incompressible Flow Simulation Using the Moment-of-fluid Method,* Int. J. Numer. Meth. Fluids, DOI: 10.1002/fld.2108.

Schofield, S.P. and M.A. Christon M.A., *Effects of Element Order and Interface Reconstruction in FEM/volume-of-fluid Incompressible Flow Simulations*, Int. J. Numer. Meth. Fluids (submitted) 2010.

Schofield, S.P., R.V. Garimella, M.M. Francois, and R. Loubere, *A Second-order Accurate Material-order-Independent Interface Reconstruction Technique for Multi-material Flow Simulations*, J. Comput. Phys. Vol. 228, 731-745, 2009.

Scott, R.B., B.K. Arbic, E.P. Chassignet, A.C. Coward, M.E. Maltrud, W.J. Merryfield, A. Ashwanth Srinivasan, and A. Anson Varghese, *Total Kinetic Energy in Four Global Eddying Ocean Circulation Models and over 5000 Current Meter Records*, Ocean Modell. (in press).

Seifter, A., G.A. Kyrala, S.R. Goldman, N.M. Hoffman, J.L. Kline, and S.H. Batha, *Demonstration of Symcaps to Measure Implosion Symmetry in the Foot of the NIF Scale 0.7 Hohlraums*, Laser Part. Beams Vol.27, iss.1, 123-127, 2009.

Shen, T., and S. Gnanakaran, *The Stability of Cellulose: A Statistical Perspective from a Coarse Grained Model of Hydrogen Bond Network*, Biophys. J. 96, 3032-3040, 2009. (highlighted on cover)

Shen, T., P. Langan, A.D. French, G.P. Johnson, and S. Gnanakaran, *Conformational Flexibility of Soluble Cellulose Oligomers: Chain Length and Temperature Dependence,* J. Am. Chem. Soc. 131, 14786-14794, 2009.

Siranosian, A.A., M. Krstic, A. Smyshlyaev, and M. Bement, *Motion Planning and Tracking for Tip Displacement and Deflection Angle for Flexible Beams*, J. Dyn. Syst. Meas. Contr. -Transactions of the ASME Vol.131, iss.3, 031009, 2009.

Stephens, D.C, S.K. Leggett, M.C. Cushing, M.S. Marley, D. Saumon, T.R. Geballe, D.A. Golimowski, X.H. Fan, and K.S. Noll, *The 0.8-14.5 μM Spectra of Mid-L to Mid-T Dwarfs: Diagnostics of Effective Temperature, Grain Sedimentation, Gas Transport, and Surface Gravity*, Astrophys. J. Vol.702, iss.1, 154-170, 2009.

Svidzinski, V.A., H. Li, B.J. Albright, and K.J. Bowers, *Particle-in-cell Simulations of Tearing Modes in Reversed-field-pinch-like Plasma*, Phys. Plasma. Vol.16, iss.2, 022504, 2009.

Svidzinski, V.A., H. Li, H.A. Rose, B.J. Albright, and K.J. Bowers, *Particle in Cell Simulations of Fast Magnetosonic Wave Turbulence in the Ion Cyclotron Frequency Range*, Phys. Plasma. Vol.16, iss.12, 122310, 2009.

Theiler, J., C. Scovel, B. Wohlberg, and B.R. Foy, *Elliptically Contoured Distributions for Anomalous Change Detection in Hyperspectral Imagery*, IEEE Geosci. Remote Sensing Lett. 7:2, doi:10.1109/LGRS.2009.2032565, 271-275, 2010.

Theiler, J., N.R. Harvey, R. Porter, and B. Wohlberg, *Simulation Framework for Spatio-spectral Anomalous Change Detection*, Proc. SPIE: Algorith. Technol. Multispectral Hyperspectral Ultraspectral Imagery XV 7334, doi:10.1117/12.818632, 73340P, 2009.

Thuburn, J., T. Ringler, J. Klemp, and W. Skamarock, *Numerical Representation of Geostrophic Modes on Arbitrarily Structured C-grids*, J. Comput. Phys. 228 (22), 8321-8335, doi:10.1016/j.jcp.2009.08.006, 2009.

Thulasidasan, S. and S. Eidenbenz, *Accelerating Traffic Microsimulations: A Parallel Discrete-Event Queue-based Approach for Speed and Scale,* Proc. ACM/SIGSIM Winter Simulation Conference, December 2009.

Thulasidasan, S. et al, *Designing Systems for Large-Scale, Discrete-Event Simulations: Experiences with the FastTrans Parallel Microsimulator,* Proc. Int. Conf. High Perf. Comput. (HiPC), December 2009.

Thulasidasan, S., S. Kasiviswanathan, S. Eidenbenz, and P. Romero, *Explicit Spatial Scattering for Load Balancing in Distributed Discrete Event Simulations with Conservative Time Synchronization,* Proc. ACM/IEEE/SCS Workshop on Principles of Advanced and Distributed Simulation, 2010.

Titarenko, Y., V. Batyaev, A. Titarenko, M. Butko, K. Pavlov, S. Florya, R. Tikhonov, N. Sobolevsky, S. Mashnik, W. Gudowski, N. Mokhov, and I. Rakhno, *Residual Radioactive Nuclide Formation in 0.8-GeV Proton-irradiated Extended Pb Target*, Nucl. Tech. Vol.168, iss.3, 631-636, 2009.

Titarenko, Y., V. Batyaev, A. Titarenko, M. Butko, K. Pavlov, S. Florya, R. Tikhonov, P. Boyko, A. Kovalenko, N. Sobolevsky, V. Anashin, S. Mashnik, W. Gudowski, N. Mokhov, and I. Rakhno, *Beam Dump and Local Shielding Layout Around the ITEP Radiation Test Facility*, Nucl. Tech. Vol.168, iss.2, 472-476, 2009.

Titarenko, Y.E., V.F. Batyaev, A.Y. Titarenko, V.M. Zhivun, K.V. Pavlov, M.A. Butko, S.N. Florya, R.S. Tikhonov, and S.G. Mashnik, *Experimental Determination and Computational Modeling of Threshold Reaction Rates in 0.8 Gev Proton-irradiated Lead Target*, Atom. Energ. Vol.107, iss.1, 48-59, 2009.

Toole G.L, et al., *Electric Power Transmission Network Design for Wind Generation in the Western United States: Algorithms, Methodology, and Analysis*, in IEEE Transaction on Power Engineering (PES), 2010.

Toole G.L, et al., *Interdependent Energy Infrastructure Simulation System*, in Handbook of Science and Technology for Homeland Security, D. Kamien, Ed, Wiley and Sons, 2009.

Toole, L., M. Fair, A. Berscheid, and R. Bent, *Electric Power Transmission Network Design for Wind Generation in the Western United States: Algorithms, Methodology, and Analysis,* Proc. 2010 IEEE Power Engineering Society Transmission and Distribution Conference and Exposition, New Orleans, LA, April 2010.

Torres, D.J., Y.H. Li, and S.-C. Kong, *Partitioning Strategies for Parallel KIVA-4 Engine Simulations*, Comput. Fluids Vol. 39, no. 2, 301-309, 2010.

van der Sluijs, M.A. and A.L. Peratt, AL. *The Ouroboros as an Auroral Phenomenon*, J. Folklore Res. Vol.46, iss.1, 3-41, 2009.

Van Hentenryck, P., R. Bent, and C. Coffrin, *Strategic Planning for Disaster Recovery with Stochastic Last Mile Distribution,* Proc.7th International Conference on Integration of Artificial Intelligence and Operations Research Techniques in Constraint Programming, June 2010.

Van Hentenryck, P., R. Bent, L. Mercier, and Y. Vergados, *Online Stochastic Reservation Systems,* Ann. Oper. Res. Volume 171(1), 101-126, 2009.

Vrugt, J.A., C.J.F. Ter Braak, C.G.H. Diks, B.A. Robinson, J.M. Hyman et al., *Accelerating Markov Chain Monte Carlo Simulation by Differential Evolution with Self-adaptive Randomized Subspace Sampling,* Int. J. Nonlinear Sci. Numer. Simulat. **10**(3), 273-290, 2009.

Vrugt, J.A., J.M. Hyman, C.J.F. Ter Braak, C.G.H. Diks, B.A. Robinson et al., *Accelerating Markov Chain Monte Carlo Simulation by Self-adaptive Differential Evolution with Randomized Subspace Sampling*, Int. J. Nonlinear Sci. Numer. Simulat. **10**(3), 273-290, 2009.

Wang, M., and Q. Kang, *Electrokinetic Transport in Microchannels with Random Roughness*, Analyt. Chem. **81**(8), 2953–2961, doi: 101021/Ac802569n, 2009.

Wang, X, D.B. Carrington, and D.W. Pepper, *An Adaptive FEM Model for Unsteady Turbulent Convective Flow Over a Backward-Facing Step*, J. Comput. Therm. Sci. Vol 1, no. 2, 121-135, 2009.

Weijer, W., S.T. Gille, and F. Vivier, *Modal Decay in the Australia-Antarctic Basin,* J. Phys. Oceanogr. 39, 2893-2909, 2009.

Welser-Sherrill, L., J.H. Cooley, and D.C. Wilson, *Interactive Tools Designed to Study Mix in Inertial Confinement Fusion Implosions,* Comput. Phys. Comm. Vol.180, iss.6, 835-841, 2009.

White, M., A. Pope, J. Carlson, K. Heitmann, S. Habib, P. Fasel, D. Daniel, and Z. Lukic, *Particle Mesh Simulations of the Lyα Forest and the Signature of Baryon Acoustic Oscillations in the Intergalactic Medium*, Astrophys. J. Vol. 713, Issue 1, 383-393, 2010.

Wohlberg, B. and D.M. Tartakovsky, *Delineation of Geological Facies from Poorly Differentiated Data*, Adv. Water Res. 32, doi:10.1016/j.advwatres.2008.10.014, 225-230, 2009.

Wohlberg, B. and J. Theiler, *Symmetrized Local Co-registration Optimization for Anomalous Change Detection*, Proc. SPIE Computational Imaging VIII 7533, doi:10.1117/12.845210, 753307, 2010.

Wohlberg, B. and P. Rodríguez, *An l1-TV Algorithm for Deconvolution with Salt and Pepper Noise*, Proc. IEEE Int. Conf. Acoustics, Speech, Signal Process. (ICASSP), doi:10.1109/ICASSP.2009.4959819, 1257-1260, 2009.

Wohlberg, B., *Inpainting with Sparse Linear Combinations of Exemplars*, Proc. IEEE Int. Conf. Acoustics, Speech, Signal Process. (ICASSP), doi:10.1109/ICASSP.2009.4959677, 689-692, 2009.

Wu, P., D. Winske, S.P. Gary, N.A. Schwadron, and M.A. Lee, *Energy Dissipation and Ion Heating at the Heliospheric Termination Shock,* J. Geophys. Res. Space Phys. Vol.114, A08103, 2009.

Wu, Y., A.D. Kaiser, Y. Jiang, and M.S. Alber, *Periodic Reversal of Direction Allows Myxobacteria to Swarm*, Proc Natl Acad Sci USA. 106, 1222-7, 2009.

Yan, G., P. Datta, S. Eidenbenz, S. Thulasidasan, and V. Ramaswamy, *Criticality Analysis and Assessment of National Internet Infrastructure*, Computer Networks, 2010.

Yin, L., B.J. Albright, H.A. Rose, K.J. Bowers, B. Bergen, D.S. Montgomery, J.L. Kline, and J.C. Fernandez, *Onset and Saturation of Backward Stimulated Raman Scattering of Laser in Trapping Regime in Three Spatial Dimensions*, Phys. Plasma. Vol.16, iss.11, 113101, 2009.

Conference Proceedings, White Papers, and Reports

The following list includes xxx conference proceedings, white papers, and reports. The list was compiled via submissions by staff in this capability area.

Agouzal, A., K. Lipnikov, Yu. Vassielvski, *Edge-based a Posteriori Error Estimators for Generating Quasi-optimal Simplicial Meshes*, Report LA-UR 09-02773, Los Alamos National Laboratory; submitted to Math. Mod. Nat. Phenom.; 2009.
Ambrosiano, J., and R. Bent, *HCSim: An Agent Model for Urban-scale Healthcare Facility Impact*, Modeling and Analysis Coordination Working Group (MACWG) Workshop, August 2009.
Ambrosiano, J., and R. Newkirk, *Food Risk Assessment Based on a System of Systems Approach*, National Center for Food Safety and Defense (NCFPD) System Based Risk and Vulnerability Assessment Workshop, May 2009.
Ambrosiano, J., D. Powell, R. Roberts, and S. Mniszewski, *Planning in the Agent Framework Simulation*, LA-UR-09-01005, 2009.
Beirao da Veiga, L., L. Lipnikov, and G. Manzini, *A Mimetic Discretization of the Stokes Problem with Selected Edge Bubbles*, Report LA-UR-09-02870, Los Alamos National Laboratory; submitted to SIAM J. Sci. Comput.; 2009.
Boettger, J.C., *Theoretical Zero-temperature Isotherm and Structural Phase Stability of Thorium Dioxide.* 49th Annual Sanibel Symposium, St. Simons Island, GA, February 26-March 3 2009, 20090226-20090303; Int. J. Quantum Chem. Vol.109, iss.15, spec. iss.SI, 3564-3569, 2009.
Booth, T.E., K.C. Kelley, and S.S. McCready, *Monte Carlo Variance Reduction Using Nested Dxtran Spheres,* 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, 765-767, 2009.
Brambilla, S., M.D. Williams, A. Gowardhan, D. Manca, and M.J. Brown, *A Shallow Water Model for Dense Gas Simulation in Urban Areas*, AMS 8th Symp. Urban Env., Phoenix, AZ, LA-UR-09-00601, 2009.
Brown, M., A. Gowardhan, M. Nelson, M. Williams, and E. Pardyjak, *Evaluation of the QUIC Wind and Dispersion Models Using the Joint Urban 2003 Field Experiment*, AMS 8th Symp. Urban Env., Phoenix, AZ, 2009.
Brown, M., M. Nelson, A. Gowardhan, D. Zajic, M. Williams, and G. Streit, *The QUIC Special Event Collector Siting Tool for the BioWatch Program: An Update on New Capabilities*, Official Use Only, LA-CP-09-0319, 2009.
Brumby, S.P., G. Kenyon, W. Landecker, et al., *Large-scale Functional Models of Visual Cortex for Remote Sensing*, 38th IEEE Applied Imagery Pattern Recognition, Vision: Humans, Animals, and Machines, Washington DC, October 14-16 2009.
Carrington, D.B, *Adaptive Finite Element Methods for Turbulent Reactive Flow*, Los Alamos ADTSC Science Highlights, 2010.
Carrington, D.B., *A Characteristic-based Split hp-adaptive Finite Element Method for Combustion Modeling in KIVA-hpFE*, Los Alamos National Laboratory Report, LA-UR-09-06527, 2009.
Carrington, D.B., and D.J. Torres, *KIVA Modeling to Support Diesel Combustion Research*, 2009 DOE/EERE Advanced Combustion Merit Review, Washington D.C., May 2009. (LA-UR-09-01740)
Carrington, D.B., *KIVA-4 Development FY 2009 Year End Report*, DOE/EERE Advanced Combustion Program report, September 2009. (LA-UR-06672)

Carrington, D.B., *KIVA-4 Development*, 2010 DOE/EERE Advanced Combustion Merit Review, Washington D.C., June 2010. (LA-UR-10-01879)

Carrington, D.B., *T-3 Combustion Modeling KIVA Combustion Model Development*, DOE/CFR meeting, Los Alamos, NM, April 21, 2010. (LA-UR 10-01878)

Carrington, D.B., *T-3 Combustion Modeling KIVA-4mpi and KIVA-hpFE Development*, AEC/HCCI Working Group Meeting, Livermore, CA, February 23, 2010. (LA-UR-10-00727)

Carrington, D.B., X. Wang, and D.W. Pepper, *An h-Adaptive Finite Element Method for Turbulent Heat Transfer*, Int. Conf. Comput. Exper. Eng. Sci., Las Vegas, NV, March 23, 2010. (LA-UR 10-01692)

Coon, E.T., S.P. MacLachlan, and J.D. Moulton, *Local Post-processing for Locally Conservative Fluxes in the Galerkin Method for Groundwater Flows*, LA-UR 09-08292, Los Alamos National Laboratory, 2009.

Dale, C.B., K.T. Kern, and S.C. Scott, *Modeling Human Resource Needs For Nuclear Power Expansion*, Technical Meeting on Workforce Planning to Support New Nuclear Power Programmes, IAEA, Vienna, Austria, March 31, 2009.

Daniel, W.B., D. Powell, and M. Rivera, *GlobalCURE*, LA-UR-09-02332, 2009.

Del Valle, S., D. Powell, et al., *National Population and Economic Impacts for 2009 Influenza A(H1N1)*, LA-UR-09-06335, 2009.

Durkee, J.W., M.R. James, and L.S. Waters, *MCNPX Graphics and Arithmetic Tally Updates*, ANS 2009 Intl. Conf. Adv. Math. Comp Methods Reactor Phys., Saratoga Springs, NY, May 3, 2009.

Eagle, N., Y.A. de Monjouye, and L.MA. Nettencourt, *Community Computing: Comparisons between Rural and Urban Societies Using Mobile Phone Data*, 2009 International Conference on Computational Science and Engineering, Vancouver, Canada, August 29-August 31 2009; ISBN: 978-0-7695-3823-5.

Espy, M. M. Flynn, J. Gomez, C. Hanson, R. Kraus, P. Magnelind, K. Maskaly, A. Matlashov, S. Newman, T. Owens, M. Peters, H. Sandin, I. Savukov, L. Schultz, A. Urbaitis, P. Volegov, and V. Zotev, *Ultra-low-field MRI for the Detection of Liquid Explosives*, 9th European Conference on Applied Superconductivity (EUCAS '09), Dresden, Germany, September 13-17 2009, 20090913-20090917; Supercond. Sci. Tech. Vol.23, iss.3, 034023, 2010.

Espy, M., M. Flynn, J. Gomez, C. Hanson, R. Kraus, P. Magnelind, K. Maskaly, A. Matlashov, S. Newman, M. Peters, H. Sandin, I. Savukov, L. Schultz, A. Urbaitis, P. Volegov, and V. Zotev, *Applications of Ultra-low Field Magnetic Resonance for Imaging and Materials Studies*, Applied Superconductivity Conference, Chicago, IL, August 17-22 2008, 20080817-20080822; IEEE Trans. Appl.Supercond. Vol.19, iss.3, pt.1, 835-838, 2009.

Francois M.M. and N.N. Carlson, *The Balanced-Force Volume Tracking Algorithm and Global Embedded Interface Formulation for Droplet Dynmaics with Mass Transfer*, NEAMS Safeguards and Separation progress report, April 2010.

Francois M.M., *A Unified Multi-Fluid Flow Computational Formulation*, ER proposal 20110243ER, submitted April 2010.

Francois, M.M. and N.N. Carlson, *Simulation of Droplet Dynamics with Mass Transfer Using the Balaced-Force Volume Tracking Algorithm for Fuel Reprocessing*, Proc. American Nuclear Society annual meeting, June 13-17, 2010.

Francois, M.M., R.B. Lowrie, and E.D. Dendy, *Five-Equation and Six-Equation Models with Interface-Preserving for Two-Material Compressible Flows*, LA-UR-10-00271, LANL, 2010.

Francois, M.M.and N.N. Carlson N.N., *Numerical Simulation of Droplet Dynamics with Species Diffusion*, NEAMS Safeguards and Separation progress report, LA-UR-09-06987, LANL, 2009.

Gutfraind, A. and K. Ahmadizadeh, K., *Markovian Network Interdiction and the Four Color Theorem*, SIAM J. Discrete Math (in review) 2009. http://arxiv.org/abs/0911.4322.

Gutfraind, A., *Constructing Networks for Cascade Resilience*, 2009. http://arxiv.org/abs/0906.0786.

Gyrya, V., K. Lipnikov, I. Aronson, and L. Berlyand, *Effective Shear Viscosity and Dynamics of Suspensions of Micro-swimmers at Moderate Concentrations*, Report LAUR-09-06018, Los Alamos National Laboratory; submitted. to J. Math. Bio.; 2009.

Haffenden, R., *Disposal of Legacy Nerve Agent GA and Lewisite Stocks at Deseret Chemical Depot* (contributing author), National Research Council of the National Academies, Letter Report, November 5, 2009.

He, K., Y. Jiang, and S.A. Dong, *Hybrid Parallel Framework for the Cellular Potts Model Simulations*, The Fifteenth International Conference on Parallel and Distributed Systems (ICPADS'09), 2009.

Herrmann, H.W., J.R. Langenbrunner, J.M. Mack, J.H. Cooley, D.C. Wilson, S.C. Evans, T.J. Sedillo, G.A. Kyrala, S.E. Caldwell, C.S. Young, A. Nobile, J. Wermer, S. Paglieri, A.M. McEvoy, Y. Kim, S.H. Batha, C.J. Horsfield, D. Drew, W. Garbett, M. Rubery, V.Y. Glebov, S. Roberts, and J.A. Frenje, *Anomalous Yield Reduction in Direct-drive Deuterium/Tritium Implosions Due to He-3 Addition*, 50th Annual Meeting of the Division of Plasma Physics of the American Physical Society, Dallas, TX, November 17-21 2008, 20080201; Phys. Plasma. Vol.16, iss.5, 56312-56312, 2009.

Jiang Y., *Cell-based Model of Tumor Angiogenesis*, Chapter in Modeling Tumor Vasculature: Molecular, Cellular, and Tissue Level Aspects and Implications, Springer, 2010.

Jordanova, V.K., *New Insights on Geomagnetic Storms from Observations and Modeling*, AIP Proceedings from the School and Workshop on Space Plasma Physics, Sozopol, Bulgaria, CP1121, 129-134, 2009.

Jordanova, V.K., *Self-consistent Simulations of Plasma Waves and their Effects on Energetic Particles*, in The Dynamic Magnetosphere, ed. by W. Liu and M. Fujimoto, Springer, 2010.

Kiedrowski, B.C. and F. Brown, *Adjoint-weighted Kinetics Parameters with Continuous Energy Monte Carlo,* 2009 American Nuclear Society Annual Meeting and Embedded Topical Meeting: Nuclear and Emerging Technologies for Space (NETS 2009), Atlanta, GA, June 14-18 2009, 20090614-20090618; Trans. Am. Nucl. Soc. Vol.100, 297-299, 2009.

Kwan, T.J.T., M. Berninger, C. Snell, T.S.F. Wang, and L. Yin, *Simulation of the Cygnus Rod-Pinch Diode Using the Radiographic Chain Model,* 35th IEEE International Conference on Plasma Science; Karlsruhe, Germany, June 15-19 2008, 20080615-20080619; IEEE Trans. Plasma Sci. Vol.37, iss.4, pt.1, 530-537, 2009.

LeClaire, R., D. Powell, R. Haffenden, and D. Belasich, *CEMSA Event Historical Survey*, LA-UR-09-02332, 2009.

LeClaire, R.J., *CEMS Simulation Methodology*, LA-UR-09-00484, January 2009.

LeClaire, R.J., *CEMSA Execution Plan*, LA-UR-09-00486, January 2009.

Letellier, B.C., R.J. Pawar, and D. Sanzo, *Statistical Abstraction of High-Fidelity CO2 Pressure Histories in 2-D, Uniform, Cylindrical Domains*, LA-UR-10-02526, Proc. 9th Annual Carbon Capture and Sequestration Conference, Pittsburgh, Pennsylvania, May 10-13, 2010.

Lipnikov, K., and M. Shashkov, *A Mimetic Tensor Artificial Viscosity Method for Arbitrary Polyhedral Meshes* Report LA-UR 10-00043, Los Alamos National Laboratory; Proc. of ICC10 Conference; 2010.

Lipnikov, K., and M.J. Shashkov, *A Mimetic Tensor Artificial Viscosity for Lagrangian Hydrocodes on Arbitrary Polygonal Meshes*, Los Alamos Report LA-UR 10-00006, Los Alamos National Laboratory, submitted to J. Comp. Phys. 2010.

Lipnikov, K., J. D. Moulton, and D. Svyatskiy, *Adaptive Strategies in the Multilevel Multiscale Mimetic (M^3) Method for Two-phase Flows in Porous Media*, LA-UR 10-01228, Los Alamos National Laboratory, 2010. Submitted to SIAM Multiscale Modeling and Simulation.

Livescu, D., J.R. Ristorcelli, and R.A. Gore R.A., *Mixing Asymmetry in Variable-density Turbulence*, Bull. Am. Phys. Soc. 54(19), 203, 2009.

McDonald, M.P., S. Mahadevan, J. Ambrosiano, and D.R. Powell, *Risk-Based Policy Optimization for Protection of Critical Infrastructures against a Pandemic Influenza Outbreak*, Decision Support Systems (in review) 2010.

Miyoshi, Y. and V.K. Jordanova, *Numerical Simulation of Energetic Electrons in the Inner Magnetosphere during the October 2001 Storm*, edited by M. Hirahara, I. Shinohara, Y. Miyoshi, N. Terada, and T. Mukai, AIP Conference Proceedings from the International Conference on Future Perspectives of Space Plasma and Particle Instrumentation, Rikkyo University, Japan, Volume 1144, 142-145, 2009.

Moore, L., D. Powell, J. Fair, R. LeClaire, and M. Wilson, *Comparing Mitigation Effects under Uncertainty in a Simulated Disease Outbreak*, LA-UR-10-00592, 2010.

Nelson, M. and M. Brown, *QUIC Start Guide (v. 5.6)*, LA-UR-10-01062, 2010.

Nelson, M.A., M.D. Williams, D. Zajic, E.R. Pardyjak, and M.J. Brown, *Evaluation of an Urban Vegetative Canopy Scheme and Impact on Plume Dispersion*, AMS 8th Symp. Urban Env., Phoenix AZ, LA-UR-09-00068, 2009.

NISAC Team, *H1N1 Influenza Pandemic Study, Phase 1*, September 2009.

NISAC Team, *H1N1 Influenza Pandemic Study, Phase 2*, December 2009.

NISAC Team, *Improvised Nuclear Device (IND) Study*, April 2010.

Pepper, D.W, X. Wang, and D.B. Carrington, *A Meshless Method for Modeling Convective Heat Transfer*, Int. Heat Tran. Conf. 14 - IHTC'14, Washington D.C. (accepted) 2010. (LA-UR 10-00726)

Petersen, M.R., D. Livescu, J. Mohd-Yusof, and S. Dean, *High Resolution Numerical Simulations of Compressible Isotropic Turbulence*, Bull. Am. Phys. Soc. 54(19), 161, 2009.

Pierrard, V., J. Goldstein, N. André, V.K. Jordanova, G.A. Kotova, J.F. Lemaire, M.W. Liemohn, and H. Matsui, *Recent Progress in Physics-based Models of the Plasmasphere*, Space Sci. Rev. special issue on The Earth's Plasmasphere: Cluster and IMAGE - A Modern Perspective, DOI 10.1007/s11214-008-9480-7, 2009.

Pineda-Porras, O., *New Perspectives on the Damage Estimation for Buried Pipeline Systems due to Seismic Wave Propagation*, Proc. Technical Council on Lifeline Earthquake Engineering Conference of the American Society of Civil Engineering, 2009.

Powell, D.R., R. Haffenden, and R.J. LeClaire, *CEMSA Event Historical Survey*, LA-UR-09-00480, January 2009.

Reckinger, A.J., D. Livescu, and O.V. Vasilyev, *Wavelet-based Simulations of Single-mode Rayleigh-Taylor Instability*, Bull. Am. Phys. Soc. 54(19), 287, 2009.

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.

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., *Natural Gas Asset Ranking Results and Methodology*, report to Dept. of Homeland Security-RDMB, 2010.

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

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

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

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.

Toole G.L, et al., *Electric Service Statistics Sept. 2008 to Aug. 2009*, report to Santa Teresa, New Mexico Industrial Park Association, 2009.

Toole G.L, et al., *Electromagnetic Pulse (EMP) Impacts on Extra High Voltage (EHV) Power Transformers*, report to Dept. of Homeland Security-RDMB, 2010.

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.

Toole G.L, et al., *Regional Infrastructure Protection Plan Outage Analysis for the New York City Metropolitan Area*, National Infrastructure and Simulation Analysis Center report, report to Dept. of Homeland Security-RDMB, 2010.

Toole G.L, et al., *Y Bar Ranch Renewable Energy Site Assessment, Dell City NM*, report to New Mexico small business, 2009.

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.

Van Cuyk, S., A. Deshpande, A. Hollander, L. Ticknor, L. Veal, M. Brown, N. Duval, L. Gallegos-Graves, and K. Omberg, *Bacillus thuringensis var. kurstaki (Btk): Agent Fate Characterization*, 2008 Final Report, LA-UR-09-05794, 2009.

Van Cuyk, S., A. Deshpande, A. Hollander, L. Ticknor, L.A. Veal., M. Brown, N. Duval., L. Gallegos-Graves, and K.M. Omberg, *Bacillus Thuringiensis var Kurstaki (Btk): Agent Fate Characterization,* 2008 final report, LA-UR-09-05794, 2009.

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.

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.

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.

Abdel-Fattah A, Tarimala S, Garcia E, Martinez B, Ware D, Lichtner P, Reimus P, Roback R, Los Alamos National Laboratory SFA Progress Report: II Plutonium Transport By Calcite Colloids, 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, Kennewick WA, September 21 2009
Abdel-Fattah AI, Microscopic and macroscopic scale behavior of colloidal particles subject to elastic-wave stimulations, 14th Intl Conf on Surface Forces, Moscow to St Petersburg Russia, June 21, 2010, LA-UR-09-07802
Abdel-Fattah AI, Roberts PM, Tarimala SI, Reem IH, Acoustically-induced microparticle orbiting and clustering on a solid surface: origin and implications, Particles 2008 conf, Orlando FL, May 10, 2008, LA-UR-08-01610
Anderson BE, Griffa M, Ulrich TJ, Johnson PA, Selective source reduction to identify masked smaller sources using time reversal acoustics (TRA), 2007 Review Of Progress in Qualitative Nondestructive Evaluation, Proceedings, LA-UR-07-5914
Arrowsmith MD, Arrowsmith SJ, Miller KC, Stump BW, The bighorns regional array: an uprecedented opportunity for seismo-acoustic discrimination, Seismological Society of America, Portland OR, April 21, 2010, LA-UR-10-00233
Arrowsmith SJ, Hartse H E, Whitaker R, Infrasound from Earthquakes: A Robust Study of Epicentral Infrasound from Earthquakes in the Western US, LA-UR-09-08144
Arrowsmith SJ, Hartse HE, Whitaker R, Burlacu R, Low frequency sound from earthquakes: What can we uniquely learn from seismo-acoustics? Seismological Society of America, Portland OR, April 21, 2010, LA-UR-10-00112
Arrowsmith SJ, Stump BW, Johnson JB, Drob DP, The seismo-acoustic wavefield: A new paradigm in studying geophysical phenomena, Seismological Society of America, Portland OR, April 21, 2010, LA-UR-10-00110
Arrowsmith SJ, Taylor S R, Real-Time Acoustic Detection of Moving Vehicles, LA-UR-09-08316
Arrowsmith SJ, The Use of Seismo-Acoustics for Proliferation Detection LA-UR-09-07822
Arrowsmith SJ, Whitaker RW, Modrak RT, Anderson DN, Robust detection and location of infrasound and seismo-acoustic events, Seismological Society of America, Portland OR, April 21, 2010, LA-UR-10-00111
Becker N M, Levitt D G, Modeling Infiltration Through N-Tunnel Ponds At Rainier Mesa Nevada Test Site, UGTA Technical Information Exchange (Tie) Meeting Spring 2009
Beckham RE, Tarimala S, Abdel-Fattah AI, Enhanced Micromixing In Porous Media Lattice-Boltzmann Modeling And Microfluidic Experimental Results, 2009 American Geophysical Fall Meeting, San Francisco CA, December 14-18 2009
Beckham RE, Tarimala S, Abdel-Fattah AI, Enhanced micromixing in porous media Lattice-Boltzmann modeling and microfluidic experimental results, 2009 American Geophysical Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05649
Beckham RE, Tarimala S, Roberts P, Abdel-Fattah AI, Enhanced Micromixing In Porous Media Lattice-Boltzmann Modeling And Microfluidic Experimental Results, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Birdsell KH Reid KD, Katzmann D, Rapid Recharge to Perched Intermediate Groundwater Zones Pajarito Plateau Los Alamos New Mexico, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-19, 2008, LA-UR-08-05882
Boukhalfa H., et al., Los Alamos National Laboratory SFA Progress Report: I Biogeochemical Processes Governing the Subsurface Speciation of Plutonium, Environmental Remediation Sciences Program Science Focus Area Annual Meeting, Lansdowne VA, April 20-24-2009
Boukhalfa H., et al., Los Alamos National Laboratory SFA Progress Report: III Plutonium(VI) Adsorption onto Goethite and Manganese Oxide, Environmental Remediation Sciences Program Science Focus Area Annual Meeting, Lansdowne VA, April 20-24-2009
Brommer D B, Monte Carlo Fault Generation For CO2 Sequestration, 2009 Science And Energy Research Challenge, Oak Ridge TN, August 14 2009
Broxton D, Google Earth Kml File Of Well Locations And Stratigraphy For The Geologic Model Of The Espanola Basin, LA-UR-09-01190
Broxton D, Groundwater Monitoring Well Network Evaluations And Optimizing The Locations Of Additional Monitoring Wells At Los Alamos National Laboratory, 8th Annual Espanola Basin Workshop, Santa Fe NM, March 3–4 2009
Carey J W, Lichtner P C, Computational Studies Of Two-Phase Cement-Co2-Brine Interaction In Wellbore Environments, 2009 SPE International Conference On Co2 Capture & Storage, San Diego CA, November 2-4 2009
Carey JW, Abdel-Fattah AI, Backhaus S, Kang Q, Lichtner PC, Moulton D, Zhao Y, Integrated experimentation and hybrid modeling for prediction and control of multi-phase flow and reaction in CO2 injection and storage, Immigration Exhibit, LA-UR-09-07803
Carey JW, Crow W, CCP2 well integrity survey - analysis program and way forward, 2008 UIC Conf, New Orleans LA, January 14, 2008, LA-UR-07-8437
Carey JW, Lichtner PC, Computational studies of two-phase cement-CO2-brine interaction in wellbore environments, 2009 SPE International Conference on CO2 Capture & Storage, San Diego CA, November 2-4, 2009, LA-UR-09-05560
Carey JW, Science of geological carbon sequestration: integration of experimentation and simulation, NNSA LDRD Energy Security Symposium, Washington DC, September 18, 2008, LA-UR-08-05146
Carey JW, Williams MR, Hakala JA, Fessenden JE, Keating EH, Experimental Study Of Sediment-CO2 Reactions With Application to Changes in Groundwater Quality Due To Leakage of Sequestered CO2, 2009 AGU Fall Meeting, San Francisco CA, December 14-18 2009
Carey JW, Williams MR, Hakala JA, Fessenden JE, Keating EH, Experimental study of sediment-CO2 reactions with application to changes in groundwater quality due to leakage of sequestered CO2, 2009 AGU Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05837
Cheng A, Huang L, Rutledge J, Time-phase VSP Data Processing for Monitoring CO2 Injection, Society of Exploration Geophysicists Annual Meeting, Houston TX, October 25-30, 2009, LA-UR-09-02388
Cheng Arthur, Huang L, Rutledge James Time-Lapse VSP Data Processing For Monitoring Co2 Injection Society Of Exploration Geophysicists Annual Meeting, Houston TX, October 25-30 2009
Chrystal AE, Heikoop JM, Longmire P, Dale M, Larson TE, Perkins GB, Fabryka-Martin JT, Simmons AM, Fessenden-Rahn J, Using Isotopes To Define Background Groundwater Nitrate At The Los Alamos National Laboratory In North Central New Mexico USA, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Chrystal AE, Heikoop JM, Longmire P, Dale M, Larson TE, Perkins GB, Fabryka-Martin JT, Simmons AM, Fessenden-Rahn J, Isotopic Composition of Natural Nitrate in Groundwater in Los Alamos New Mexico, EBTAG 2010, Santa Fe NM, March 4, 2010, LA-UR-10-01238
Cisneros-Dozal L M, Fessenden J, Block C, Feddema R, Engel R, Miller P, Wallander R, Evaluating the Carbon Sequestration Potential of Agricultural Fields, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7 2009
Cisneros-Dozal LM, Fessenden J, Heikoop JM, et al., Novel Insights to the factors controlling the monsoon precipitation in the SW US from a mid-Pleistocene lake sediment record Valles Caldera Northern New Mexico, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-19, 2008, LA-UR-08-05880
Clayton DJ, Gable CW, 3-D Thermal Analysis of High-Level Waste Emplaced In a Generic Salt Repository, LA-UR-09-00589
Cole G L, Coblentz D, Jacobs E P, Koning D, The 2009 Three-Dimensional Geologic Models Of The Los Alamos National Laboratory Site Southern Espanola Basin And Espanola Basin, LA-UR-09-03701
Cole G. L., New Geologic Framework Models For the Pajarito Plateau and Espanola Basin Regions, Espanola Basin Advisory Group Meeting, Santa Fe NM, March 3 2009
Dai Z, Deng H, Wolfsberg A, Lu Z, Ye Ming, Reimus P, Upscaling of Reactive Mass Transport in Fractured Rocks with Multimodal Reactive Mineral Facies, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05667
Dai Z., Deng H., Wolfsberg A. V., Lu Z., Reimus P., Upscaling of Reactive Mass Transport In Fractured Rocks With Multimodal Reactive Mineral Facies, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Dai Z., Deng H., Wolfsberg A., Lu Z., Ye M., Reimus P., Upscaling Of Reactive Mass Transport In Fractured Rocks With Multimodal Reactive Mineral Facies, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Dai Z., Kwicklis E., Eddebbarh A., Wolfsberg A., Gable C., Sensitivity Analysis of the Pahute Mesa Pumping Tests: Strategy to Evaluated the Observation Well Design, UGTA Technical Information Exchange Meeting Las Vegas NV, April 20 2009
Dean CA, Reimus PW, Effective Kd values for radionuclides in Yucca Mountain saturated alluvium, 2008 International High-Level Radioactive Waste Management, Las Vegas NV, September 7, 2008, LA-UR-08-00564
Dean CA, Reimus PW, Transport of uranium and neptunium in the saturated volcanic tuff and alluvium at Yucca mountain, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-19, 2008, LA-UR-08-05845
Denli H Quantitative Monitoring For Geologic Carbon Sequestration Using Double- Difference Elastic Waveform Inversion2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Denli H, Huang L Differential Waveform Tomography Using Time-Lapse VSP Data for Monitoring Co2 Migration8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh Pa, May 4-7 2009
Denli H, Huang L Elastic Reverse-Time Migration with Eigenstructure-Based Coherency Decomposition for Fault and Fracture Detection 8th Annual Conf on Carbon Capture & Sequestration, Pittsburgh Pa, 2009
Denli H, Huang L Quantitative Monitoring For Geologic Carbon Sequestration Using Double-Difference Elastic Waveform Inversion American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Denli H, Huang L, Differential waveform tomography using time-lapse VSP data for monitoring CO2 migration, 8th Annual Conf on Carbon Capture & Sequestration, Pittsburgh PA, 2009, LA-UR-09-00810
Denli H, Huang L, Differential Waveform Tomography Using Time-Lapse VSP Data for Monitoring CO2 Migration, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7, 2009, LA-UR-09-00410
Denli H, Huang L, Double-Difference Elastic Waveform Tomography in the Time Domain, Society of Exploration Geophysists Annual Meeting 2009, Houston TX, October 25, 2009, LA-UR-09-02289
Denli H, Huang L, Elastic Reverse-Time Migration with Eigenstructure-based Coherency Decomposition for Fault and Fracture Detection, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7, 2009, LA-UR-09-00411
Denli H, Huang L, Elastic reverse-time migration with Eigenstructure-based coherency decomposition for fault and fracture detection, 8th Annual Conf on Carbon Capture & Sequestration, Pittsburgh PA, 2009, LA-UR-09-03601
Denli H, Huang L, Elastic-wave sensitivity analysis for seismic monitoring, 70th EAGE Conf & Exhibition incorporating SPE EUROPEC 2008, Rome Italy, June 9, 2008, LA-UR-LA-UR-08-00383
Denli H, Huang L., Elastic Reverse-Time Migration with Eigenstructure-Based Coherency Decomposition for Fault and Fracture Detection, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7 2009
Denli H., Huang L., Double-Difference Elastic Waveform Tomography in the Time Domain, Society of Exploration Geophysics Annual Meeting 2009, Houston TX, October 25 2009
Denli H., Huang L., Double-Difference Elastic Waveform Tomography in the Time Domain, Society of Exploration Geophysicists Annual Meeting 2009, Houston TX, October 26 2009
Denli H., Huang L., Differential Waveform Tomography Using Time-Lapse VSP Data for Monitoring CO2 Migration, 8th Annual Conf on Carbon Capture & Sequestration, Pittsburgh Pa, 2009
Ding M, Longmire P, Vaniman D, Broxton D, Rearick M, Ware D, Katzman D, Barger J, Webb S Experimental Characterization Of Chromium Fate And Transport In Sandia Canyon Los Alamos National Laboratory New Mexico 2009 Geological Society Of America Annual Meeting, Portland Or, October 18-21 2009
Ding M, Longmire P, Vaniman D, Broxton D, Rearick M, Ware D, Katzman D, Barger J, Webb S Experimental Characterization Of Chromium Fate And Transport In The Sandia Canyon Vadose Zone And Regional Aquifer Los Alamos New Mexico 2009 AGU Fall Meeting, San Francisco CA, December 14-18 2009
Ding M, Longmire P, Vaniman D, Broxton D, Rearick M, Ware D, Katzman D, Barger J, Webb S Experimental Characterization Of Chromium Fate And Transport In The Vadose Zone And Regional Aquifer At Sandia Canyon Los Alamos New Mexico American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Dixon Paul 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 Paul R, Stroud Cliff D Sustainable Nuclear Energy for the 21st Century Brochure LA-UR-09-00437
Dubey Manvendra K Feasibility of Greenhouse Gas Monitoring From Space LDRD Day Meeting, Santa Fe NM, September 14 2009
Dubey Manvendra K, Costigan Keeley, Chylek P., WRF Simulations of Los Angeles Region Carbon-Dioxide Emissions: Comparisons with Column Observations2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Dubey Manvendra K, Costigan Keeley, Wunch Debra, Wennberg Paul Simulations Of Los Angeles Region Carbon-Dioxide Emissions: Comparisons With Observations American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Dubey MK, Costigan K, Chylek P, WRF simulations of Los Angeles region carbon-dioxide emissions: Comparisons with column observations, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05650
Dubey MK, Mazzoleni C, Emerging observations aerosol-cloud processes from Department of Energy field campaigns to inform cloud models, Advances on modelling and observing clouds and convection, Toulouse France, June 2, 2008, LA-UR-08-03285
Dubey MK, Quantifying aerosol radiactive forcing to constrain climate sensitivity for an optimal transition to a carbon-neutral clean-air world, NNSA LDRD Energy Security Symposium, Washington DC, September 18, 2008, LA-UR-08-05145
Fabryka-Martin June T, Simmons Ardyth M, Longmire Patrick Data Reliability For Groundwater Monitoring Wells At Los Alamos National Laboratory8th Annual Espanola Basin Workshop, Santa Fe NM, March 3–4 2009
Fehm: Finite Element Heat and Mass Brochure LA-UR-09-01662
Fessenden J, Cisneros-Dozal L M, Feddema R, 13C and 14C measurements as tracing of carbon movement and storage in agricultural fields, 7th Annual Conf on Carbon Capture & Sequestration, Pittsburgh PA, May 5, 2008, LA-UR-08-00946
Fessenden-Rahn J, Clegg S, Humphries S, Dobeck L, Spangler L, Seepage CO2 Detection using ZERT controlled release site in Boseman MT, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05598
Fessenden-Rahn Julianna Stable Isotope Signatures of Nuclear Processingla-Ur-09-01834
Fessenden-Rahn Julianna, Clegg Samuel, Humphries Seth, Dobeck Laura, Spangler Lee Seepage Co2 Detection Using ZERT Controlled Release Site In Bozeman Mt2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Flowers BA, Dubey MK Observations Of Aerosol Long-Range Transport For Asia Using A New 3-Laser Photoacoustic Spectrometer Gordon Research Conf On Atmospheric Chemistry, Waterville Valley NH, August 23-28 2009
Flowers BA, Mazzoleni Claudio Field Observations Linking Organic Carbon Content To Optical Properties In Atmospheric Aerosols 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Gable CW, Clayton DJ, Lu Z, Inverse Modeling To Determine Thermal Properties of Salt Due To Heating from High-Level Waste Emplaced In a Generic Salt Repositoryla-Ur-09-00587
Gable CW, Clayton DJ, Lu Z, Modeling Coupled Thermomechanical Phenomena For Disposal Strategies In A Nuclear Waste Salt Repository Impact Of THMC Process On The Safety Of Underground Radioactive Waste Repositories, Luxembourg, September 29-October 1 2009
Gable CW, LaGrit: Los Alamos Grid Toolbox Brochure, LALP-LA-UR-09-019
Han J, Carey JW, Zhang J, A coupled water chemistry and corrosion model for high salinity-high CO2 environments with application to wellbore integrity in CO2 sequestration, 2009 AGU Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05836
Han J, Carey JW, Zhang J, A water chemistry model applied to corrosion under geologic conditions, NACE 2010, San Antonio TX, March 14-18, 2010, LA-UR-09-07787

Han J, Carey JW, Zhang J, Assessing the effect of cement-steel interface on well casing corrosion in aqueous CO2 environments, 9th Annual conf on Carbon Capture and Sequestration, Pittsburgh PA, May 10, 2010, LA-UR-10-00781

Han J, Carey JW, Zhang JA, Coupled Water Chemistry and Corrosion Model for High Salinity-High CO2 Environments with Application to Wellbore Integrity in Co2 Sequestration 2009 AGU Fall Meeting, San Francisco CA, December 14-18 2009

Harp DR, Dai Z, Wolfsberg AV, Vrugt JA, Robinson BA, et al., Aquifer structure identification and uncertainty evaluation using evolutionary stochastic inversion, Computational methods in water resources XVII, San Francisco CA, July 6, 2008, LA-UR-08-00793

Harp DR, Vesselinov VV, Birdsell KH, Hydrogeologic property inference using spatially-dependent aquifer parameters, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05607

Harp DR, Vesselinov VV, Birdsell KH, Hydrogeologic Property Inference Using Spatially-Dependent Aquifer Parameters 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Harp DR, Vesselinov VV, Estimation of hydrostratigraphy by optimization of Markov-chain geostatistical model using mean facies and transition lengths as adjustable parameters, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05610

Harp Dylan R, Vesselinov V. V., Birdsell Kay H Hydrogeologic Property Inference Using Spatially-Dependent Aquifer Parameters American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Harp Dylan R, Vesselinov V. V., Estimation of Hydrostratigraphy by Optimization of Markov-Chain Geostatistical Model Using Mean Facies and Transition Lengths as Adjustable Parameters2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Harp Dylan R, Vesselinov V. V., Identification of Hydrostratigraphy: Optimization of Markov-Chain Geostatistical Model by Adjusting Facies Conductivity Mean Facies Lengths and Mean Transition Lengths American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Hartse Hans E, Denli H, Huang L Time-Reversal Location Of Small Mining Explosions And Earthquakes2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Hartse Hans E, Denli H, Huang L, Zou R., Time-Reversal Location Of Small Mining Explosions And Earthquakes, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Hartse HE, Denli H, Huang L, Time-Reversal Location of Small Mining Explosions and Earthquakes, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05720

Heikoop Jeffrey M, Chrystal Abbey E, Longmire Patrick A, Larson T. E, Perkins George B, Fabryka-Martin June T, Simmons Ardyth M, Fessenden-Rahn Julianna E, Dale Michael R Isotopic Composition Of Natural Nitrate In Groundwater At Los Alamos National Laboratory Los Alamos New Mexico Usa2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Heikoop Jeffrey M, Unkefer Pat J, Toshima Munehiro, Larson T. E, Perkins George B Application Of Carbon And Nitrogen Isotopes To Culturing Of Algae For Production Of Biofuels Algae Biomass Summit, San Diego CA October 7-9 2009

Heikoop JM, Chrystal AE, Longmire PA, Larson TE, Perkins GB, Fabryka-Martin JT, Simmons AM, Fessenden-Rahn JE, Dale MR, Isotopic composition of natural nitrate in groundwater at Los Alamos National Laboratory Los Alamos New Mexico USA, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05613

Heikoop JM, Longmire P, Birdsell KH, Isotopic Evidence for Partial Natural Attenuation of chromium contamination at Los Alamos National Laboratory New Mexico, Espanola basin technical advisory group annual meeting, Santa Fe NM, March 6, 2008, LA-UR-08-00944

Hickmott Donald D, Shimizu Nobu, Spear Frank S Trace Element Zoning In Garnets - Retrospective And Prospective2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Hickmott Donald D, Shimizu Nobu, Spear Frank S Trace Element Zoning In Garnets - Retrospective And Prospective American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Hickmott Donald D, Xu H., Zhao Y., Luo J., Lokshin K, Mao W Applications Of Neutron Diffraction Studies At LANSCE To Environment And Energy Problems2009 Goldschmidt Conference, Davos Switzerland, June 21-26 2009

House LS, Roberts PM, Tencate JA, Romero-Yeske MD, Seismicity of the Rio Grande Rift and surrounding regions north-central New Mexico, 2008 Seismological Society of America Annual Meeting, Santa Fe NM, April 16, 2008, LA-UR-LA-UR-08-00189

Huang L Seismic Imaging and Monitoring For Geologic Carbon Sequestration2009 Seismological Society of America Annual Meeting Monterey CA, April 8-10 2009

Huang L, Cheng Arthur, Rutledge James Time-Lapse VSP Data Processing For Monitoring Co2 Injection2009 SEG Annual Meeting, Houston TX, October 25-30 2009

Huang L, Denli H Double-Difference Elastic Waveform Tomography Using Time-Lapse Seismic Data for Monitoring Co2 Migration8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh Pa, May 4-7 2009

Huang L, Denli H How to Design A Sparse Array for Seismic Monitoring?, 2009 SEG Summer Research Workshop, Banff Canada, August 23-27 2009

Huang L, Denli H, How to design a sparse array for seismic monitoring?, 2009 SEG Summer Research Workshop, Banff Canada, August 23-27, 2009, LA-UR-09-02144

Huang L, Double-Difference Waveform Tomography for Imaging Spatial and Temporal Changes in EGS Reservoirs, 34th Annual Meeting of the Geothermal Resources Council, Sacramento CA, October 24-27, 2010, LA-UR-10-01324

Huang L, Li C., Duric Neb Breast Ultrasound Tomography with Total-Variation Regularization2009 SPIE Medical Imaging, Orlando Fl, February 7-12 2009

Huang L, Li C., Duric Neb Breast Ultrasound Tomography with Total-Variation Regularization2009 SPIE Medical Imaging, Orlando Fl, February 7-12 2009

Huang L, Rutledge J, Denli H, Zhou R, Time-Lapse VSP Surveys for Monitoring CO2 Migration at the Aneth Oil Field in Utah, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7, 2009, LA-UR-09-00408

Huang L, Rutledge J, Wang Yi, Denli H, et al., VSP Monitoring of CO2 Injection at the SACROC Oil Field in Texas, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05748

Huang L, Rutledge James, Denli H, Zhou R., Time-Lapse VSP Surveys For Monitoring Co2 Migration At The Aneth Oil Field In Utah8th Annual Conf On Carbon Capture And Sequestration, Pittsburgh Pa, May 4-7 2009

Huang L, Rutledge James, Wang Yi, Denli H, et al., VSP Monitoring Of Co2 Injection At The SACROC Oil Field In Texas2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009

Huang L, Rutledge James, Zhou R.,, Denli H, Peron J., Zhao Michelle, Cheng Arthur Time-Lapse VSP Surveys For Monitoring Co2 Migration At The Aneth Oil Field In Utah8th Annual Conf On Carbon Capture And Sequestration, Pittsburgh Pa, May 4-7 2009
Huang L, Simonetti F, Detecting breast microcalcifications using super-resolution ultrasound imaging: A numerical phantom study, SPIE Medical Imaging, San Diego CA, February 13-18, 2010, LA-UR-09-04695
Huang L, Simonetti F, Huthwaite P, The Different Structural Scales of the Breast and their Impact on Time-of-Flight and Diffraction Tomography, SPIE Medical Imaging, San Diego CA, February 13-18, 2010, LA-UR-09-04694
Huang L, Simonetti Francesco A Novel Synthetic Aperture Technique for Breast Tomography with Toroidal Arrays2009 SPIE Medical Imaging, Orlando Fl, February 7-12 2009
Huang L, Simonetti Francesco A Novel Synthetic Aperture Technique for Breast Tomography with Toroidal Arrays2009 SPIE Medical Imaging, Orlando Fl, February 7-12 2009
Huang L, Wang Yi, Zhang Z, Rutledge J, Time-Lapse Offset and Walkaway VSP Monitoring of CO2 Injection at SACROC, 9th Annual conf on Carbon Capture and Sequestration, Pittsburgh PA, May 10, 2010, LA-UR-10-01128
Huang L, Waveform Tomography of Time-Lapse Seismic Data for Monitoring CO2 Injection, 9th Annual conf on Carbon Capture and Sequestration, Pittsburgh PA, May 10, 2010, LA-UR-10-01132
Huang L, Zhou R., Rutledge James, Denli H Double-Difference Tomography of Microseismic Data for Monitoring Carbon Sequestratio2009 SEG Annual Meeting, Houston TX, October 25-30 2009
Johnson P. A., Perturbation by Acoustic Waves during Stick-Slip Behavior in Sheared Granular Media with Implications to Earthquake Processes International Congress on Ultrasonics, Santiago Chile, January 11 2009
Johnson PA, Anderson BE, Griffa M, Huang L, Larmat C, et al., Time reversal analysis of acoustic signatures: sensor and imaging development, CLES capability review: sensors remote sensing and sensor systems, Los Alamos NM, May 20, 2008, LA-UR-08-03253
Johnson PA, Perturbation by acoustic waves during stick-slip behavior in sheared granular media with implications to earthquake processes, International Congress on Ultrasonics, Santiago Chile, January 11, 2009, LA-UR-08-05813
Johnson Paul, LeBas Pierre-Yves et al., Effects Of Acoustic Waves On Stick—Slip Behavior In Sheared Granular Media Intnl School On Complexity 11th Course Grains Friction And Faults, Erice Sicily, July 20 2009
Kang Q, Lichtner PC, Mukherjee PP, A multiscale continuum formulation for reactive transport in hierarchical porous media, Computational methods in water resources XVII, San Francisco CA, July 6, 2008, LA-UR-08-00561
Kang Q, Wang M Pore Scale Modeling Of Electrosmosis Of Dilute Electrolyte Solution In Porous Media 2009 AGU Fall Meeting, San Francisco CA, December 14-18 2009
Kang Q, Wang M, Lichtner PC, Pore-scale studies of multiphase flow and reaction involving CO2 sequestration in geologic formations, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2008, LA-UR-08-06260
Kanjorski N, Keating E, Fessenden J, Pawar R, The impact of CO2 on shallow groundwater chemistry in Chimayo New Mexico, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-19, 2008, LA-UR-08-05785

Keating E, Doherty J, Vrugt JA, Wolfsberg A, The applicability of calibration-constrained predicitive uncertainty analysis techniques to strongly non-linear models with high parameter dimensionality, Computational methods in water resources XVII, San Francisco CA, July 6, 2008, LA-UR-08-00560
Keating Elizabeth, Kang Q., Dash Z., Kwicklis Edward Particle Tracking-Based Strategies For Simulating Transport In A Transient Groundwater Flow Field At Yucca Flat Nevada Test Site USA, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Keating GN, Pasqualini D, Middleton R, Pawar R, Stauffer P, How storage uncertainty will drive CCS infrastructure, 10th Intl Conf on Greenhouse Gas Control Technologies, Amsterdam Netherlands, September 19, 2010, LA-UR-09-08222
Keating Gordon N, Pasqualini Donatella Integrated System Dynamics Model to Assess Options for Emissions Reductions Related To Energy-Water Sustainability in Sonoma County 2nd Forum on Energy & Water Sustainability, Santa Barbara CA, April 10 2009
Keating Gordon N, Pasqualini Donatella, Geernaert Gary Web Technologies and System Dynamics for Community Sustainability Local and Regional Sustainability Workshop, Odense Denmark, March 16-17 2009
Keating Gordon N, Pasqualini Donatella, Geernaert Gerald L, Perry Frank VA Model For Partnerships Between National Laboratories And County Agencies For Climate Change Adaptation2009 Geological Society Of America Annual Meeting, Portland Or, October 18-21 2009
Keating Gordon N, Pasqualini Donatella, Geernaert Gerald L, Perry Frank VA Model For Partnerships Between National Laboratories And County Agencies For Climate Change Adaptation2009 Geological Society Of America Annual Meeting, Portland Or, October 18-21 2009
Keating Gordon, Pasqualini Donatella Integrated System Dynamics Model To Assess Options For Emissions Reductions Related To Energy-Water Sustainability In Sonoma County2nd Forum On Energy & Water Sustainability, Santa Barbara CA, April 10 2009
Keating Gordon, Pasqualini Donatella, Geernaert Gary, Barnett Larry Web Technologies And System Dynamics For Community Sustainability, Applied Solutions Workshop, Rohnert Park CA, February 2009
Kwicklis Edward M, Ruskauff Gregory Investigation Of The Effects Of Withdrawals For Water Supply On 3h Plume Migration In Central Frenchman Flat Nevada Test Site, UGTA Technical Exchange Meeting, Las Vegas NV, April 20 2009
Le Bas Pierre-Yves, Carey James W, Johnson Paul A Probing Rock For Chemical-Induced Mechanical-Change Due To Exposure To Super Critical C02 Applying Nonlinear Elastic Wave Spectroscopy (News)Intl Congress On Ultrasonics Universidad De Santiago De Chile January 11-17 2009
Le Bas Pierre-Yves, Carey James W, Johnson Paul A Probing Rock For Chemical-Induced Mechanical-Change Due To Exposure to Super Critical C02 Applying News, ICU, Santiago Chile, January 11th-18th 2009
Le Bas PY, Carey JW, Johnson PA, Probing rock for chemical-induced mechanical-change due to exposure to super critical C02 applying nonlinear elastic wave spectroscopy (NEWS), Intl Congress on Ultrasonics Universidad de Santiago de Chile January 11-17, 2009, LA-UR-08-06713
LeBas PY, Anderson B, Griffa M, Ulrich T, Johnson PA, On the use of time reversal in the detection of buried nonlinear features, 13th Int'l Conf on Nonlinear Elasticity in Material, Aix-En-Provence France, June 21, 2008, LA-UR-08-03051
Levitt D, Wilson C, Herr J, Wolfsberg A, Eddebbarh A, Simulating the Impacts of Energy Production Climate Variability and Climate Change on Water Resources in the Upper Colorado River Basin with the WARMF Model, Water/Energy Sustainability at the GWPC Annual Forum 2009, Salt Lake City UT, September 13, 2009, LA-UR-LA-UR-09-02402

Levitt Daniel G, Kwicklis Edward M, Sully Michael J, Witkowski Marc S Runoff And Infiltration Into Nuclear Subsidence Craters At Yucca Flat Nevada Test Site2009 Devil's Hole Workshop Furnace Creek Ranch Death Valley CA May 6-8 2009
Levitt Daniel, Eddebbarh Al, Wilson Cathy, Wolfsberg Andrew, Herr Joel Assessing Surface Water Resource Availability For Oil Shale Development Using The WARMF Model29th Oil Shale Symposium, Golden Co, October 19-23 2009
Levitt Daniel, Wilson Cathy, Herr Joel, Wolfsberg Andrew, Eddebbarh A., Simulating The Impacts Of Energy Production Climate Variability And Climate Change On Water Resources In The Upper Colorado River Basin With The WARMF Model, Water/Energy Sustainability At The GWPC Annual Forum 2009, Salt Lake City UT, September 13 2009
Lichtner P. C., PFLOTRAN: Application to Uranium Migration at the Hanford 300 Area ERSP PI Meeting, Lansdowne VA, April 23 2009
Lichtner P. C., PFLOTRAN: Next-Generation Model for Simulating Reactive Flow and Transport At The Petascale ERSP Pi Meeting, Lansdowne VA, April 23 2009
Lichtner PC, Hammond G, High resolution simulations of the Hanford 300 area, ERSP 3rd annual PI meeting, Lansdowne VA, April 7, 2008, LA-UR-08-01317
Lichtner PC, Kang Q, Upscaling pore-scale lattice-Boltzmann modeling of multicomponent reactive transport to the continuum scale, ERSP 3rd annual PI meeting, Lansdowne VA, April 7, 2008, LA-UR-08-01318
Lichtner PC, Kang Q, Wang M, Upscaling multi-physico chemical processes in porous media from pore to continuum scales, DOE/ERSP PI Meeting, Lansdowne VA, April 20-24, 2009, LA-UR-09-01623
Lichtner PC, Next-generation petascale reactive flow and transport code Pflotran with application to the Hanford 300 area, DOE/ERSP PI Meeting, Lansdowne VA, April 20-24, 2009, LA-UR-09-01622
Lichtner Peter C Next-Generation Petascale Reactive Flow And Transport Code PFLOTRAN With Application To The Hanford 300 Area DOE/ERSP PI Meeting, Lansdowne VA, April 20-24 2009
Lichtner Peter C, Hammond Glenn E Massively Parallel Simulation Of Uranium Migration At The Hanford 300 Area American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Lichtner Peter C, Kang Q., Wang Moran Upscaling Multi-Physico Chemical Processes In Porous Media From Pore To Continuum Scales DOE/ERSP PI Meeting, Lansdowne VA, April 20-24 2009
Linhoff Benjamin, Longmire Patrick, Rearick Michael, Mcquillan Dennis, Gallegos Robert, King Amanda, Torres Karen Uranium In Santa Fe County Groundwater, New Mexico Symposium On Water Resources, Socorro NM, August 11 2009
Longmire Patrick, Heikoop Jeffrey M, Ding Mei, Rearick Michael S, Katzmann Danny Geochemical Processes Controlling Chromium Fixation Within The Sandia Canyon Wetland Los Alamos New Mexico American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Lucero C, Maceira MS, Rowe CK, Steck LL, Borchers B, Computational Improvements in the Three-Dimensional Shear-Wave Model Derived From the Joint Inversion of Multiple Geophysical O, 2007 American Geophysical Union Fall Meeting, San Francisco CA, December 2007, LA-UR-07-6183
Maceira M, Rowe CA, Steck LK, Simultaneous joint inversion of multiple geophysical data sets and 3D tomography, Seismological Society of America Annual Meeting 2009, Monterey CA, April 8, 2009, LA-UR-09-02732
Maceira M, Rowe CA, Steck LK., Simultaneous Joint Inversion Of Multiple Geophysical Data Sets And 3d Tomography Seismological Society Of America Annual Meeting 2009, Monterey CA, April 8 2009

Manga Michael, Rowland Joel C Response Of Alum Rock Springs To The October 30 2007 Alum Rock Earthquake And Implications For The Origin Of Increased Discharge After Earthquakes216th European Geophysical Union Meeting, Vienna Austria, April 2009
Middleton Richard S, Bieleiki Jeffrey M, Kuby Michael Optimal Spatial Deployment Of Carbon Capture And Storage Infrastructure Given A Price On Carbon Dioxide2009 Geological Society Of America Annual Meeting, Portland Or, October 18-21 2009
Miller Terry A, Vesselinov V. V., Integrated Approach for 3d Geology Rendering Numerical Meshing and Modeling for Flow and Transport Studies Pajarito Plateau New Mexico Espanola Basin Advisory Group Meeting, Santa Fe NM, March 3 2009
Modrak, Ryan T, Maceira Monica, Van Wijk J., Pasyanos M., Joint Inversion Of Surface Wave And Gravity Observations: Application To East Africa American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Mukherjee P. P Capillarity Wettability And Interfacial Dynamics In Polymer Electrolyte Fuel Cells, ICNMM 2009, Pohang South Korea, June 22-24 2009 Keynote Paper
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 & Exposition, Lake Buena Vista Fl, November 13-19 2009
Mukherjee P. P, Schulz v. ker P, Kang Q., Becker Jurgen, Wiegmann Andreas Two-Phase Behavior And Compression Effect In A PEFC Gas Diffusion Medium216th European Geophysical Union Meeting, Vienna Austria, April 2009
Mukherjee P. P, Wang Chao-Yang, Schultz v. ker P, Kang Q. Two-Phase Behavior And Compression Effect In The PEFC Gas Diffusion Medium216th Electrochemical Society Meeting, Vienna Austria, October 4-9 2009
Mukherjee P. P., Capillarity Wettability and Interfacial Dynamics in Polymer Electrolyte Fuel Cells International Conference on Nanochannels Microchannels and Minichannels, Pohang South Korea, June 22 2009
Mukherjee P. P., Kang Q., Mukundan R., Borup R. L., Numerical Modeling Of Two-Phase Behavior In The PEFC Gas Diffusion Layer2009 Fuel Cell Seminar & Exposition, Palm Springs CA, November 16-19 2009
Mukherjee PP, Kang Q, Lichtner PC, Pore-Scale Modeling of Transport in Charged Porous Media, Computational methods in water resources XVII, San Francisco CA, July 6, 2008, LA-UR-08-00562
Newell Dennisco2-Rich Mineral Springs - Natural Analogs for a Leaking Carbon Sequestration Scenario Geological Society of America Annual Meeting, Portland OR, October 18-21 2009
Pasqualini Donatella, Bassie Andrea M, Wolfsberg Andrew V Carbon and Water Resources (UES Impacts and Management Assessment for Oil Shale Development Int'l Oil Shale Symposium, Tallinn Estonia, June 7 2009
Pasqualini Donatella, Keating Gordon N Resilient Climate-Energy Systems IGPP External Review, Los Alamos National Laboratory, June 3 2009
Pasqualini Donatella, Patelli Paolo Clear Model For Energy And Climate Impacts2009 Geological Society Of America Annual Meeting, Portland Or, October 18-21 2009

Perkins George B, Larson T. E, Longmire Patrick, Heikoop Jeffrey M Differentiation Among Multiple Sources Of Anthropogenic Nitrate In A Complex Groundwater System Using Dual Isotope Systematics: A Case Study From Mortandad Canyon New Mexico American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Perry Frank V The Role Of Earth Scientists And The Public In Complex Climate And Energy (ues2009 Geological Society Of America Annual Meeting, Portland Or, October 18-21 2009
Phillips W S, Mayeda K M, Malagnini L, Rowe C A Developments In Regional Phase Amplitude Tomography2009 Seismological Society Of America Annual Meeting Monterey CA, April 8-10 2009
Phillips W S, Stead R J Source Spectral Parameters Of Aftershocks Of The Great 2008 Wenchuan Earthquake2009 Seismological Society Of America Annual Meeting Monterey CA, April 8-10 2009
Phillips W Scott, Stead Richard J Source Spectral Parameters Of Aftershocks Of The Great 2008 Wenchuan Earthquake Seismological Society Of America Annual Meeting 2009, Monterey CA, April 8 2009
Rahn Thom, Lee Hanna, Throop Heather Abiotic Litter Decomposition In Dryland Ecosystems American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Randall George E, Hartse Hans E Identification Of Deep Earthquakes (A Proposal To Nnsa/Na22) NNSA Proposal LA-UR-09-01989
Rehfeldt Kenneth R Geothermal Research At Los Alamos National Laboratory: Past Present And Future Advanced Energy 2009, Hauppauge NY, November 18-19 2009
Reimus P, Schafer T, Hauser W, Walther C, Geckeis H, et al., The CFM (Colloid Formation and Migration) Project at the Grimsel Test Site (GTS Switzerland): Model interpretations of first field experiments, Migration '09, Kennewick WA, September 20-25, 2009, LA-UR-09-01912
Reimus P, Schafer T, Hauser W, Walther C, Geckeis H, et al., The CFM (Colloid Formation And Migration) Project At The Grimsel Test Site (GTS Switzerland): Model Interpretations Of First Field Experiments Migration '09, Kennewick WA, September 20-25 2009
Reimus P, Schafer T, Hauser W, Walther C, Geckels H, Degueldre C, Trick T The CFM (Colloid Formation And Migration) Project At The Grimsel Test Site (GTS Switzerland): Model Interpretations Of First Field Experiments Migration 09, 12th Intl Conf On The Chemistry And Migration Behaviour Of Actinides And Fission Products In The Geosphere, Kennewick WA, September 20-25 2009
Roberts Peter M, Abdel-Fattah Amr I Investigation Of Nonlinear Stress/Strain Mechanisms For Mobilizing Colloids In Porous Media Doe Office Of Science LA-UR-09-01000
Roberts PM, Abdel-Fattah AI, Acoustic effects on colloid interactions and porous fluid transport, Immigration Exhibit, LA-UR-09-07805
Roberts PM, Abdel-Fattah AI, Elastic wave effects on colloid interactions and their influence on porous fluid transport, Immigration Exhibit, LA-UR-09-07804
Rowe CA, Bilek SL, Ruhl CJ, Aster RC, Stankova-Pursley J, Johnson J Characterization Of The August 2009 New Mexico Earthquake Swarm In The Central Rio Grande Rift 2009 AGU Fall Meeting, San Francisco CA, December 14-18 2009
Rowe CA, Dionicio V, Maceira M, Zhang H, Londono H Simultaneous Joint Inversion Of Seismic Body Wave Travel Times And Satellite Gravity Data For Three-Dimensional Tomographic Imaging Of Western Colombia 2009 AGU Fall Meeting, San Francisco CA, December 14-18 2009
Rowe CA, Dionicio V, Maceira M, Zhang H, Londono H, Simultaneous joint inversion of seismic body wave travel times and satellite gravity data for three-dimensional tomographic imaging of western Colombia, 2009 AGU Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05928

Rowe CA, Maceira M, Steck LK, Allen RC, Obrebski M Validation Of 3d Ray-Theoretical And Finite-Frequency Tomographic Images Of The Western US Lithosphere: Comparison Of Synthetic Seismograms Generated Via The Spectral Element Method 2009 AGU Fall Meeting, San Francisco CA, December 14-18 2009
Rowe CA, Maceira M, Steck LK, Allen RC, Obrebski M, Validation of 3D ray-theoretical and finite-frequency tomographic images of the western US lithosphere: comparison of synthetic seismograms generated via the spectral element method, 2009 AGU Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05557
Rowland JC, Wilson CJ, Brumby S, Pope P, River mobility in a permafrost dominated floodplain, European geosciences union general assembly 2008, Vienna Austria, April 13, 2008, LA-UR-09-00171
Rowland JC, Wilson CJ, Brumby SP, Pope PA, Arctic River Mobility: A baseline assessment, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05573
Rowland Joel C, Wilson Cathy J, Brumby Steven P, Pope Paul A Arctic River Mobility: A Baseline Assessment2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Rowland Joel C, Wilson Cathy J, Brumby Steven P, Pope Paul A Arctic River Mobility: A Baseline Assessment American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Rowland Joel C, Wilson Cathy J, Brumby Steven, Pope Paul River Mobility In A Permafrost Dominated Floodplain 216th European Geophysical Union Meeting, Vienna Austria, April 2009
Satriano Claudio, Rowe Charlotte Automatic Correlation-Based Picking For Iterative Refining Of Tomographic Images Seismological Society Of America Annual Meeting 2009, Monterey CA, April 8 2009
Schultz-Fellenz Emily 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 PH, Kwicklis EM, Sully MJ, Modeling evaporation from a non-vegetated lysimeter experiment, Computational methods in water resources XVII, San Francisco CA, July 6, 2008, LA-UR-08-00481
Stauffer PH, Pawar R J, Lettelier BC, Viswanathan HS, Sanzo DL, Keating GN, CO2-PENS: development of a spatially coherent system-level tool for performance assessment of geologic carbon dioxide sequestration, Hedberg Conference of the American Association of Petroleum Geologists, Vancouver Canada, August 16, 2009, LA-UR-09-02596
Stauffer Philip H Numerical Analysis Of The MDA-G Soil-Vapor Extraction Test Material Disposal Area G Technical Area 54 LA-UR-LA-UR-09-00995
Stauffer Philip H, Pawar Rajesh J, Lettelier Bruce C, Viswanathan Hari S, Sanzo Dean L, Keating Gordon NCo2-Pens: Development Of A Spatially Coherent System-Level Tool For Performance Assessment Of Geologic Carbon Dioxide Sequestration Hedberg Conference Of The American Association Of Petroleum Geologists, Vancouver Canada, August 16 2009
Steck Lee, Begnaud Michael, Romero-Yeske Marian, Mackey Kevin, Fujita Kazuya, Stead Richard, Seismic Event Relocation In Northeastern Russia American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Steck Lee, Phillips W Scott, Begnaud Michael, Stead Richard Tomography Of Pg And Sg Across The Western United States Using US Array Data, American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Teixidor G. T, Mukherjee P. P, Park B. Y, Madou M. J., Theoretical Evaluation Of Fractal-Like Electrode Characteristics For Lithium-Ion Batteries, 215th ECS Meeting, San Francisco CA, May 24-29 2009

Ulrich T J, Van Den Abeele K, LeBas P.-Y., Anderson B. E., Griffa M., Guyer R. A., Three Component Time Reversal Imaging Using Nonlinear Elasticity, ICU Santiago Chile, January 11th-18th 2009
Ulrich TJ, TenCate JA, Sutin Alexander M, Wide band Time Reversal Acoustic nonlinear diagnostics, 18th Intl Symposium on Nonlinear Acoustics (ISNA), Stockholm Sweden, July 7, 2008, LA-UR-08-01290
Vaniman D. T., Bassanite On Mars40th Lunar And Planetary Science Conference, Houston TX, March 23-27 2009
Vaniman D., Chipera S., Brown-Holland K., Bish D., The Todilto Formation As An Analog Of Short-Lived Martian Flood Evaporites, LA-UR-09-08141
Vesselinov V, Characterization of medium heterogeneity using pneumatic and tracer testing, International Groundwater Symposium, Istanbul Turkey, June 18, 2008, LA-UR-08-00656
Vesselinov V. V., Mishra Phoolendra Kumar, Neuman Shlomo P Analytical Solution For Flow To A Partially Penetrating Well With Storage In A Confined Aquifer 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18 2009
Vesselinov VV Harp D Birdsell KH, Tomographic inverse estimation of aquifer properties based on pressure variations caused by transient water-supply pumping, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-19, 2008, LA-UR-08-06233
Vesselinov VV, Birdsell K, Broxton D, Characterization of conceptual model uncertainties and estimation of their impact on contaminant transport predictions, 2008 Ground Water Summit, Memphis TN, March 30, 2008, LA-UR-07-7466
Vesselinov VV, Harp D, Analysis of temporal high-frequency pressure and water-supply pumping data to identify aquifer properties, Computational methods in water resources XVII, San Francisco CA, July 6, 2008, LA-UR-08-00655
Vesselinov VV, Harp DR, Decision support based on uncertainty quantification of model predictions of contaminant transport, 2010 CMWR Meeting, Barcelona Spain, June 21, 2010, LA-UR-09-06553
Vesselinove VV, Mishra PK, Neuman SP, Analytical Solution for Flow to a Partially Penetrating Well with Storage in a Confined Aquifer, 2009 American Geophysical Union Fall Meeting, San Francisco CA, December 14-18, 2009, LA-UR-09-05668
Viswanathan HS, Abdel-Fattah AI, 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, Mukherjee PP, Lichtner PC, Kang Q, Modeling of transport in charged porous media - a pore-scale perspective, 54th annual meeting Center for environmental kinetics analysis, University Park PA, October 22, 2008, LA-UR-08-06250
Wang M., Kang Q., Interfacial Electrokinetic And Reactive Transport Phenomena In Micro And Nanopores Of Permeable Media Journal Article LA-UR-09-07605
Wang Moran, Kang Q. Electrokinetic Transport In Realistic Nanochannels 62nd APS Division Of Fluid Dynamics, Minneapolis MN, November 22-24 2009
Wang Moran, Kang Q. Ion Transport In Nanofluidic Channels2009 ASME 2nd Micro/Nanoscale Heat & Mass Transfer Conf, Shanghai China, December 20 2009
Wang Moran, Kang Q., Viswanathan H., Numerical Modeling Of Electrokinetic Transport And Mixing Enhancement In Heterogeneously Charged Microchannels, 2009 ASME 2nd Micro/Nanoscale Heat & Mass Transfer Conf, Shanghai China, December 20 2009

Wang Y, Huang L, Reverse-time migration of time-lapse walkaway VSP data for monitoring CO2 injection, LA-UR-10-00915
Ward L, Phillips W Scott Broad Area Yield Estimation Using Regional Phase Data NNSA Proposal LA-UR-09-01839
Wohletz K, Ogden D, 3D Numerical Simulations of Coupled Solid and Fluid Mechanics in Volcanic Conduit Erosion and Crater Formation, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-19, 2008, LA-UR-08-06056
Wohletz Kenneth H Constraining The Evolution Of volcanic Hydrothermal Systems By 3d Field-Based Thermal Models 34th Stanford Geothermal Workshop, Stanford CA, Feb 19-21 2009
Wohletz Kenneth H., Energetics Excavation And Geothermal Significance Of Marr Craters 3rd Intl Maar Conf, Malargue Mendoza Argentina, April 14-17 2009
Wohletz KH, Constraining the evolution of volcanic hydrothermal systems by 3D field-based thermal models, 34th Stanford Geothermal Workshop, Stanford CA, Feb 19-21, 2009, LA-UR-08-07469
Wohletz KH, Energetics excavation and geothermal significance of Marr craters, 3rd Intl Maar conf, Malargue Mendoza Argentina, April 14-17, 2009, LA-UR-08-07543
Xu H, Zhao Y, Zhang J, Hickmott D. D., Vogel S C, Daemen L. L., Harti M A High-P/T Neutron Diffraction Study Of Hydrous Minerals2009 American Geophysical Union Joint Assembly, Toronto Canada, May 24-27 2009
Xu H., Zhao Y, Zhang J, Hickmott D. D., Vogel S C, Daemen L. L., Hartl M A High P/T Neutron Diffraction Study Of Hydrous Minerals2009 American Geophysical Union Joint Assembly, Toronto Canada, May 24-27 2009
Yang X., Phillips W Scott, Randall George E, Hartse Hans E, Stead Richard J Developing Frequency Dependent 2d Attenuation Models For Asia2009 Seismological Society Of America Annual Meeting Monterey CA, April 8-10 2009
Zhang Z, Huang L, Rutledge J, Denli H, 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, LA-UR-09-08150
Zhang Z, Huang L, Wave-Equation Migration of Time-Lapse VSP Data for Monitoring CO2 Injection at Aneth Utah, 9th Annual conf on Carbon Capture and Sequestration, Pittsburgh PA, May 10, 2010, LA-UR-10-01120
Zhang Z., Huang L, Rutledge James, Denli H 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, Huang L, Daley T, Majer E, Denli H, Rutledge J, Monitoring of Geological Carbon Sequestration Using the Coda-Wave Interferometry Method and Time-Lapse VSP Data, 70th EAGE Conf & Exhibition incorporating SPE EUROPEC 2008, Rome Italy, June 9, 2008, LA-UR-08-00438
Zhou R, Huang L, Denli H, Rutledge J, Double-difference tomography using microearthquake data for monitoring CO2 injection at Aneth UT, 8th Annual Conf on Carbon Capture and Sequestration, Pittsburgh PA, May 4-7, 2009, LA-UR-09-00353
Zhou R, Huang L, Rutledge J, Cheng A, Zhao M, Peron J, Monitoring Temporal Changes of Seismic Velocity due to CO2 Injection Using Time-Lapse VSP Data and Coda-Wave Interferometry, 2008 American Geophysical Union Fall Meeting, San Francisco CA, December 14-19, 2008, LA-UR-08-05793

Zhou R, Huang L, Rutledge J, Daley T, Majer EL, Using the coda-wave interferometry method and time-lapse VSP data to estimate velocity changes from geological carbon sequestration in a brine aquifer, Society of Exploration Geophysicists (SEG) Annual Meeting, Las Vegas NV, November 9, 2008, LA-UR-08-02451
Zhou R, Huang L, Rutledge J, Daley T, Using the coda-wave interferometry method and time-lapse VSP data to estimate velocity changes from geological carbon sequestration in a brine aquifer, SEG Annual Meeting, Las Vegas NV, November 9, 2008, LA-UR-08-07439
Zhou R.,, Huang L, Denli H, Rutledge James Double-Difference Tomography Using Microearthquake Data For Monitoring Co2 Injection At Aneth UT 8th Annual Conf On Carbon Capture And Sequestration, Pittsburgh Pa, May 4-7 2009
Zhou R.,, Huang L, Denli H, Rutledge James Double-Difference Tomography Using Microearthquake Data For Monitoring Co2 Injection At Aneth UT 8th Annual Conf On Carbon Capture And Sequestration, Pittsburgh Pa, May 4-7 2009
Zhou R.,, Huang L, James Rutledge James, Denli H, Zhang H., Double-Difference Tomography Of Microseismic Data For Monitoring Carbon Sequestration Society Of Exploration Geophysicists Annual Meeting, Houston TX, October 25-30 2009
Zhou R.,, Huang L, Rutledge James, Denli H, Zhang H., Double-Difference Tomography Using Microearthquake Data For Monitoring Co2 Injection At Aneth UT 8th Annual Conf On Carbon Capture And Sequestration, Pittsburgh Pa, May 4-7 2009
Ziock Hans J, Colgate Sterling A Is Information Possible Without Life? Decade Of The Mind Iv, Santa Ana Pueblo NM, January 14-15 2009
Zou R., Larson T. E, Hickmott Donald D, Zhao Y. Hydrogen Storage On Nanoporous Metal-Organic Framework Materials LANL-NEDO/AIST Workshop On Hydrogen Storage, Boston Ma, December 4 2009
Zyvoloski G, Pawar R, Predicting the performance of geothermal reservoirs: some useful numerical techniques, Computational methods in water resources XVII, San Francisco CA, July 6, 2008, LA-UR-08-00619
Zyvoloski G., Calibrating Coupled Heat-Mass-Stress Simulations Constrained With Seismic Data Energy Wind And Water Workshop, Auckland University, February 9-12 2009
Zyvoloski GA, Stress-Dependent Fracture-Aperture Relationships For Geothermal Energy Applications 2009 AGU 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 - 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.
DREAM - Real-Time DREAM (Dynamic Radiation Environment Assimilation Model) installed at the AFRL Space Weather Forecast Lab in Albuquerque, Novemeber 2009.
Garimella, R.V., *MSTK: A Flexible Infrastructure Library For Developing Mesh Based Applications*, in Proc. 12th Int. Meshing Roundtable, Williamsburg, VA, 2004. http://Math.Lanl.Gov/~Rao/Meshing-Projects/MSTK
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
Hagberg, A.A., D.A. Schult, and P.J. Swart, *Exploring Network Structure, Dynamics, And Function Using Networkx*,in Proc. 7th Python in Science Conference (Scipy2008), Pages 11–15, Pasadena, CA, August 2008. http://networkx.lanl.gov
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. Particpated 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 Phyics 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., 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., 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
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
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
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
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
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
Jordanova, V.K., Geophysical Research Letters
Jordanova, V.K., Journal of Geophysical Research
Kiedrowski, B., Nuclear Science and Engineering
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
Lowrie, R.B., International Journal for Numerical Methods in Fluids
Lowrie, R.B., Journal of Computational Physics
Lowrie, R.B., Monthly Weather Review
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
Parsons, D., Nuclear Science and Engineering
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
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
Tonks, D., Journal of Applied Physics
Tonks, D., Physical Review Letters
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
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

Johnson, P. A., Applied Physics Letters, Referee
Johnson, P. A., Science, Referee
Johnson, P. A., Physical Review Letters, Referee
Johnson, P. A., Journal of Geophysical Research, Referee
Johnson, P. A., Geophysical Research Letters, Referee
Johnson, P. A., Journal of the Acoustical Society of America, Referee
Johnson, P. A., Physical Review E, Referee
Johnson, P. A., Physical Review B, Referee
Johnson, P. A., Chu, S., Atmospheric Chemistry and Physics, referee
Coblentz, D., Earth and Planetary Sciences, referee
Coblentz, D., Tectonics, referee
Coblentz, D., National Science Foundation, referee.
Coblentz, D., Tectonophysics, referee
Fryer, C., Astrophysical Journal, referee
Hartse, H., Bulletin of Seismological Society of America, Referee.
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
Keating, G., Bulletin of Volcanology, Referee
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
Louis, W. C., Physical Review Letters referee
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
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
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
Porch, W., Journal of Atmospheric Chemistry and Physics, Referee
Porch, W., Journal of Optics Letters, Referee
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
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
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., 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
Wang, M., Communications in Computational Physics, Referee

Classified Reports

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

2008 NECDC Conference Proceedings: 3 LA-CPs submitted
JOWOG 42, 6/8-13, 2009, AWE United Kingdon: 11 LA-CPs submitted
2009 NEDPC 10/26-30, 2009, LLNL: 17 LA-CPs submitted
08-0009, 1/1/08, SRD, An Unclassified Title (U)
2/26/2009 Presentation to Secretary of Energy, Washington, DC: 2 classified videos prepared
Weapon Science Capability Review, LANL 3/25/09: 1 LA-CP submitted
Boost Fest April 7-10, 2009, Sandia National Laboratories, NM: 2 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)

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) 12/463,796
Patent application (2009) 12/463,796
Patent application (2009) 12/463,796
Patent application (2009) 12/463,802
Patent application (2009) 12/463,802
Patent application (2009) 12/463,802
Patent application (2009) 12/476,081
Patent application (2009) 61/170,070
Patent application (2009) 61/170,070
Patent application (2009) 61/170,070
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
Koby, Joseph R., Science & Energy Research Challenge (SERCh) Award, DOE - Dept. of Energy's Office of Science, Poster - Environmental Science (2nd Place), 11/08
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 A., 2007 Hydrology Prize, Dutch Hydrological Society (NHV), Best Publication (2004 - 2006) in the field of Hydrology, 11/07
Vrugt, Jasper A., S-1 Early Career Award,Soil Science Society of America (SSSA), Soil Physics, 01/07
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
Zyvoloski, George, Mid-Continent Regional Technology Transfer Award, Federal Laboratory Consortium, Finite Element Heat and Mass, 10/08