SAND 2014-XXXX

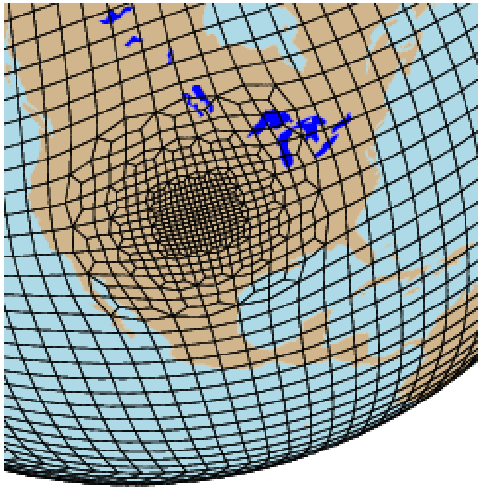
SAND2014-19946PE

HPC Mod/Sim at Sandia

Robert Hoekstra & Randy Summers

Computing Research Center

Sandia National Laboratories



Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Outline

- HPC at Sandia
- Extreme Computing
- Transformational Modeling & Simulation
- Application Highlights
- Collaboration

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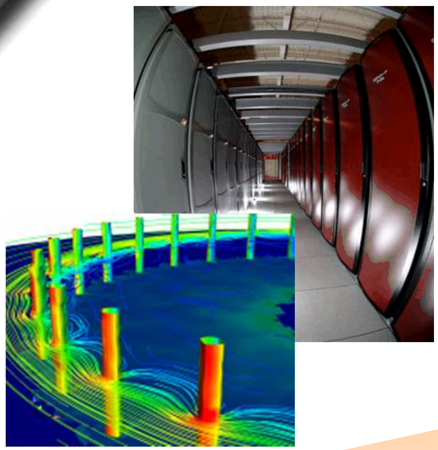
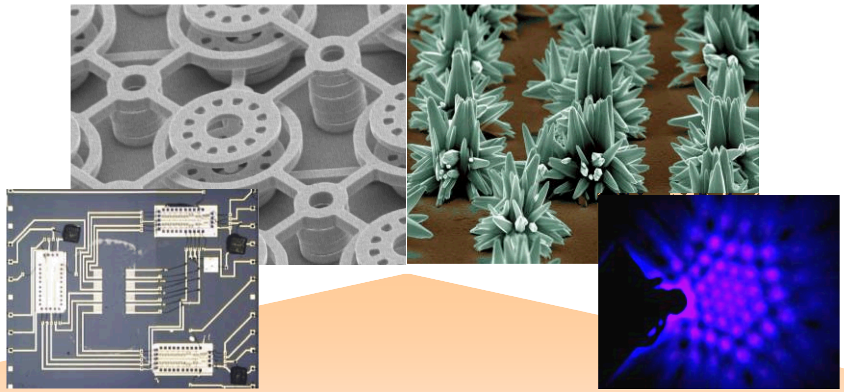
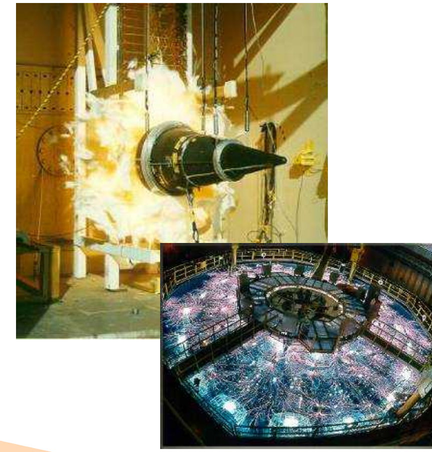
Research Disciplines Drive Capabilities





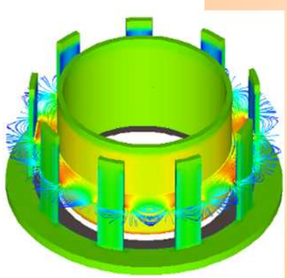


High Performance Computing

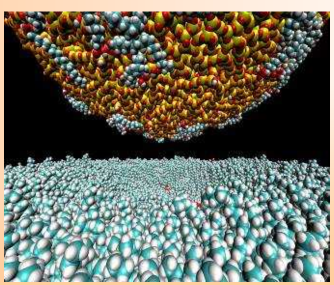
Nanotechnologies & Microsystems

Extreme Environments

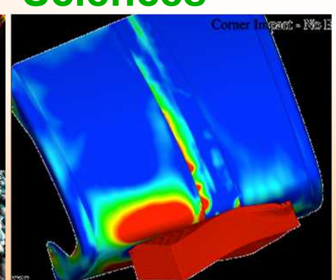
Computer Science



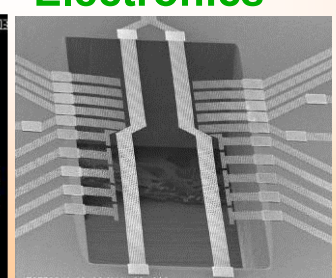
Materials



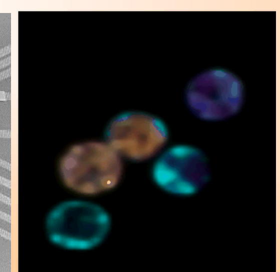
Engineering Sciences



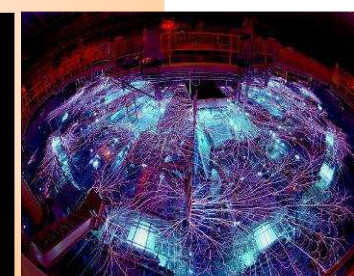
Micro Electronics



Bioscience



Pulsed Power



Research Disciplines

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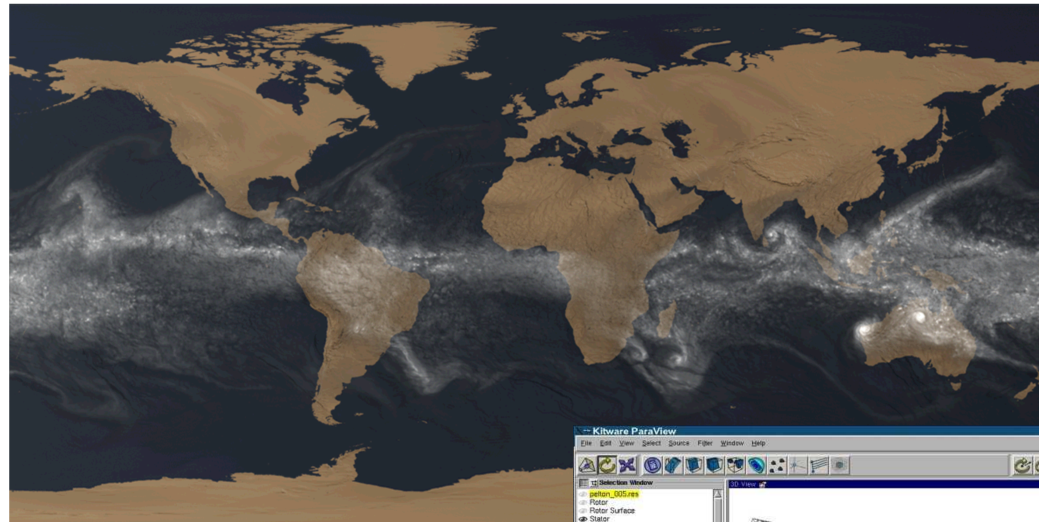
(Some of)

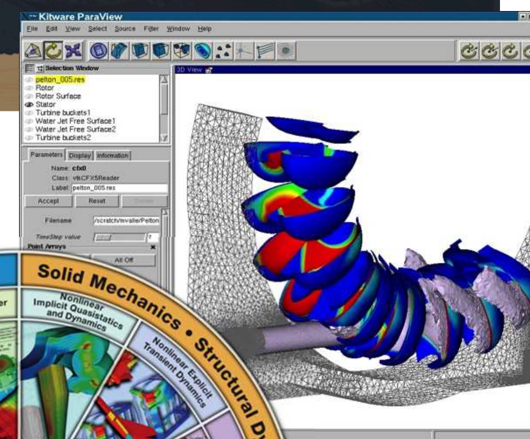
What do we do?

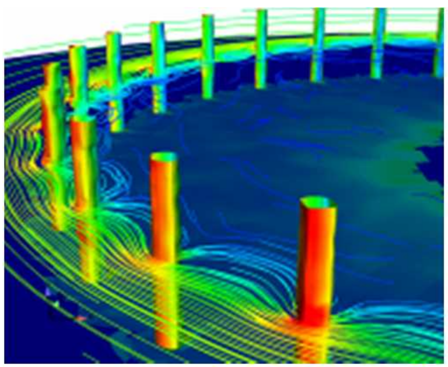
Trilinos

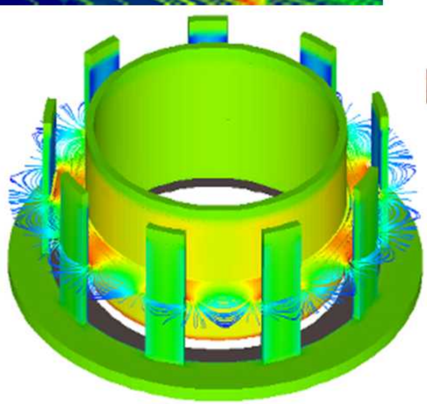
CUBIT

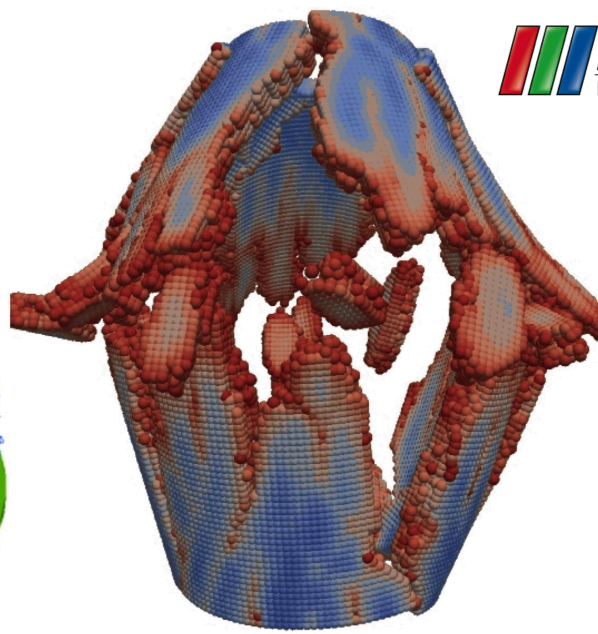
DAKOTA



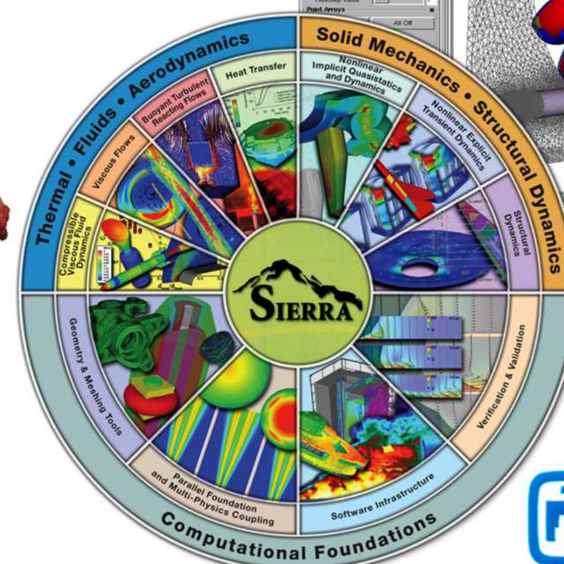








ParaView
Parallel Visualization Application



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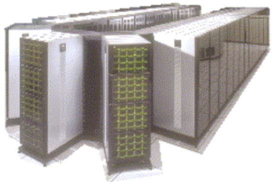
Track Record of HPC Accomplishments


CM-2


nCUBE-2


iPSC-860


Paragon


ASCI Red


Cplant


Red Storm

1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009

Gordon Bell Prize

R&D 100
Parallel Software

R&D 100
Signal Processing

Karp Challenge

Patent
Parallel Software

R&D 100
Meshing

Patent
Meshing

R&D 100
Dense Solvers

Gordon Bell Prize

SC96 Gold Medal
Networking

World Record
281 GFlops

World Record
143 GFlops

Patent
Paving

R&D 100
Storage

Gordon Bell Prize

World Record
Teraflops

Mannheim
SuParCup

Patent
Partitioning

R&D 100
Salvo

R&D 100
Aztec

Fernbach
Award

R&D 100
Xyce

R&D 100
Allocator

Patent
Data Mining

R&D 100
Catamount

R&D 100
Trillinos

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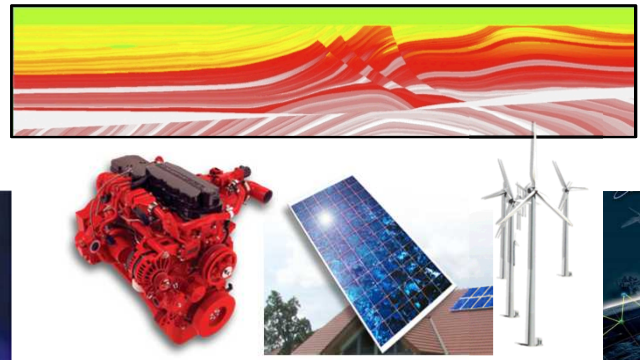
Sandia Strategies and HPC Research



Sandia Strategic Thrusts	Nuclear Security	Energy Security	Cyber Security
Computer Science Application Themes	Nuclear Weapons Engineering	Energy/Climate Security	Cyber Assurance
	Decision Support		
Computer Science Technology Themes	Predictive Simulation, Scalable Computing	Scalable Informatics	Cognitive Science
	Enabling Technologies		

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National code strategy: Sandia as the engineering simulation capability provider

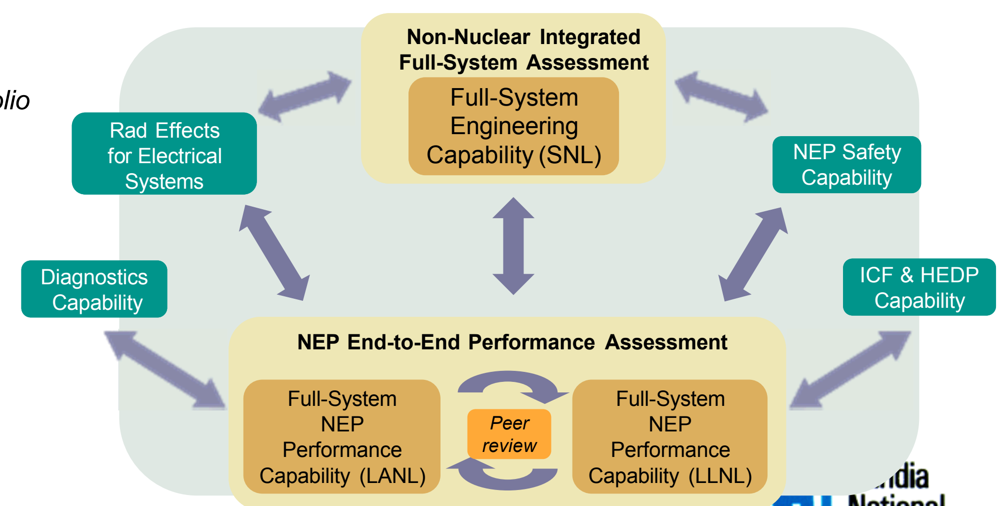
Focus Areas	Current State	Strategies	Future State
Integrated Simulation Capabilities (Application Codes)	• 14 modern + numerous legacy codes across 6 broad application areas • Core physics simulation competencies established	Establish the National Simulation Portfolio for Stockpile Certification	• 7 modern national capabilities • End legacy development • Core competencies sustained
Computational Science	• Tera scale computational science established (MPI programming model) • Basic capabilities for uncertainty quantification	Advance computational algorithms to enable predictive simulation and QMU	• Algorithms & programming models supporting predictive simulation at petaFLOP and exaFLOP scales • Advanced capabilities for uncertainty quantification and QMU studies
Scope of Applications	• ASC simulation capabilities focused on certification for tail numbers	Broaden the impact of ASC simulation capabilities in national security	• Capabilities for broader national security applications, including NNSA nuclear security and non-proliferation missions

Strategic Components

1. Establish the National Simulation Portfolio for Weapons Science and Engineering, and Stockpile Certification
   - *Define the core simulation capabilities needed*
   - *End development funding for legacy codes*
   - *Establish the capability to couple between codes of national portfolio*
2. Advance Computational Algorithms to Enable Predictive Simulation and QMU
   - *Advance scalability of computational algorithms*
   - *Collaborate on evolution of programming models*
   - *Deliver advanced capabilities for QMU and UQ*
3. Broaden the Impact of ASC Simulation Capabilities in National Security
   - *Develop a business "prospectus" for major capabilities*
   - *Develop and support interagency partnerships*
   - *Develop enhanced capabilities for expanded national security missions*

Objectives

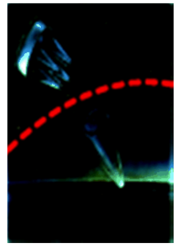
1. *Advance world-leading predictive science*, providing the capability to sustain stockpile stewardship without returning to underground nuclear testing as weapons age and we move further from the test base.
2. *Enable Quantification of Margins and Uncertainties (QMU)-based certification*, transforming the broader certification process to allow more effective and selective use of aboveground experiment, certification tests, flight tests, and other tests.
3. *Catalyze a responsive infrastructure* through pervasive simulation across all aspects of the stockpile lifecycle, such as design, certification, manufacturing, Significant Finding Investigation resolution, transportation, security, safe dismantlement, outputs and environments, etc.
4. *Enable a broadened national security mission*, in which simulation tools extend beyond stockpile stewardship and enable the next-generation mission of the Complex



The Nuclear Weapons Program is the principal driver for Sandia Computational Simulation

Delivery

Separation shock/ Aerodynamic Heating

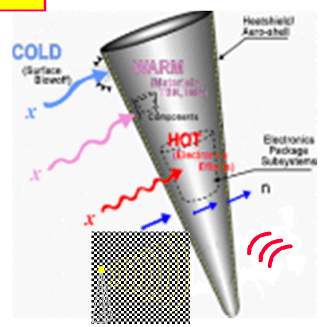


Staging shock

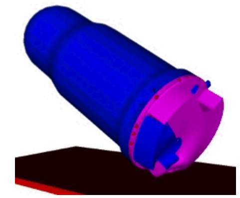
Random vibration

Survivability

Radiation Effects



Assured Safety and Security



Mechanical Insult **Thermal Insult**

Electromagnetic Insult

Security Components

Assured Performance & Manufacturing

Safe & Secure Transport

SNL Engineering Codes are positioned to support the engineering needs of the complex

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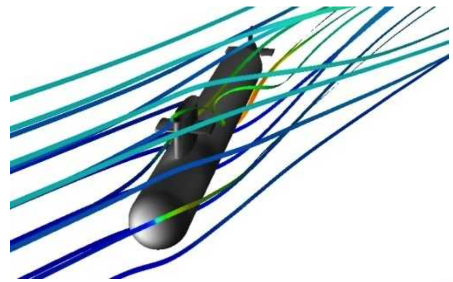
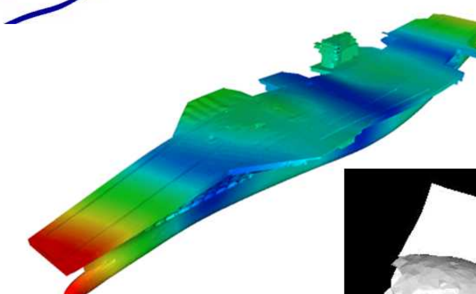
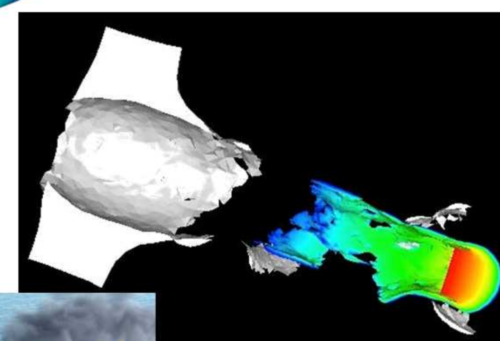
But Non-NW customers contribute significant resources

- Other Sandia mission areas and projects, for example
  - Energy
  - LNG
  - Satellite programs
- Industry
  - Goodyear,
  - Proctor & Gamble
- DoD
  - CREATE
  - ARDEC, TARDEC, Picatinny, ARL, etc.
- NASA (and JPL)

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SIERRA has a wide range of coupled mechanics simulation capabilities

- Thermal/fluids/aerodynamics
  - Compressible fluid mechanics with subsonic through hypersonic flows
  - Non-newtonian reacting flow with free surfaces, porous media, and complex material response
  - Low mach number turbulent reacting flow participating media radiation
  - Heat transfer with chemistry, phase change, and enclosure radiation
- Solid mechanics/structural dynamics
  - Nonlinear solid mechanics, quasistatics, implicit dynamics, failure and tearing
  - Nonlinear solid dynamics with explicit time integration, nodal-based tets, remeshing, particle methods, cohesive surface elements, contact, and material failure
  - Linear structural dynamics and modal analysis of complex structures

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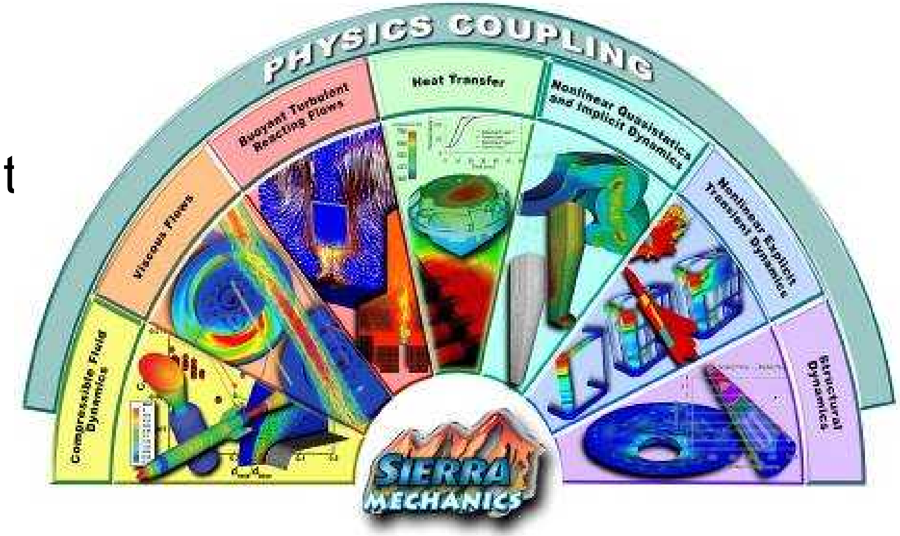
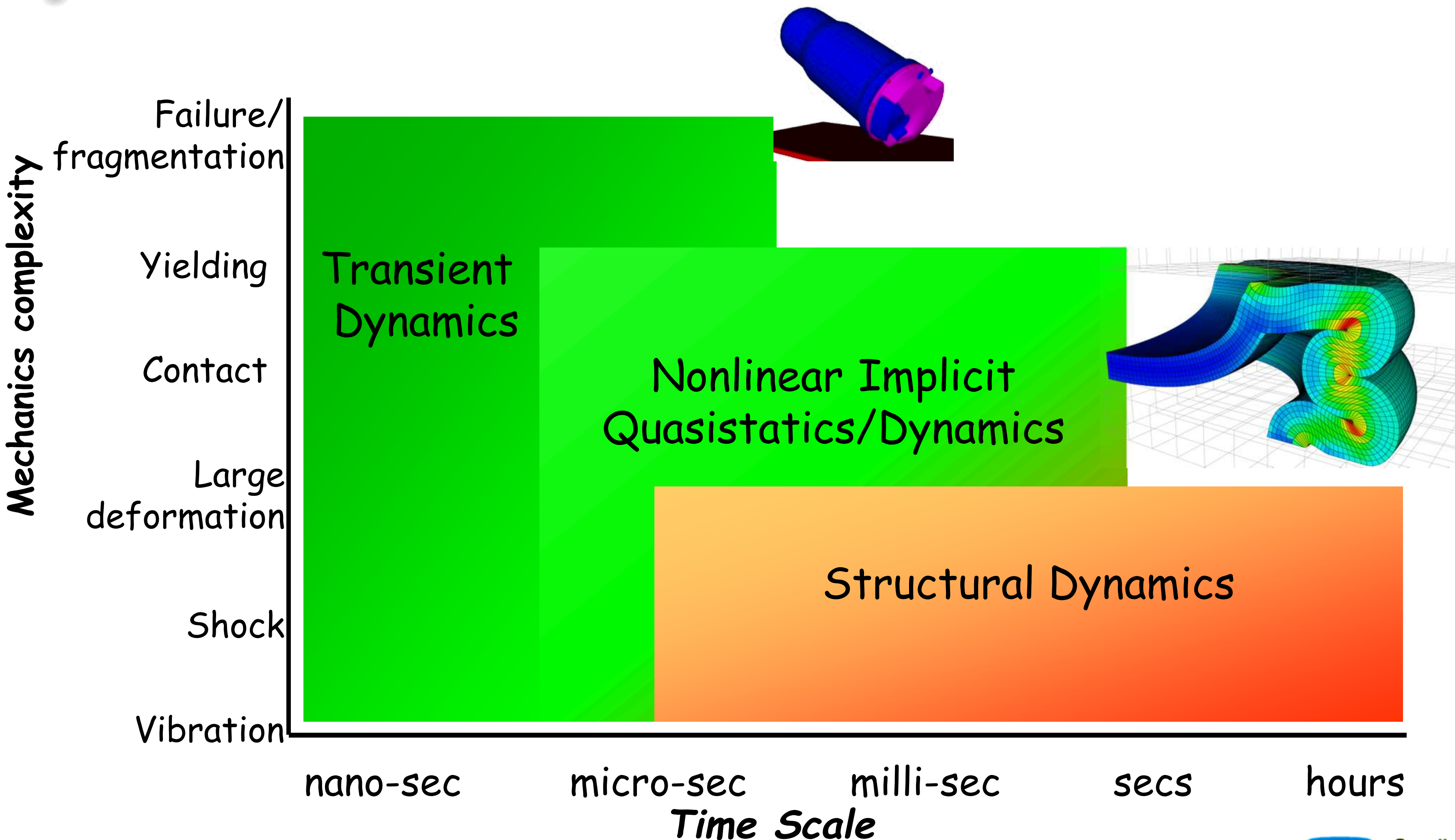
Sierra is the engineering mechanics simulation code for Sandia missions



- Distinguishing strengths
  - "Application aware" development
  - Scalable
  - SQA and V&V
  - Multiple scales
  - Coupling
- Explicit tie to SNL workflow, including
  - Geometry and meshing
  - Visualization
  - Design and optimization
- "Partner" applications include
  - CTH and ALEGRA for shock physics simulations
  - RAMSES suite for radiation effects, electrical and electronics simulations

Sierra includes solid mechanics and structural dynamics capabilities



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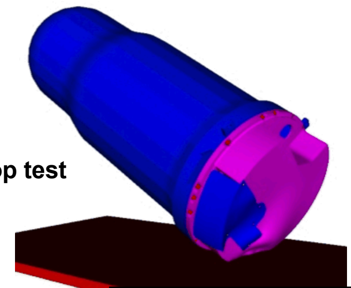
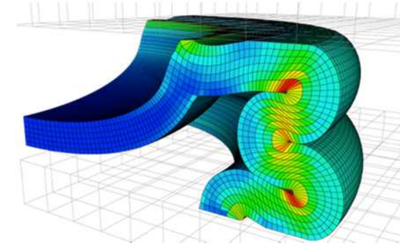
Explicit transient dynamics and implicit quasi-statics and dynamics capabilities

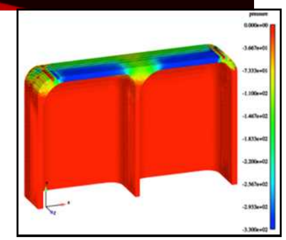
- Fully Three-Dimensional
- Finite Elements and Particles
  - Hex and Nodal Based Tets
  - Shell and Beams
  - SPH and Mass particles
- Material models: 50+, including energy-dependent materials
- Explicit contact: Massively parallel, momentum balance, accurate friction response
- Multi-length Scale
- Boundary conditions:
  - Kinematic and Force
  - Specialized: cavity expansion, silent BC
  - CONWEP integration (Analytic Blast Pressure Loads)
- Explicit Failure modeling:
  - Material failure/element death
  - Cohesive zones (elements, contact surfaces)
  - Phenomenological models (spot weld, line weld)
  - Automatic remeshing using Nodal Based Tets
  - X-FEM (pervasive failure modeling)
- Quasi-static failure modeling

W80 drop test





Large deformation/contact



Coupled Thermal/QS/Dynamic

- Provides scalable parallel solvers for highly nonlinear problems
  - Contact
  - Nonlinear material response
  - Large deformation
- Utilizes services provided by the Sierra Framework/Toolkit to enable
  - Coupled physics
  - Multi-length scale modeling techniques
  - Preloading

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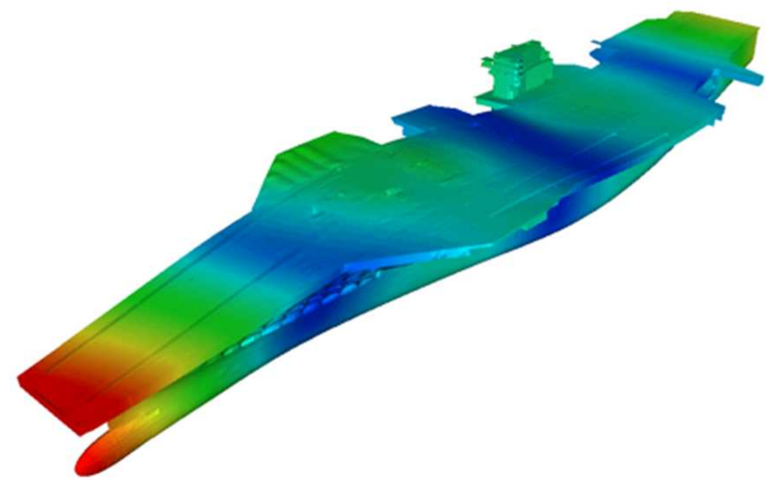
Structural Dynamics

- Predicts the response of a system under dynamic conditions.
  - Stresses (particularly in the operating regime)
  - Fatigue
  - Energy dissipation in joints
- Efficient for very large problems
  - Many millions of coupled equations
  - Serial, direct matrix solutions scale to order N^3
  - Parallel, iterative solvers are typically more complex, but scale as O(N)
- Structural Acoustics
- Inverse Problem Capability underdevelopment



Recent Past:
NASTRAN
MC2912
30,000 dof

→

Today:
Sierra MP
>10M dof

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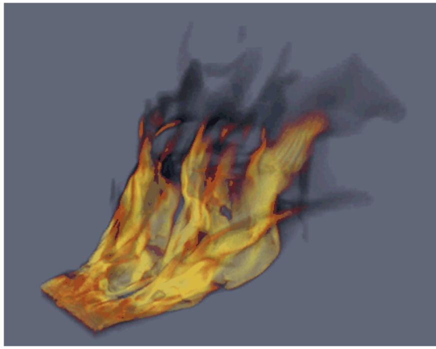
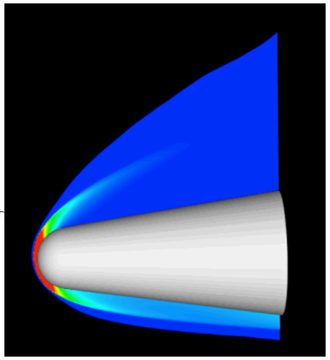
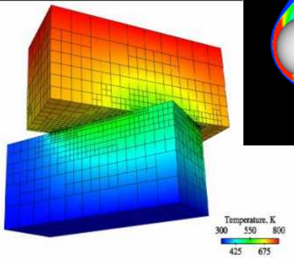
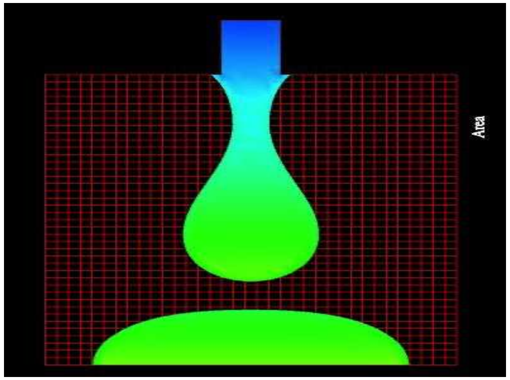
Computational Thermal & Fluid Mechanics



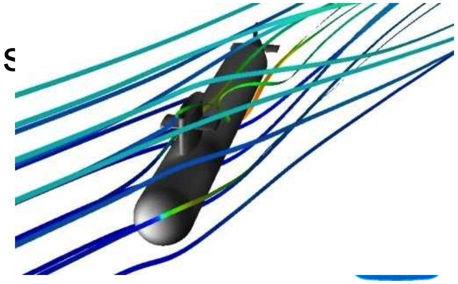




- Heat transfer, enclosure radiation and chemistry
  - Dynamic enclosures
  - Element birth/death
  - Contact
- Compressible fluid mechanics
  - Subsonic through hypersonic
  - Laminar and turbulent
  - Unstructured mesh
- Non-Newtonian, free surface, and porous media flows
  - Complex material response
  - Level sets for surface tracking
  - Flexible coupling schemes
  - Porous media, with chemical reactions and phase change



- Low Mach number, high Reynolds number, variable density, chemically reacting flows
  - Eddy dissipation and mixture fraction reaction models
  - RANS and LES based turbulence models
  - Unstructured Mesh
  - Pressurization models



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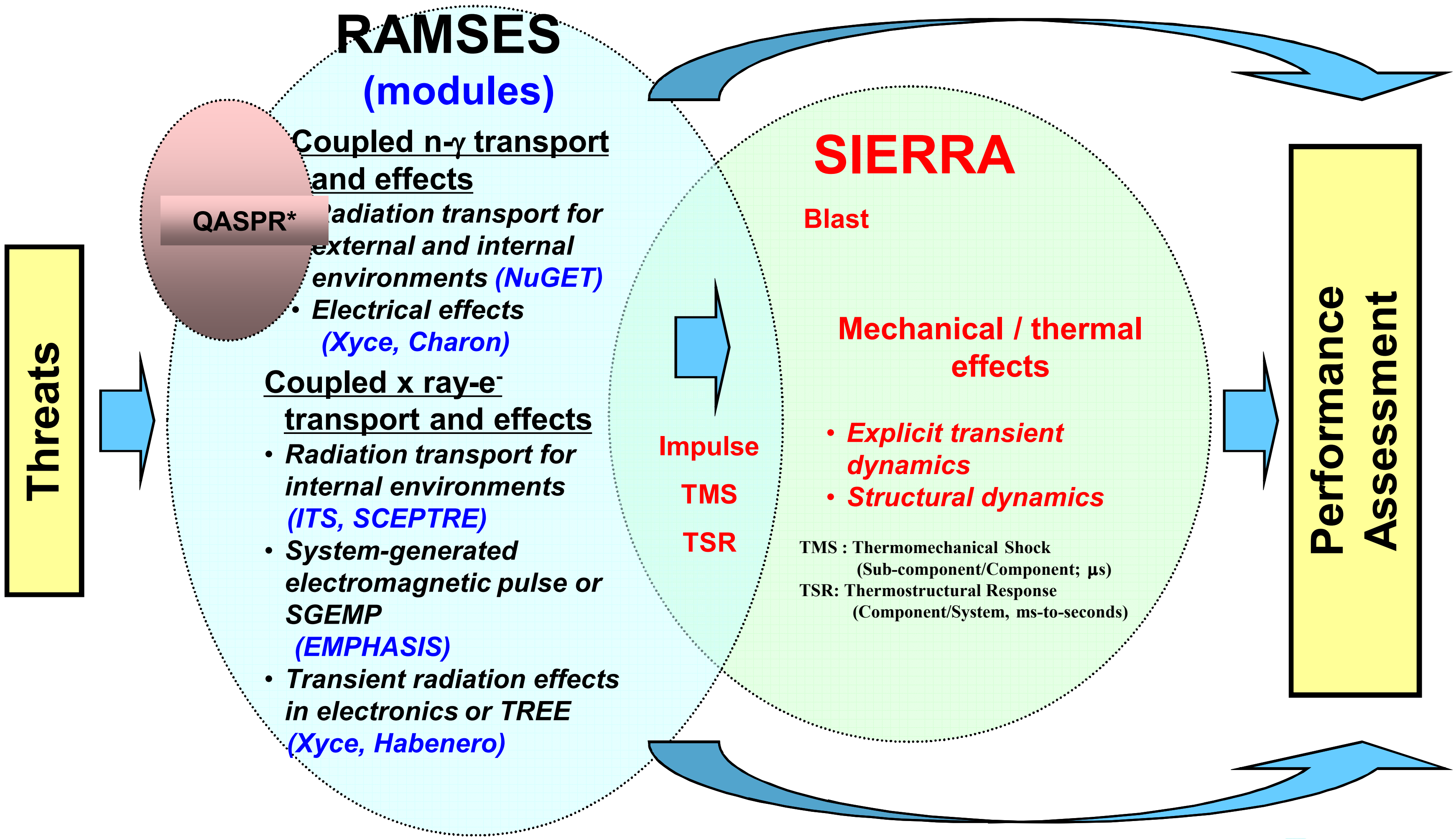
RAMSES: Radiation Analysis, Modeling and Simulation for Electrical Systems

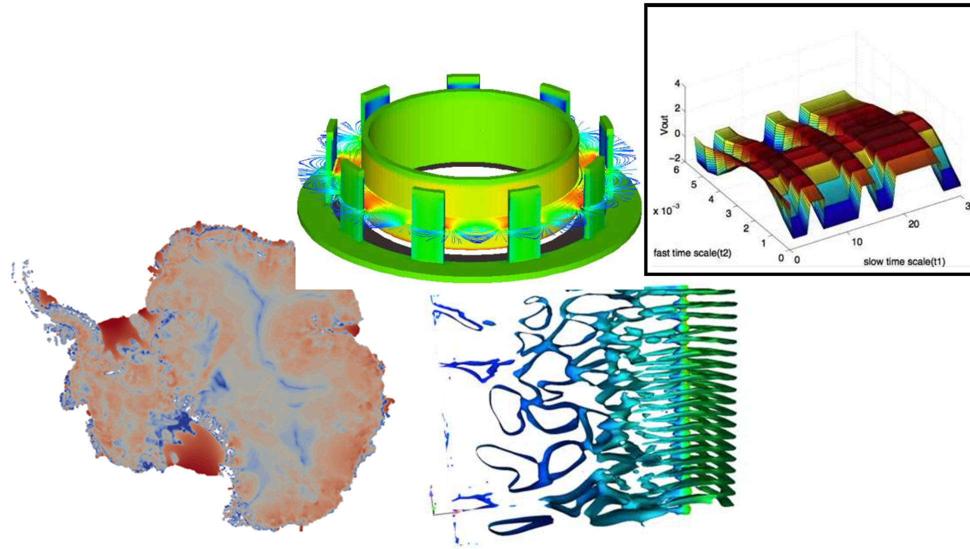
Nuclear Survivability Mission



*QASPR – Qualification Alternatives to the Sandia Pulsed Reactor (Response of electronics to short-pulse neutrons)

Multidisciplinary Research is Key to Success

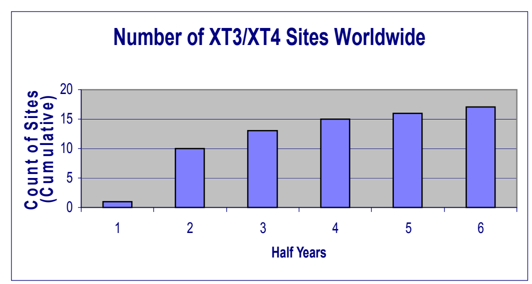
Leading Edge Algorithms and Enabling Technologies



State-of-Art Computational Science Applications

Computer Science Research Institute

Model within Sandia for External Collaborations



Scalable HPC Architectures and Systems

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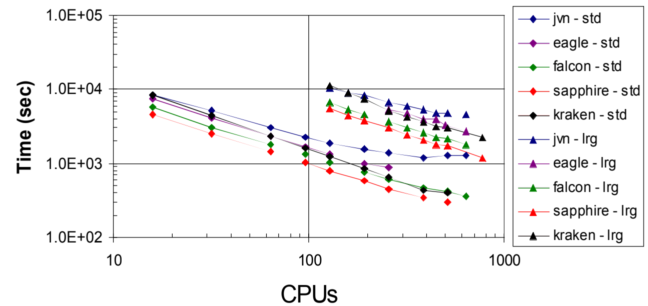
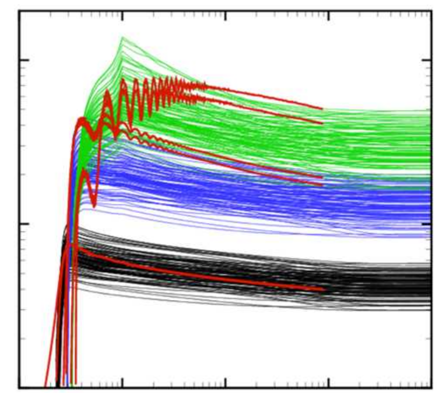
Technical Areas

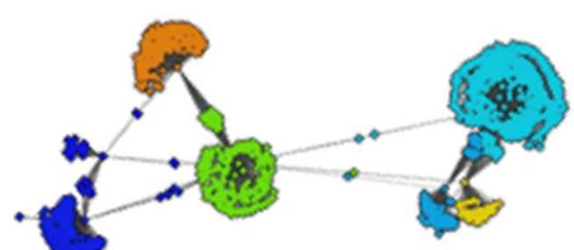
- **Scalability & Extreme Computing**
  - Build on the legacy of MP computing
  - Next generation architectures and algorithms
  - Research is driven by compelling applications
- **Transformation**
  - Change the way modeling & simulation is used
  - Focus on supporting critical decisions
  - Technologies: verification & validation, uncertainty quantification, optimization, inverse problems, …
- **Informatics**
  - New frontiers in extreme data analysis
  - Heterogeneous data, streaming data
  - Rare events, pattern recognition, cognition
  - New demands on architectures and algorithms



CTH 7.1 Scaling at DoD centers



Dakota-Charon calculations including propagation of uncertainty for 3 conditions compared to experimental data in red



Informatics: Data Clustering

HPC Software Trends

- Need to emphasize scalable HPC software
  - Of course, in terms of parallel performance
  - Developer performance
  - Capability growth
  - Maintenance and support costs
- Need robustness in HPC software design
  - Must accommodate hardware disruptions
  - Must enable both discovery science and predictive engineering
  - Software is the "true" capability – it lives on well beyond the hardware
- Need greater agility
  - Explosive potential for HPC in myriad of new domains
  - Need to quickly stand-up new HPC applications
- Cannot support one-off codes anymore
  - Particularly true for mission labs & industry

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Asking different questions…

- Scientific Discovery can utilize a single, hero calculation that lacks rigorous validation
  - **Questions**: What are key phenomena? What are first-order parameters? What physical insight can be obtained?
  - **Implications**: Simplified geometries, simple (single) physics & models, approximate boundary conditions, limited experimental data.
- Predictive Engineering often requires an ensemble of computations
  - **Questions**: What is the optimal design? What are the margins of uncertainty? Is simulation consistent with measured data? How do I optimally design a validation experiment? To what degree can I rely on the simulation to make a high-consequence decision?
  - **Implications:** Complex geometries, complex physics/chemistry, complex models, realistic boundary conditions, multi-physics & multi-scale, needs to be fused with (sometimes) extensive experimental data.

Algorithms Capabilities

- Trilinos: **HPC solution components**
  - Compatible space-time discretizations
  - Linear & nonlinear solvers
  - Partitioning and dynamic load balancing
  - Automatic differentiation
  - Optimization (fully coupled)

Full vertical Integration!

- Dakota: **Risk informed decision making**
  - Optimization (multiparallel, surrogate,..)
  - UQ (aleatory & epistemic)
  - New sparse-collocation methods…
  - Optimization under uncertainty
  - Rapid deployment of new algorithms

Ready to use optimization and UQ methods

- **Extensive algorithms R&D foundation…**

Agile Modeling & Simulation

- **Strategic Goals**
  - To align the many efforts at Sandia involved in developing software for the modeling and simulation of physical systems (mostly PDEs):
  - To enable the Rapid development of new Production codes
  - To embed the codes with Transformational design, analysis, and decision-support capabilities
  - To benefit from Synergy & reduce Redundancy

- **Consensus Vision**
  - A full range of independent yet interoperable software components ☑ **Capabilities** ☑ **Interfaces**
  - Software quality tools and procedures
  - Prototype applications that demonstrate use cases, vertical integration, and verification

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The Components Effort Expands this Effort

Analysis Tools (*black-box*)
- Optimization
- UQ (sampling)
- Parameter Studies
- V&V, Calibration
- OUU, Reliability

Analysis Tools (*embedded*)
- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Constrained Solves
- Optimization
- UQ Solver

Linear Algebra
- Data Structures
- Iterative Solvers
- Direct Solvers
- Eigen Solver
- Preconditioners
- Matrix Partitioning

Architecture-Dependent Kernels
- Multi-Core
- Accelerators

Composite Physics
- MultiPhysics Coupling
- System Models
- System UQ

Mesh Tools
- Mesh I/O
- Inline Meshing
- Partitioning
- Load Balancing
- Adaptivity
- Remeshing
- Grid Transfers
- Quality Improvement
- DOF map

Local Fill

Discretizations
- Discretization Library
- Field Manager

Derivative Tools
- Sensitivities
- Derivatives
- Adjoints
- UQ / PCE Propagation

Physics Fill
- Element Level Fill
- Material Models
- Objective Function
- Constraints
- Error Estimates
- MMS Source Terms

Utilities
- Input File Parser
- Parameter List
- Memory Management
- I/O Management
- Communicators

PostProcessing
- Visualization
- Verification
- Model Reduction

Mesh Database
- Mesh Database
- Geometry Database
- Solution Database

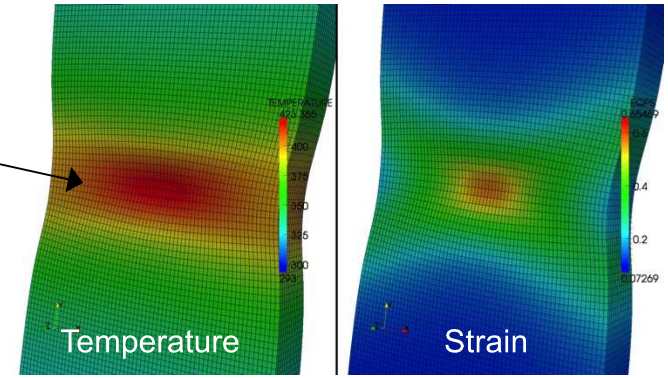
Data-Centric Algs
- Graph Algorithms
- SVDs
- Map-Reduce
- Linear Programming
- Network Models

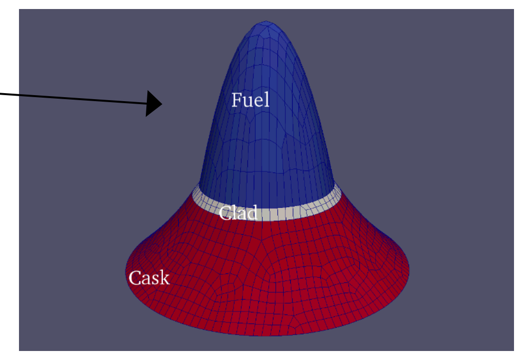
Software Quality
- Version Control
- Regression Testing
- Build System
- Backups
- Verification Tests
- Mailing Lists
- Unit Testing
- Bug Tracking
- Performance Testing
- Code Coverage
- Porting
- Web Pages
- Release Process

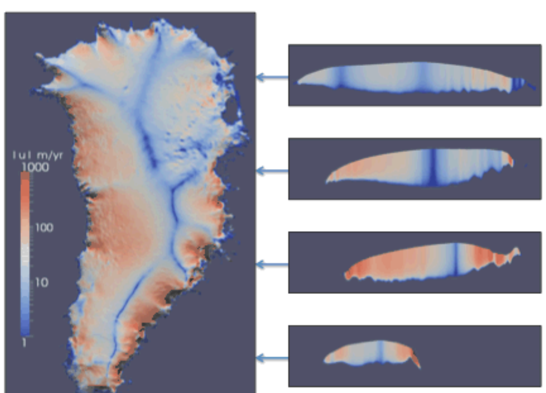
Impact: We are Developing Several New Component-Based Applications

1. Turbulent CFD for nuclear energy [NE]
2. Computational mechanics R&D [ASC]
3. Quantum device design [LDRD]
4. Extended MHD [ASCR]
5. Partner's in-house code [CRADA]
6. Peridynamics solver [ASC]
7. Biogeochemical element cycling: climate [SciDAC]
8. Fuel rod degradation modeling [NE]
9. Subsurface nuclear waste transport [NE]
10. Ice Sheet dynamics [SciDAC]

\+







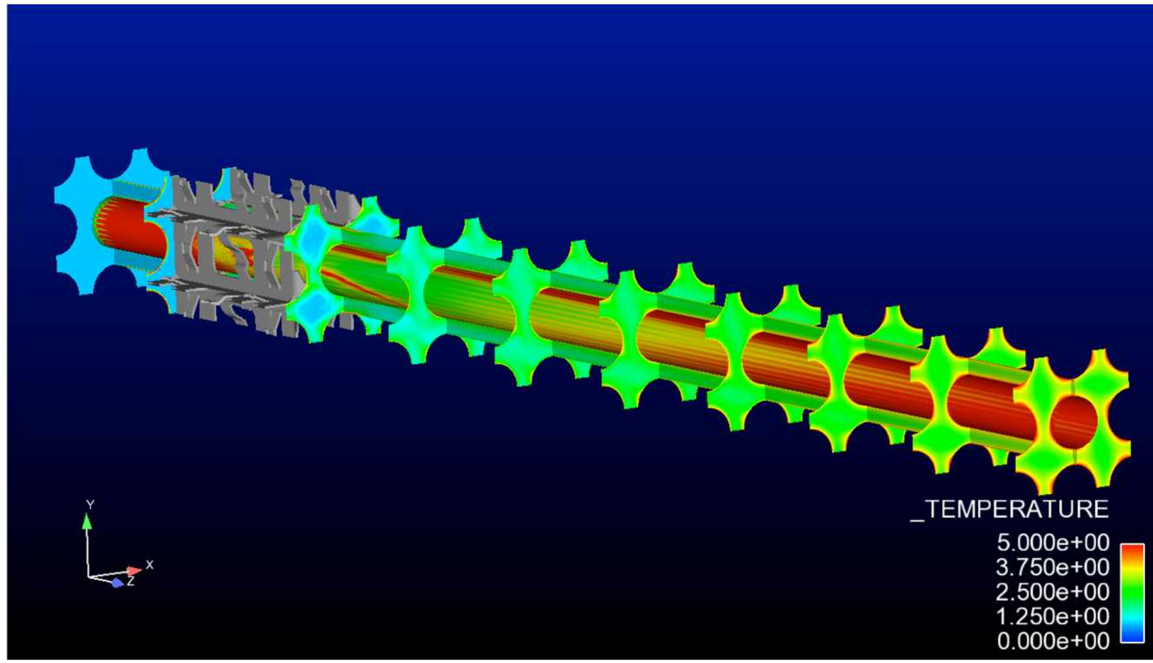
Codes are born: parallel, scalable, robust, with sensitivities, optimization, UQ

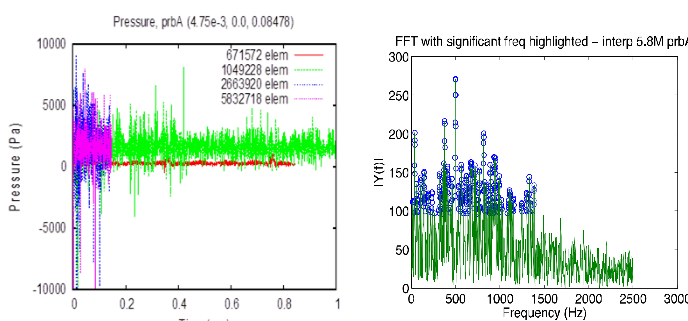
… and ready to adopt: embedded UQ, multi-core kernels, adaptivity, code coupling, ROM

Sandia National Laboratories

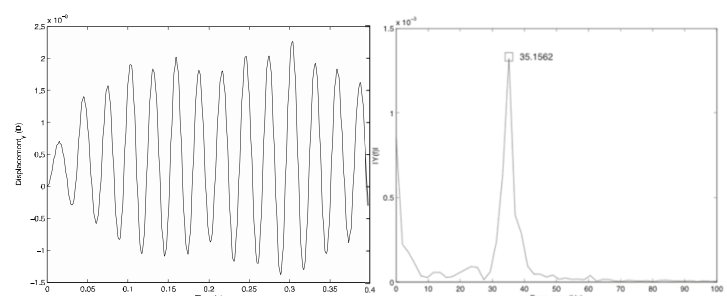
LES CFD + Rod Vibration Analysis of Nuclear Reactor Core Flow

- **Drekar went from drawing board to milestone completion on 3x3 sub-assembly in 6 months (< 3 Full time employees)!**
- **Included: Implementation + verification + validation + production runs!**
- **Assesses industry baseline tools for accuracy**
- **Challenges:**
  - **Turbulence Models**
  - **Meshing**
  - **Scalability**
  - **Time Integration**





LES Fluid Pressure Load on Fuel Rod



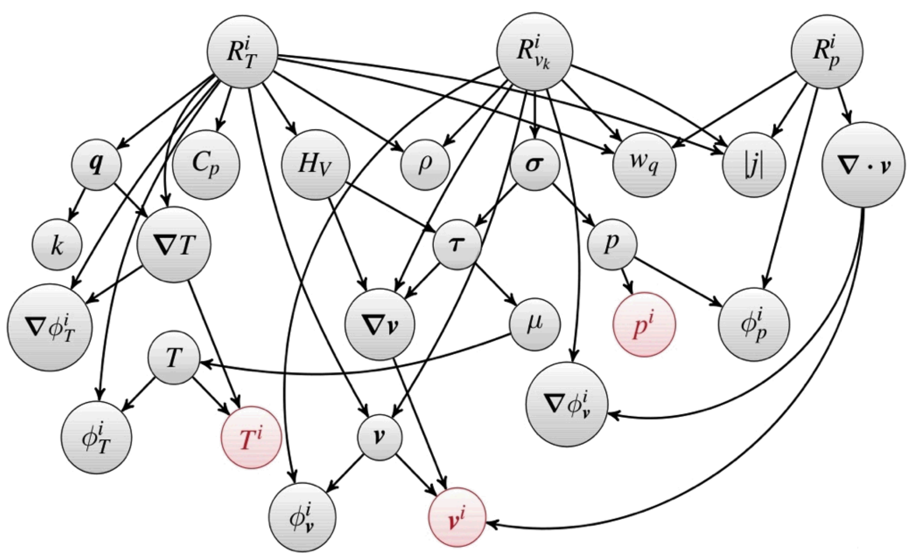
Fuel Rod Vibration Response

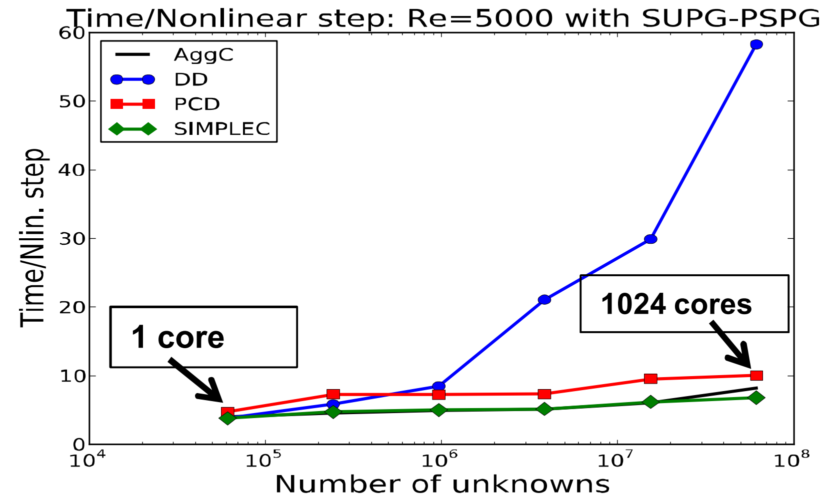
Rapid Implementation of Physics Using Graph-based Assembly Process

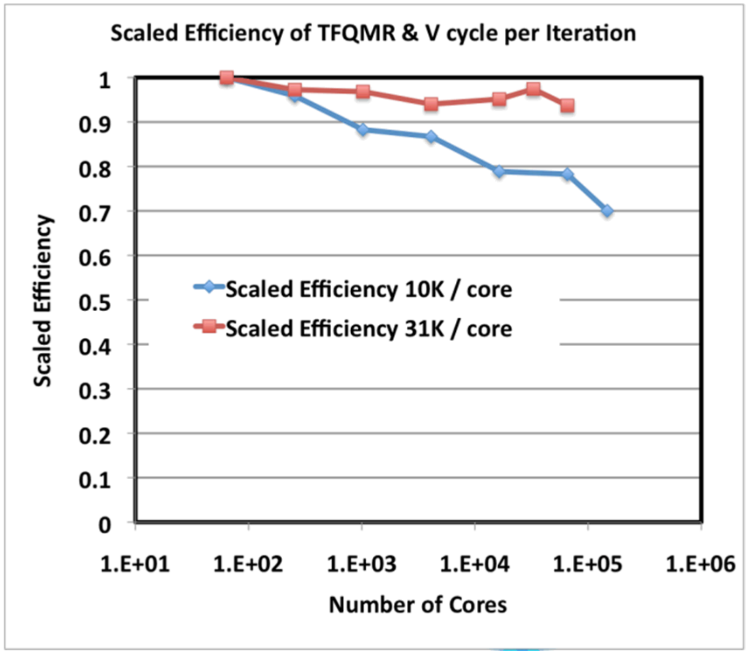
$$R_T^i = \sum_{e=1}^{N_e} \sum_{q=1}^{N_q} \left[\left(\rho C_p \boldsymbol{v} \cdot \nabla T - H_V \right) \phi_T^i - \boldsymbol{q} \cdot \nabla \phi_T^i \right] w_q |j| = 0$$

$$R_{v_k}^i = \sum_{e=1}^{N_e} \sum_{q=1}^{N_q} \left[\rho \boldsymbol{v} \cdot \nabla \boldsymbol{v} \phi_v^i + \boldsymbol{\sigma} : \nabla \left(\phi_v^i \boldsymbol{e}_k \right) \right] w_q |j| = 0$$

$$R_p^i = \sum_{e=1}^{N_e} \sum_{q=1}^{N_q} \nabla \cdot \boldsymbol{v} \phi_p^i w_q |j| = 0$$

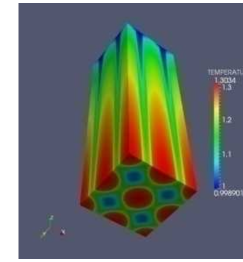




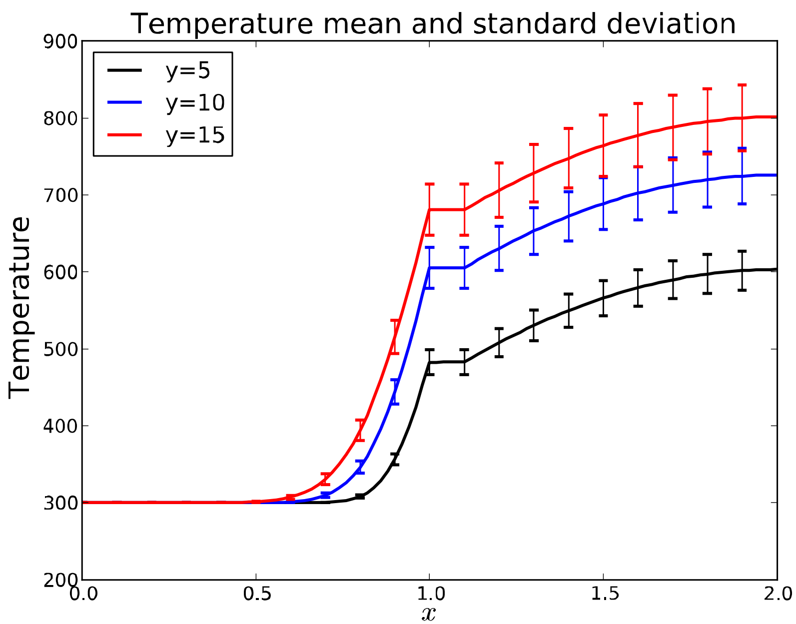


Notz, Pawlowski, Sutherland; TOMS in press

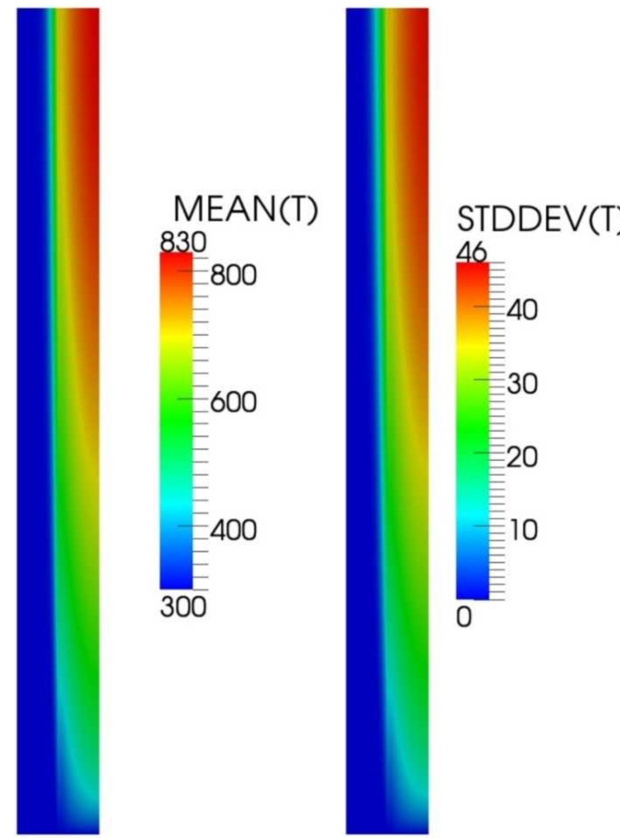
Embedded UQ in Drekar:
Multiphysics: Rod to Fluid Heat Transfer



- True multiphysics formulation: conjugate heat transfer demonstrated in Drekar
- Embedded uncertainty quantification demonstration run using TBGP concepts at the 1 year mark
- Agile components significantly decreases the time to import cutting edge research into production applications



Stochastic Galerkin UQ analysis propagating uncertainty in the magnitude of the model fuel source term and the average inflow velocity.

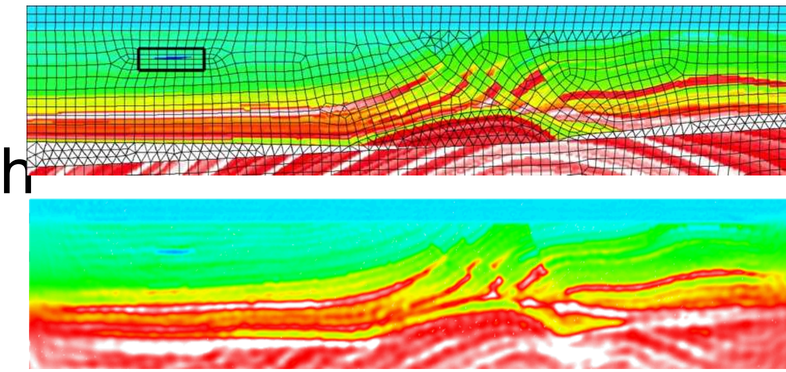


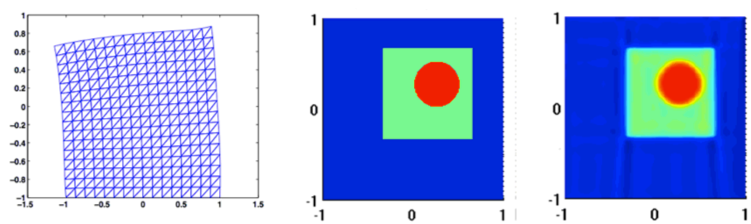
Leverages 4 ASCR funded research projects that perform R&D directly in Trilinos agile components

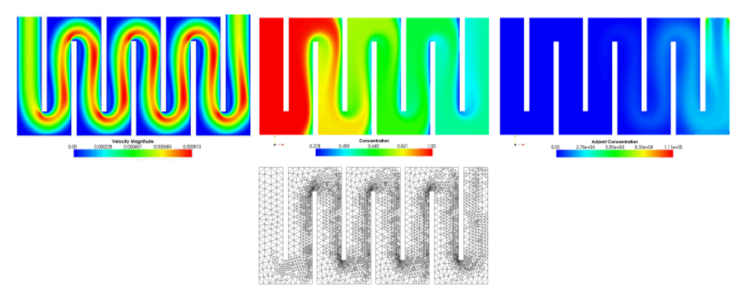
Sandia National Laboratories

Inverse Problems

- PDE-constrained optimization is “ready” for real-world problems
- Fundamental mathematics research in constrained optimization algorithms
- Both full and reduced space methods
- Utilizing compressed sensing and random projection for large data
- Careful control of in-exactness yields scalable, robust methods
- Applied to acoustics, fluids, and linear and nonlinear elasticity.
- Integrated into Sandia and partner applications – working with real data!







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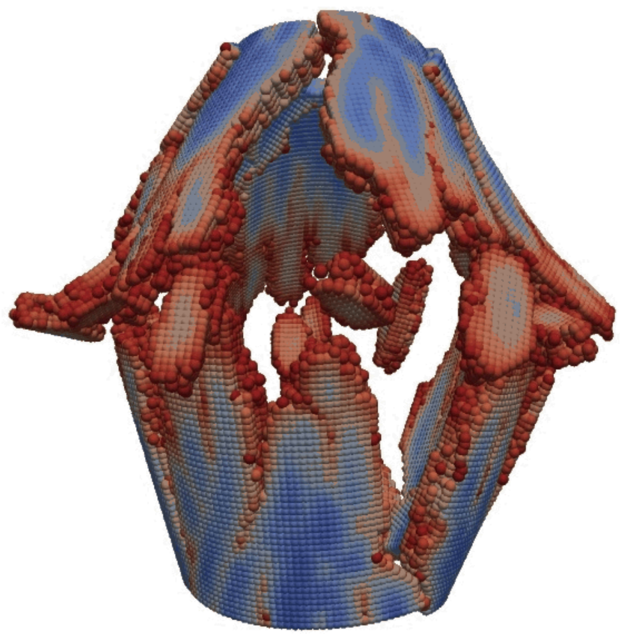
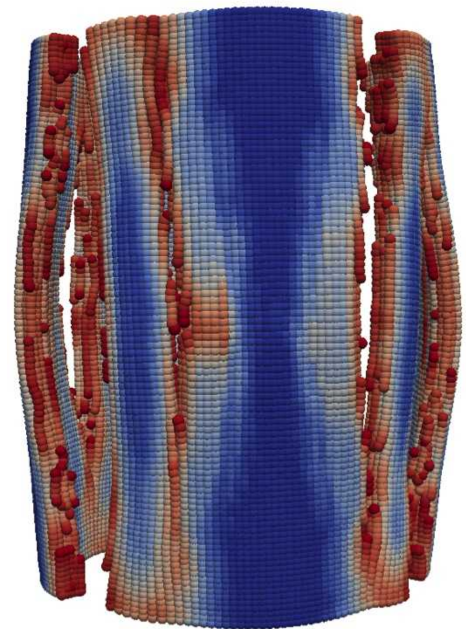
Peridynamics

Predicting material failure: Fragmenting Cylinder

Before



After
(brittle model)



After
(plastic model)

Color indicates damage

Sandia National Laboratories

Accelerating LAMMPS particle simulations

Motivation

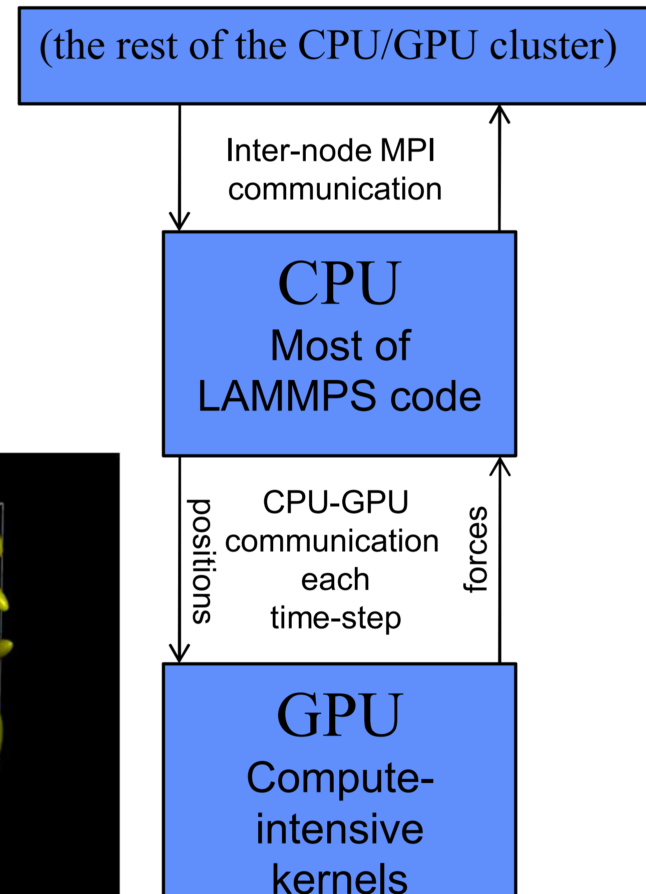
- Other MD codes are running on GPUs and showing 10-100x speedups.
- The future is many-core, and GPU computing is leading the way.
- Next generation supercomputers will have GPU accelerators

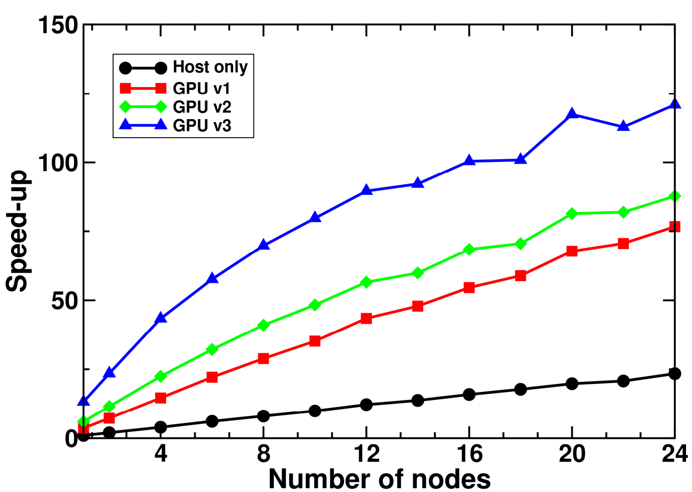
Current status, performance, and future work

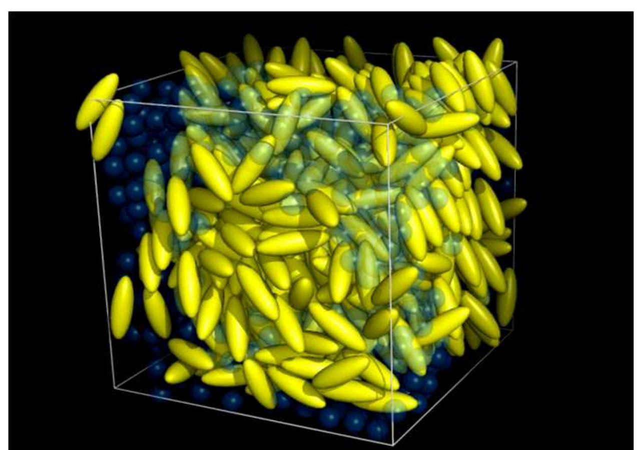
- GPU library and package available for download with LAMMPS.
- Pre-release version of GPU-LAMMPS available on Google codes.
- CUDA kernels written for three pairs styles: LJ (~6x speedup), Gay-Berne (~100x speedup), CHARMM biomolecular FF (~20x speedup)
- Code contributions from coworkers at SNL, Nvidia, ORNL, Ilmenau
- Performance improving rapidly; more pair styles coming soon…

Approach

- Enable LAMMPS to run efficiently on future CPU-based clusters with GPU accelerators.
- Rewrite the most compute-intensive LAMMPS kernels in CUDA.

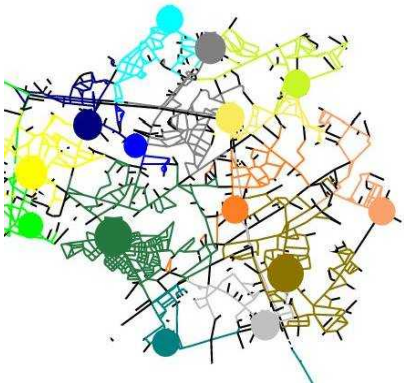






More Computational Capabilities

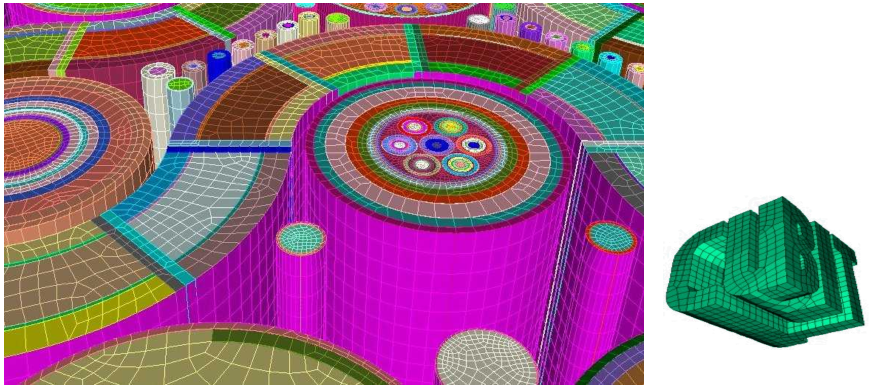
Integer Programming: Optimal Sensor Placement for Water Security (EPA)



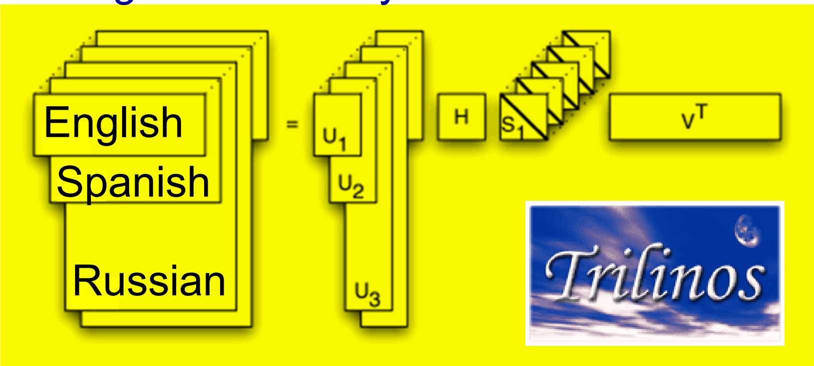
City Water Network

PICO

Mesh Generation: Accurate Geometry for Nuclear Fuels Simulation (with INL)

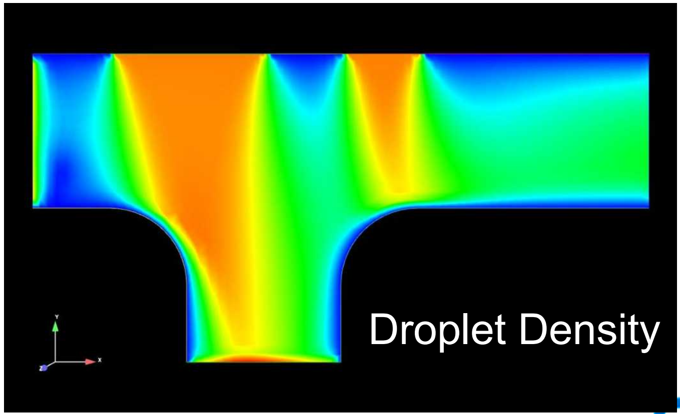


Sparse Linear Algebra: Improved Multi-Lingual Text Analysis



Precision increased from 67% to 80% on verification data

Reacting Flows on HPC: Design Capability for Chemical Lasers (AFRL)



CHARON

Sandia National Laboratories

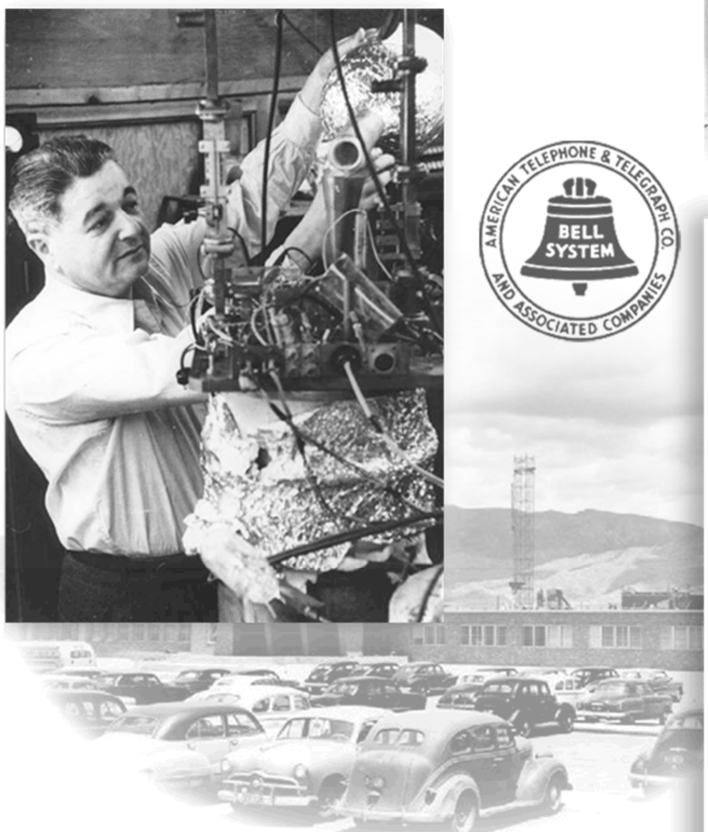
QUESTIONS?

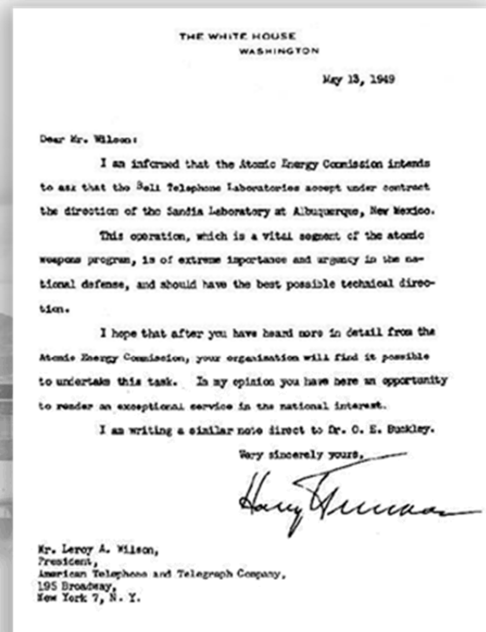
Computer Science Research Institute (CSRI)

- Annual Statistics
  - **14 projects**
  - **4 workshops**
  - **102 additional visitors from 67 institutions**
  - **37 summer students**
  - **3 sabbaticals**
- 73% of 1400's math and computer science hires in 2005-2007 had prior contact through CSRI collaborations

Sandia’s History

“Exceptional service in the national interest”





THE WHITE HOUSE
WASHINGTON

May 13, 1949

Dear Mr. Wilson:

I am informed that the Atomic Energy Commission intends to ask that the Bell Telephone Laboratories accept under contract the direction of the Sandia Laboratory at Albuquerque, New Mexico.

This operation, which is a vital segment of the atomic weapons program, is of extreme importance and urgency in the national defense, and should have the best possible technical direction.

I hope that after you have heard more in detail from the Atomic Energy Commission, your organization will find it possible to undertake this task. In my opinion you have here an opportunity to render an exceptional service in the national interest.

I am writing a similar note direct to Dr. O. E. Buckley.

Very sincerely yours,

Harry Truman

Mr. Leroy A. Wilson,
President,
American Telephone and Telegraph Company,
195 Broadway,
New York 7, N. Y.

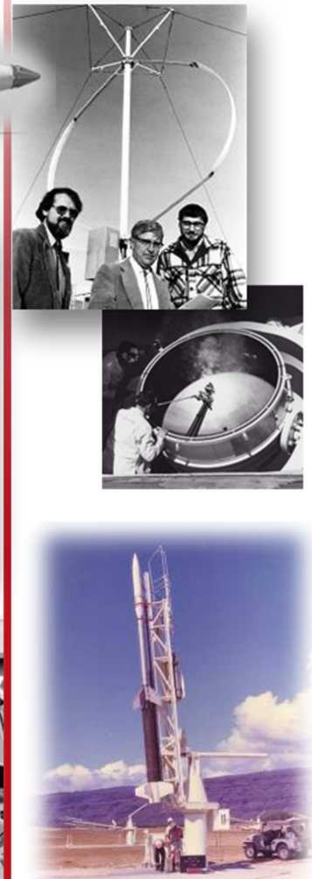
Sandia National Laboratories

The Evolution of Our Mission

1950s
Production engineering and manufacturing engineering

1960s
Development engineering

1970s
Multiprogram laboratory



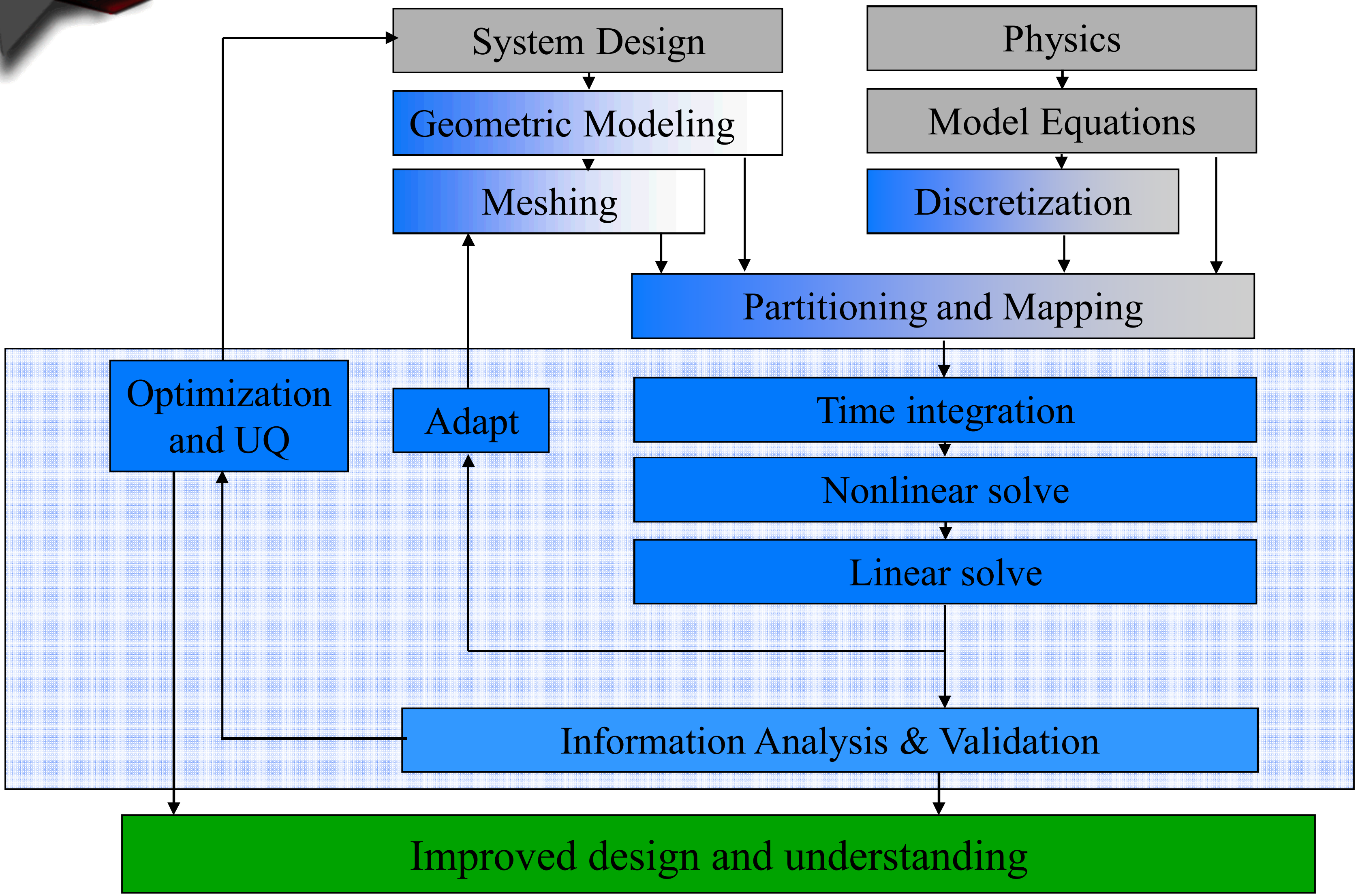
1980s
Research, development and production

1990s
Post-Cold War transition

2000s
Expanded national security role

Sandia National Laboratories

Transformational M&S



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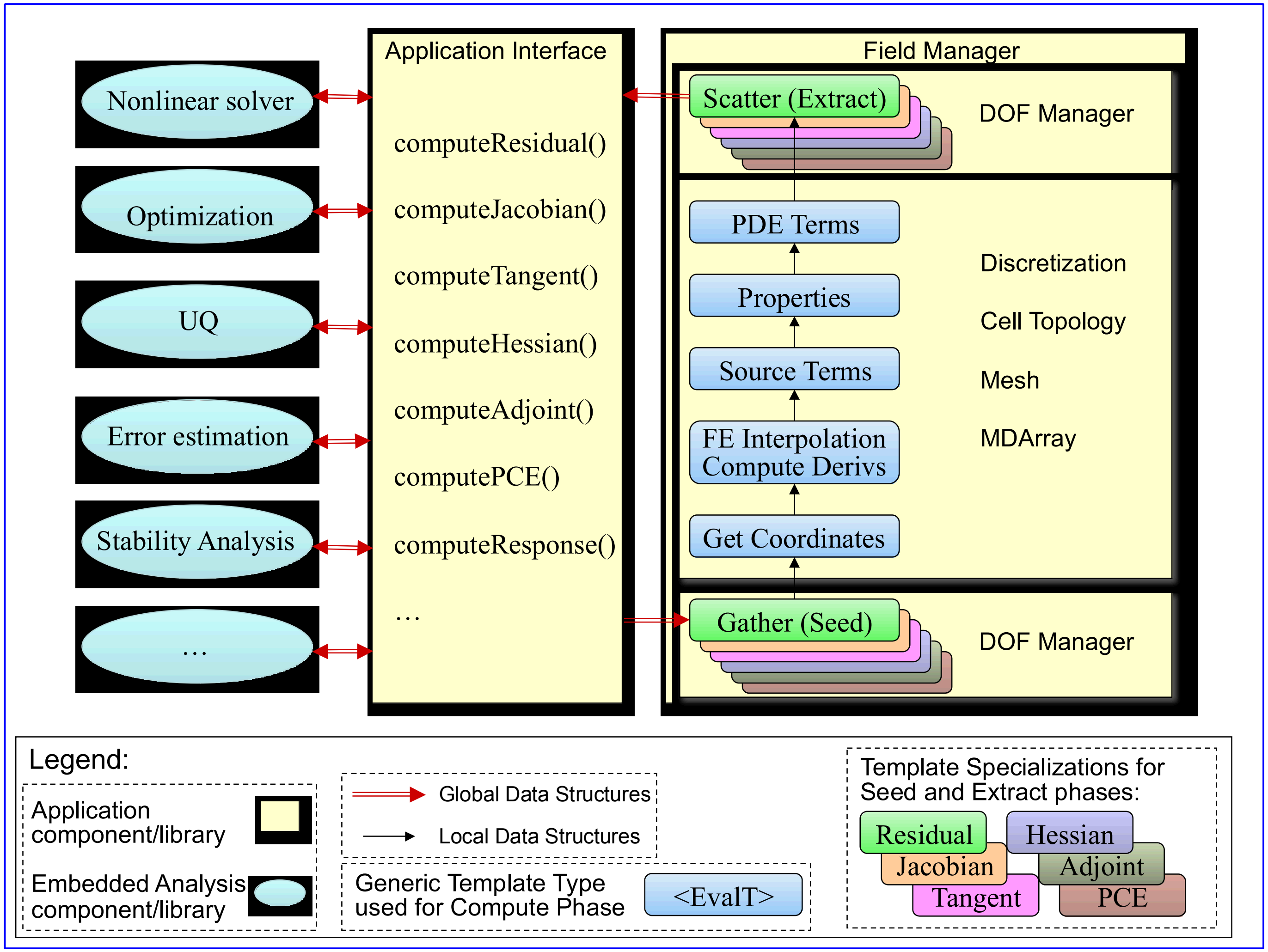
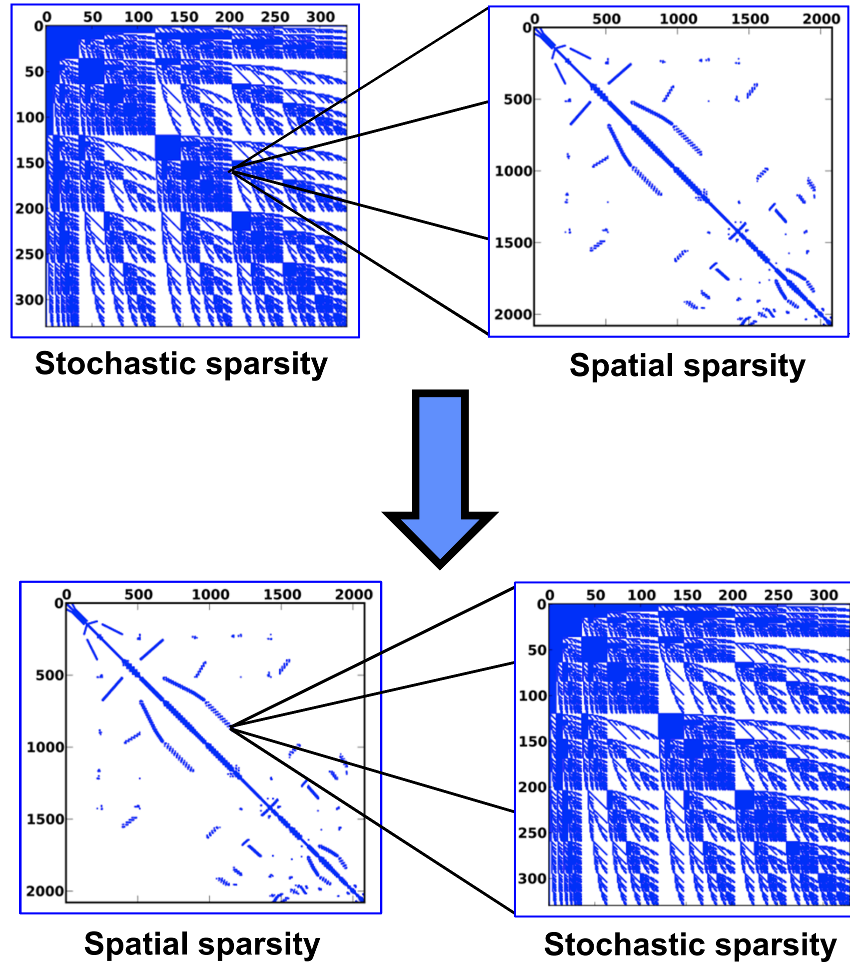
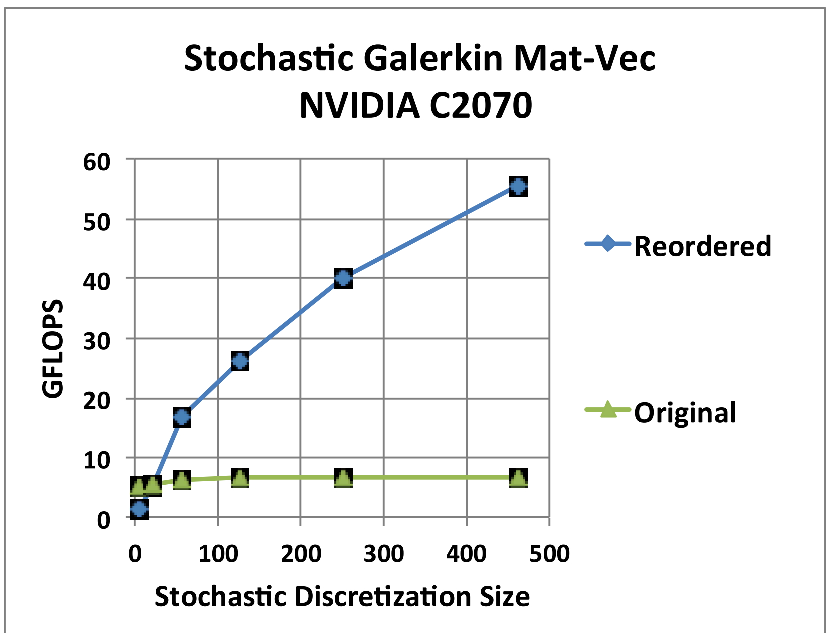
Orthogonalizing Physics and Embedded Algorithm R&D



Multicore for Embedded UQ

- **UQ approaches implemented as an outer loop**
  - Single-point forward simulations use very little available compute power
  - Emerging architectures leading to dramatically increased on-node parallelism
- **Move UQ to the inner loop: increased parallelism**
  - Embed UQ types in templated linear algebra data structures, solvers, preconditioners
  - Custom UQ-aware multicore linear algebra kernels





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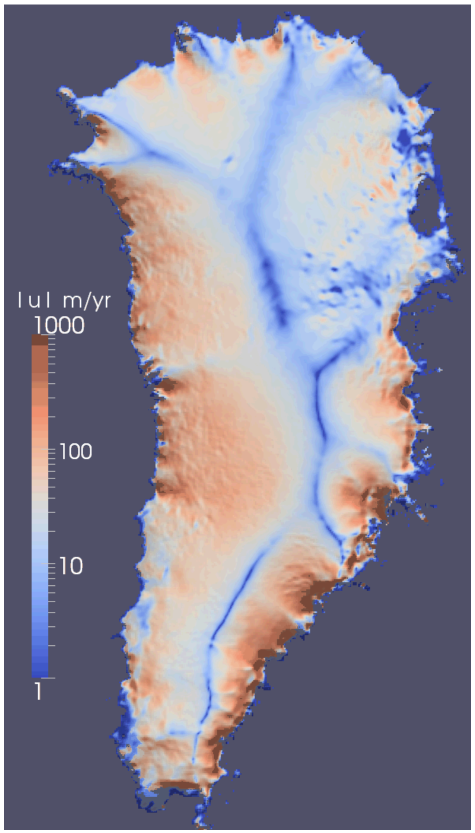
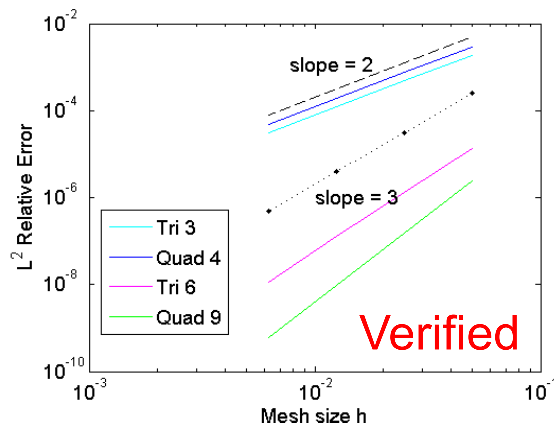
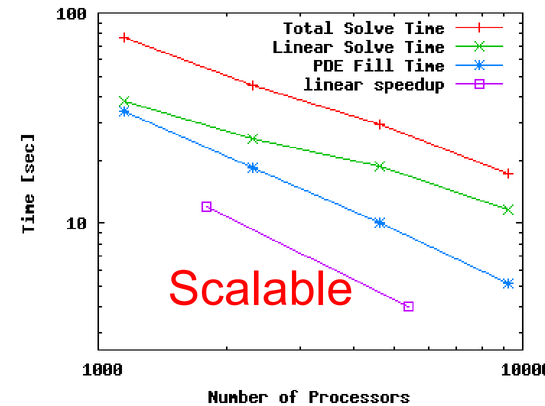
"FELIX" Ice Sheet Dycore

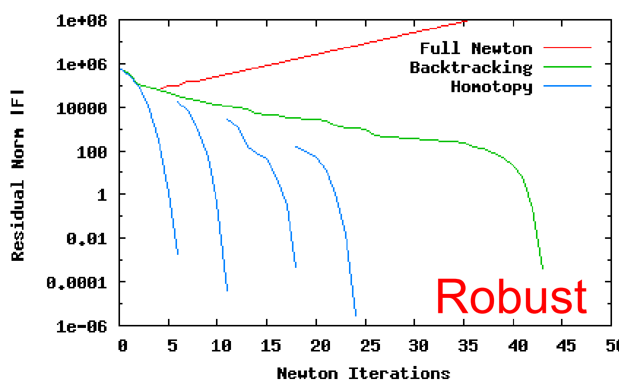
Salinger, Perego and Kalashnikova



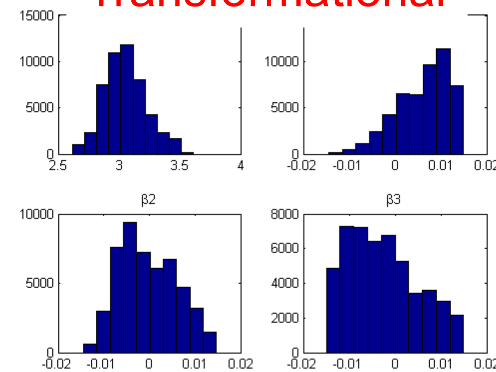
Real Geometries







Transformational



FASTMath highlight at SciDAC PI Mtg

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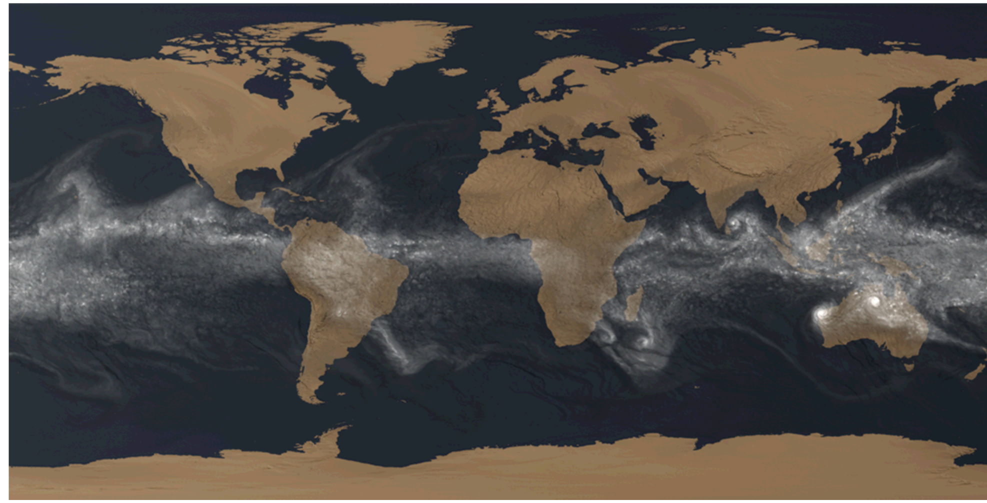
Atmospheric Climate

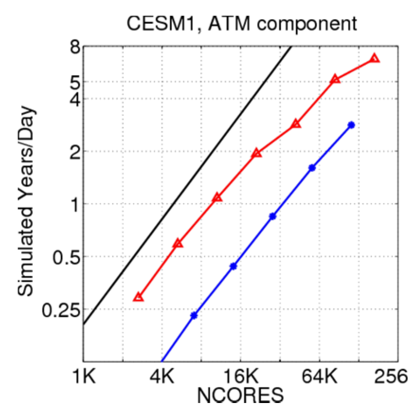


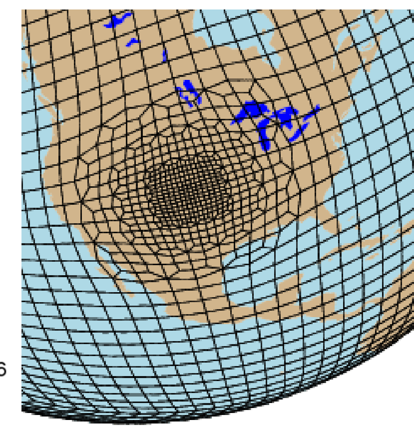
CESM next generation spectral element based atmospheric dynamical core for improved parallel scalability and variable resolution capability.

Enables ultra high resolution simulations on petascale platforms: 1/8° CESM time-slice simulations running well on 170K cores (ORNL Jaguar), achieving 4.6 SYPD. Scaling to O(500K) cores expected.

CESM's spectral element method is 4'th order accurate with local conservation of mass and energy and quasi-monotone transport.

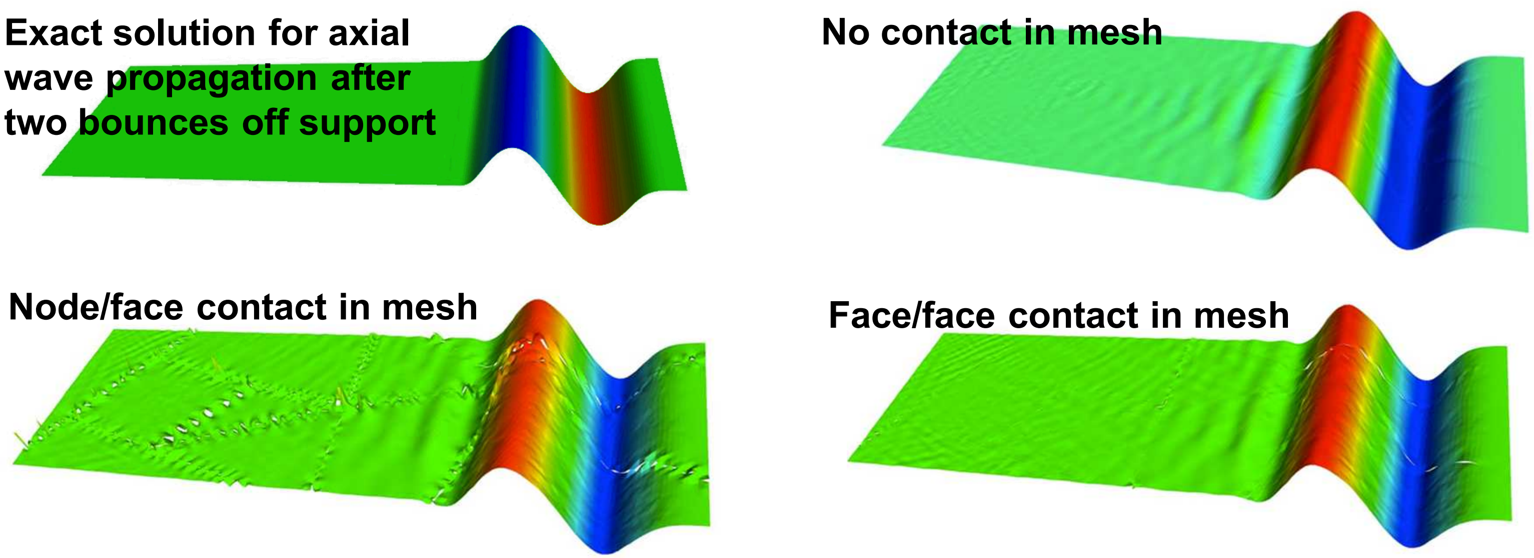
Examples: cubed-sphere grid for uniform high resolution (left), scaling to 170K cores at global 1/8° (middle), a global 1° grid smoothly transitioning to 1/8° over the SGP ARM site (right).





High Velocity Contact

- Automated contact is a core technology in Sierra
  - Recent improvements use face-face contact algorithm to handle hypervelocity contact
    - » Remedies well-known defects of node-face contact
    - » Improves accuracy and performance in remeshing



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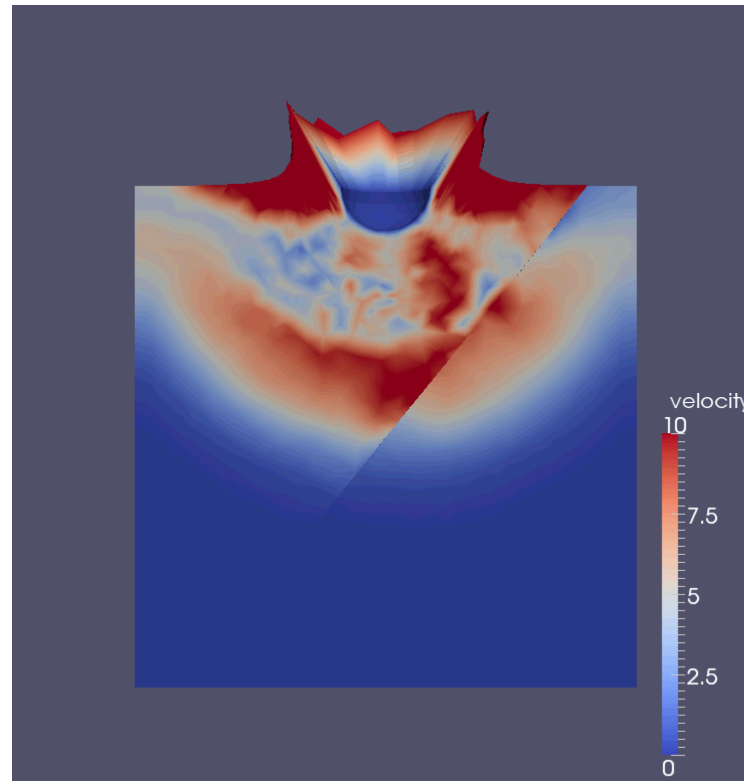
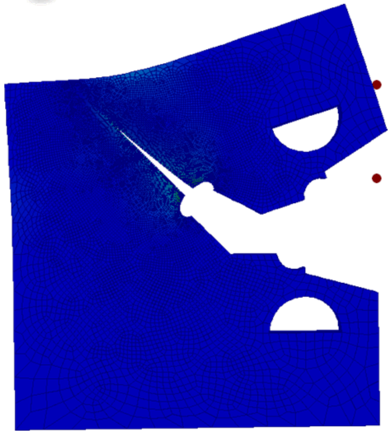
Extended FEM (XFEM)

- XFEM supports discrete localization within elems
  - Remedies one of the few weaknesses of FEM
  - Supports physics-based crack propagation
  - Permits creation of cohesive zones on interfaces
  - Allows contact between faces of interfaces
- Remaining work:
  - Crack initiation capabilities
  - Improvements in crack propagation strategies
  - Implicit solves (currently explicit dynamics only)
  - Improve scalability on MPP

XFEM used to model frictional contact on arbitrary joint within blast-loaded geologic material

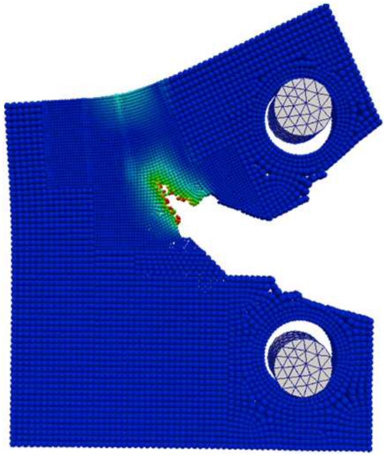


Sierra-Based X-Prize Entries



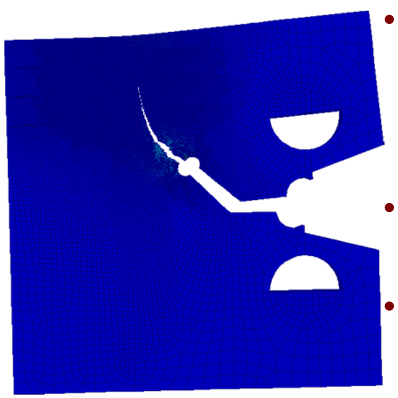
Localization Elements

- Interface elements placed in mesh *a priori*
- 3 potential crack paths competed against each other to determine most likely path



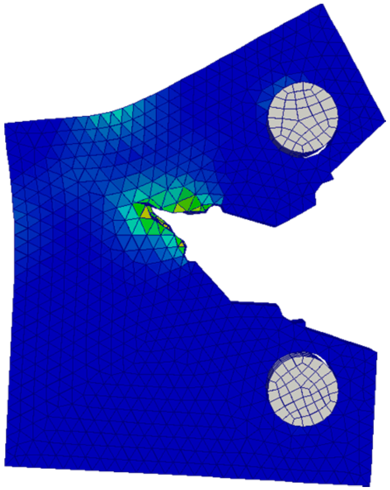
Peridynamics

- **Elastic-plastic continuum material used**
- **Bonds broken based on critical stretch**
- **Pins modeled with finite elements, interact with peridynamics via contact**



Element Death

- **Elastic-plastic material with triaxial-based tearing parameter to determine failure**
- **Elements killed when failure criterion reached**
- **Used implicit solver with limited number of failed elements per iteration**



XFEM

- **XFEM in Sierra is still in development stage. This is one of first applications**
- **Elastic-plastic continuum material used, no cohesive zone law**
- **Coarse elements used for time step and because of crack tangling**

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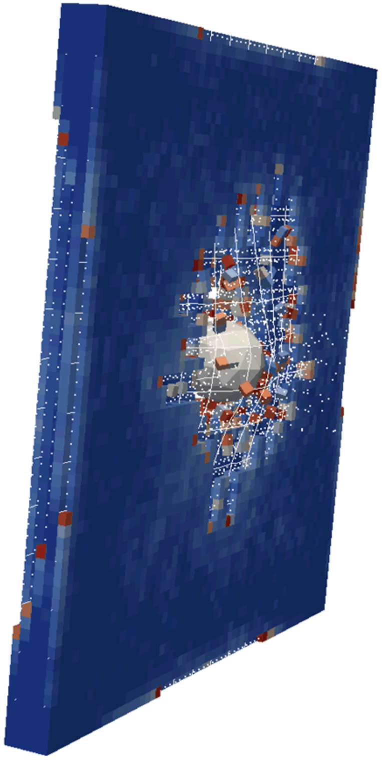
Reinforced Concrete

- Have developed robust modeling techniques for analysis of reinforced concrete structures of import to DoD
- Use K&C and other models (Epic, kayenta)
- Model reinforcing steel with embedded truss elements, which yields “exact” FE results
- Generate MPCs for composite response
- Work now in progress:
  - Implicit solvers for progressive collapse
  - Test other candidate constitutive models
  - Analysis guidelines (theory and practice)

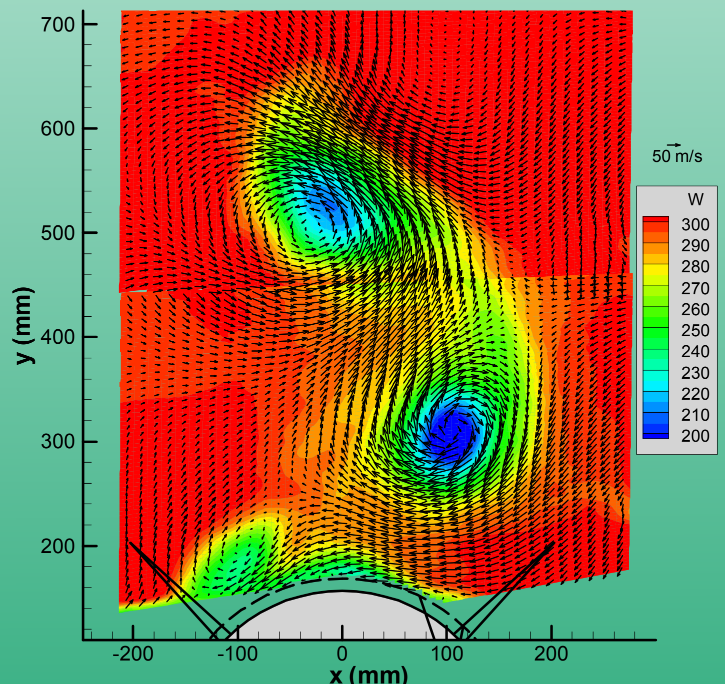


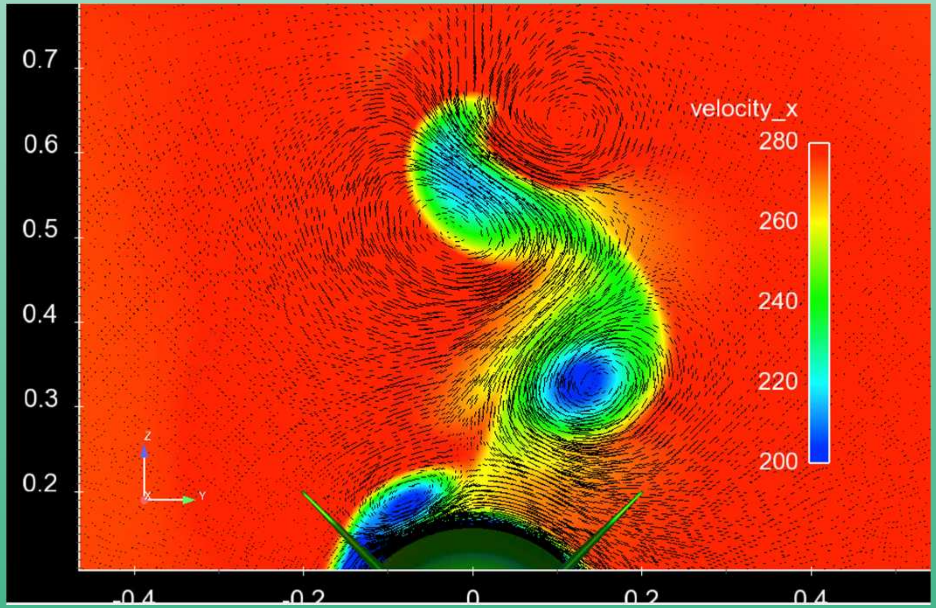
RC plate/ball impact simulation

Sandia National Laboratories

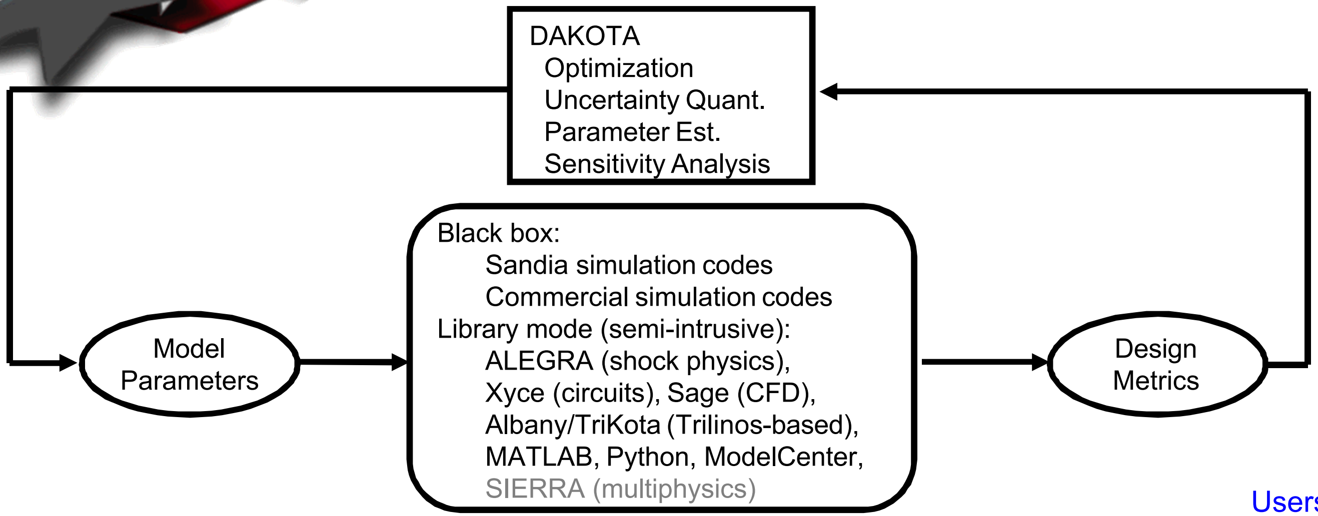
Accurate vorticity transport for transonic turbulent flows

- Currently doing RANS with 2-equation turbulence model
- Will soon extend to DES, based on validation studies.





DAKOTA



Iterative systems analysis
Multilevel parallel computing
Simulation management

http://dakota.sandia.gov
Users/Ref/Dev Manuals + training matls. online

Began as optimization LDRD in 1994

Team: 5-10 core personnel in NM/CA + TPL developers

Releases: Major/Interim, Stable/VOTD; *5.3.1 released 5/13*

DAKOTA Training: 8 sessions (~140 students) since 5.0;
26 sessions (~500 students) total since 2001.

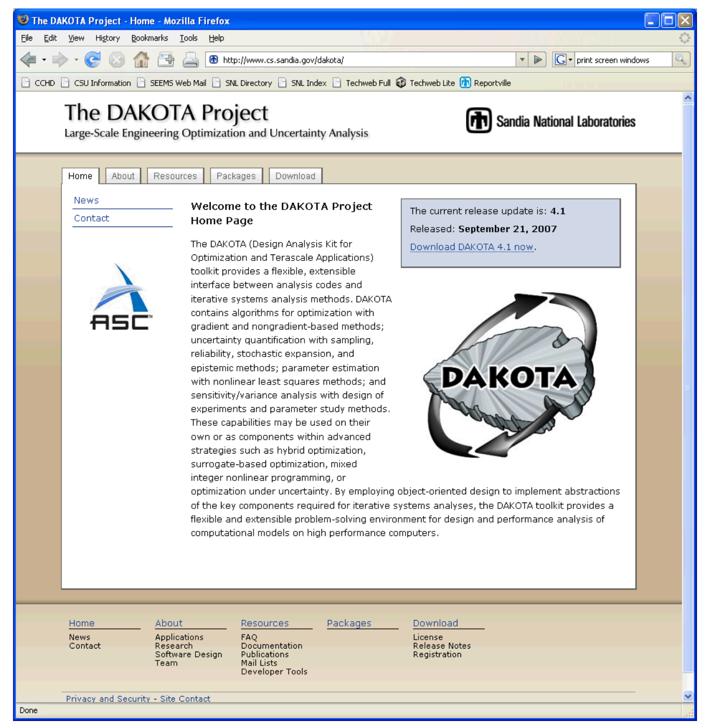
Outreach: Minitutorials at IMAC, SIAM CS&E;
SA/UQ short courses at NASA Langley, AFRL WPAFB.

Modern SQE: Linux/Unix, Mac, Windows; Nightly builds/testing;
subversion, TRAC, Cmake; Top 2008 SQE score

GNU LGPL: free downloads worldwide
(>7000 total ext. registrations, ~3500 distributions last yr.)

Community development: open checkouts now avail (→ PSAAP)

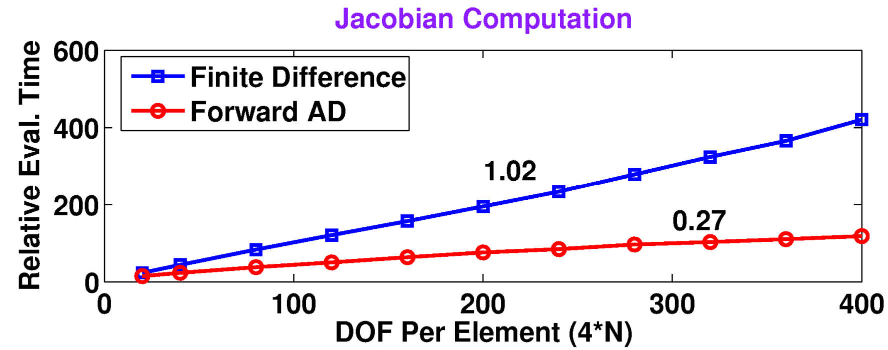
Community support: dakota-users, dakota-developers

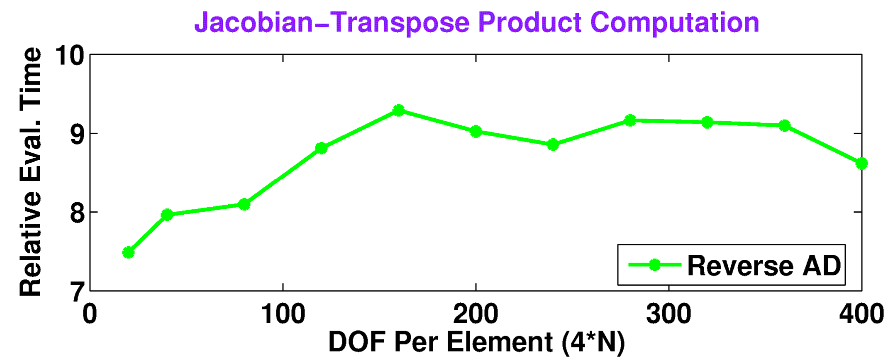


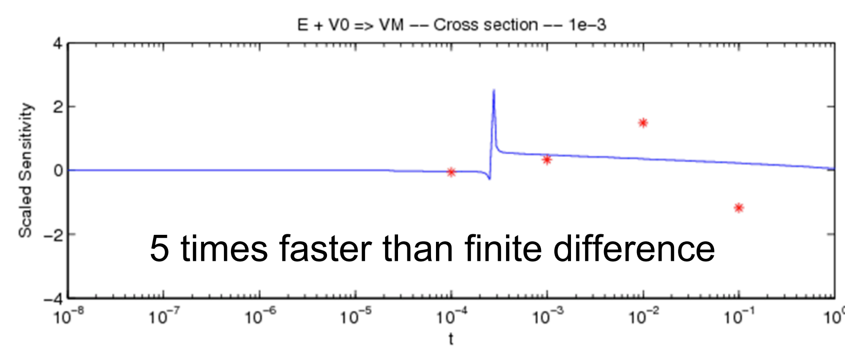
Automatic Differentiation

PI: Eric Phipps

- Use C++ templates to automatically capture derivatives
- Generates efficient derivative code
- Has begun to change the way developers use derivatives in codes
  - Much reduced complexity
  - Reduced implementation time
  - Reduced errors
  - Reduced testing/verification
- Integrates easily into existing or new C++ codes
  - Incorporated into SIERRA in 2 days!
- **Trilinos::Sacado package**







Anatomy of a Component-Based Application: