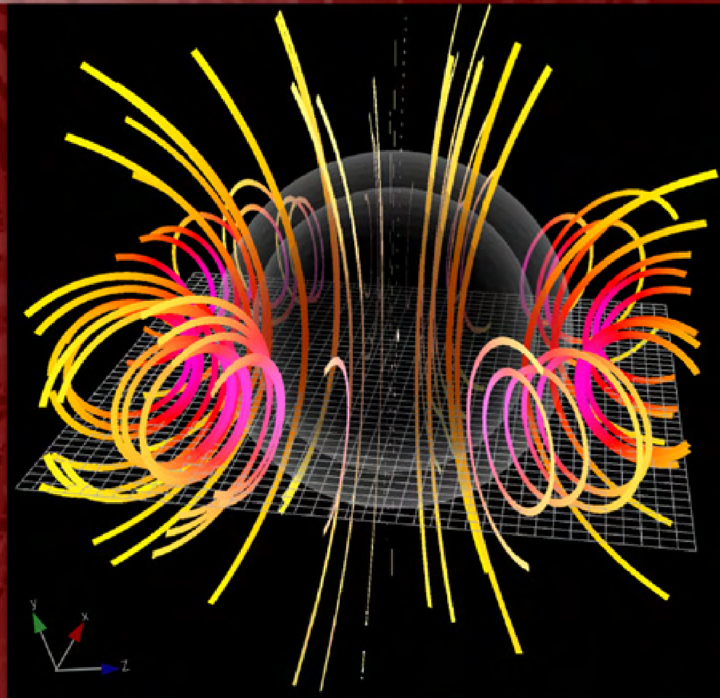
Sandia National Laboratories

Glimpses

INTO SANDIA NATIONAL LABORATORIES' ADVANCED SIMULATION AND COMPUTING PROGRAM



NNSA
National Nuclear Security Administration

ASC™

Glimpses into Sandia National Laboratories' Advanced Simulation & Computing Program

This folder provides short descriptions of *some* projects funded by the Advanced Simulation & Computing (ASC) Program at Sandia National Laboratories. A tri-laboratory program, ASC's emphasis is on high performance computing. Established in 1995 as an essential element of the U. S. National Nuclear Security Administration's (NNSA) Stockpile Stewardship Program (SSP), ASC provides advanced simulation and modeling capabilities for nuclear weapons required for the SSP. As such, ASC supports the NNSA's shift in emphasis from nuclear test-based confidence (done before the nuclear test ban in October 1992) to simulation-based confidence. Under ASC, computer simulation capabilities are developed to analyze and predict the performance, safety, and reliability of nuclear weapons and to certify their functionality.

More information on the ASC Program can be obtained at the following Web sites:
http://www.sandia.gov/NNSA/ASC/
http://www.sandia.gov/ASC/

On the cover: A representation of a magnetic field structure within a hollow sphere generated by a current carrying coil. Sandia's shock physics code, ALEGRA-HEDP, has a new capability to construct the magnetic field of a virtual source with arbitrary shape.

ASC™

Integrated Codes

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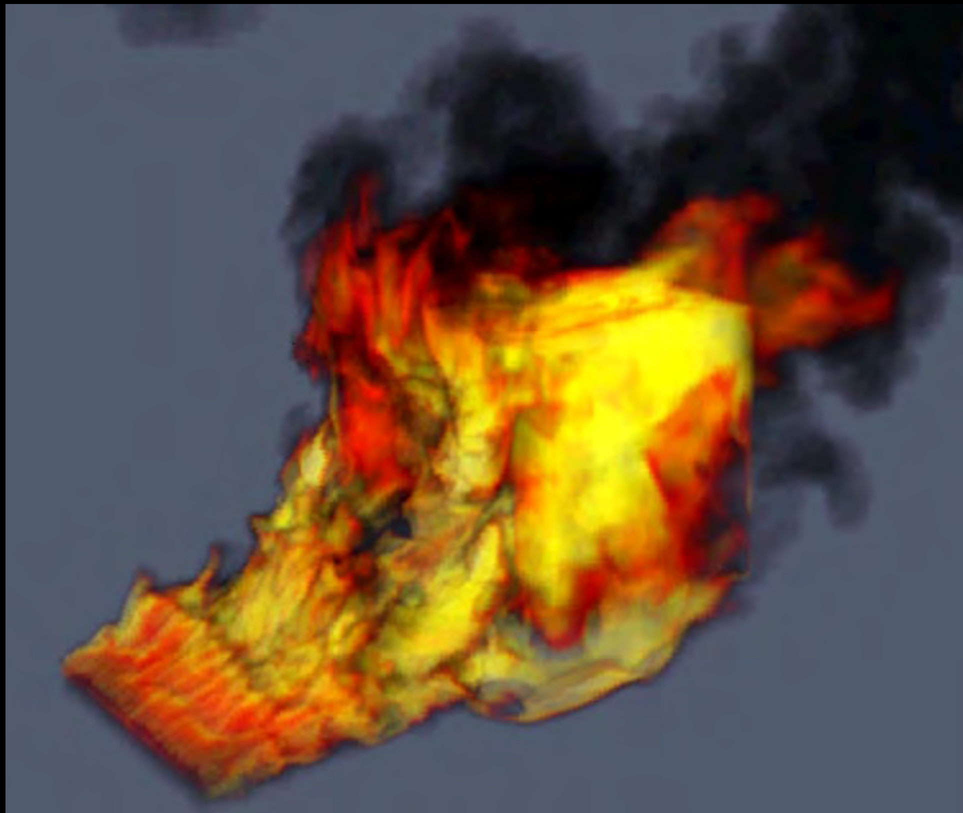

Integrated Codes

Fuego/Syrinx/Calore Model Abnormal Thermal Environments

The SIERRA/Fuego/Syrinx/Calore suite of mechanics codes provides Sandia with a comprehensive modeling capability to predict thermal response of systems in complex geometries, including enclosures as well as open-pool fires. The suite of codes is versatile enough to address the solution of flows in complex geometry involving reacting flow, radiation, and conduction. Its comprehensive verification and validation strategies ensure robustness and reliability over the entire design envelope. It also takes advantage of advanced solver and preconditioner strategies, such as those being developed in the Trilinos framework at Sandia. Characterization of abnormal thermal environments, such as those found in fires, is of key importance to ensure safety of weapon systems. The suite has a proven record in assisting engineering design applications—from heat exchangers to large-scale test facilities—in support of Sandia's mission. Fuego has been particularly useful in qualification efforts for the W76-1 weapons program and was utilized in the design of the cross-wind test facility. With a maturing software infrastructure, improving the predictive capabilities of the models in Fuego is becoming a priority.

- Fuego is a turbulent reacting flow solver including buoyancy, heat transfer, mass transfer, and combustion.
- Calore handles conduction, enclosure radiation, and foam decomposition modeling.
- Syrinx is a participating media radiation solver.

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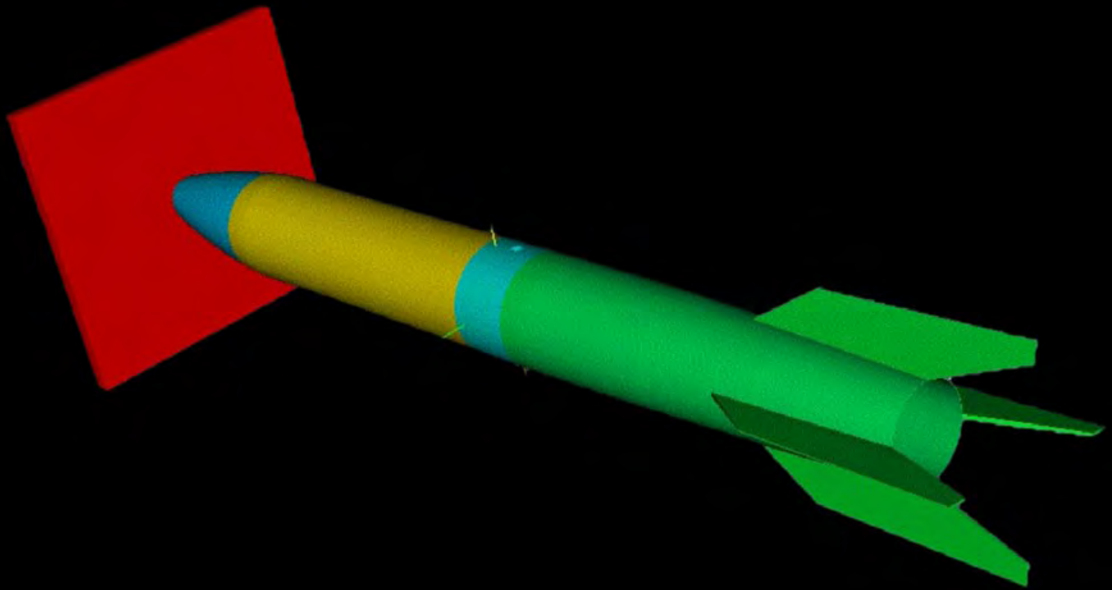
Front image: Calculation of a fire interacting with an object in a transportation container.



Presto and Adagio Codes Characterize Normal and Abnormal Mechanical Environments

This Sandia project provides reliable software to characterize normal and abnormal mechanical environments that arise from impact and accident scenarios by addressing the highly nonlinear coupling between the contact interactions, material failure, and the load path leading to eventual structural failure. To simulate impact and accident scenarios for characterizing the normal and abnormal mechanical environments, two mechanics codes, Presto and Adagio, are used. They can be coupled through SIERRA to provide a capability to simulate the static preloading of a structure (Adagio) followed by the response to a prescribed dynamic loading (Presto) in a single simulation. This capability can capture massive deformations and failure, and with scalability on massively parallel supercomputers, it is a unique and distinguishing capability—one that reinforces Sandia's leadership position for addressing complex problems of national interest. Presto and Adagio have contributed significantly to a number of programs, including the B61 ALT 357, W76-1, W80-1, and the SGT, in which high-speed crash scenarios are being investigated. Adding rational and defendable failure modeling capabilities and multiscale modeling abilities are a priority.

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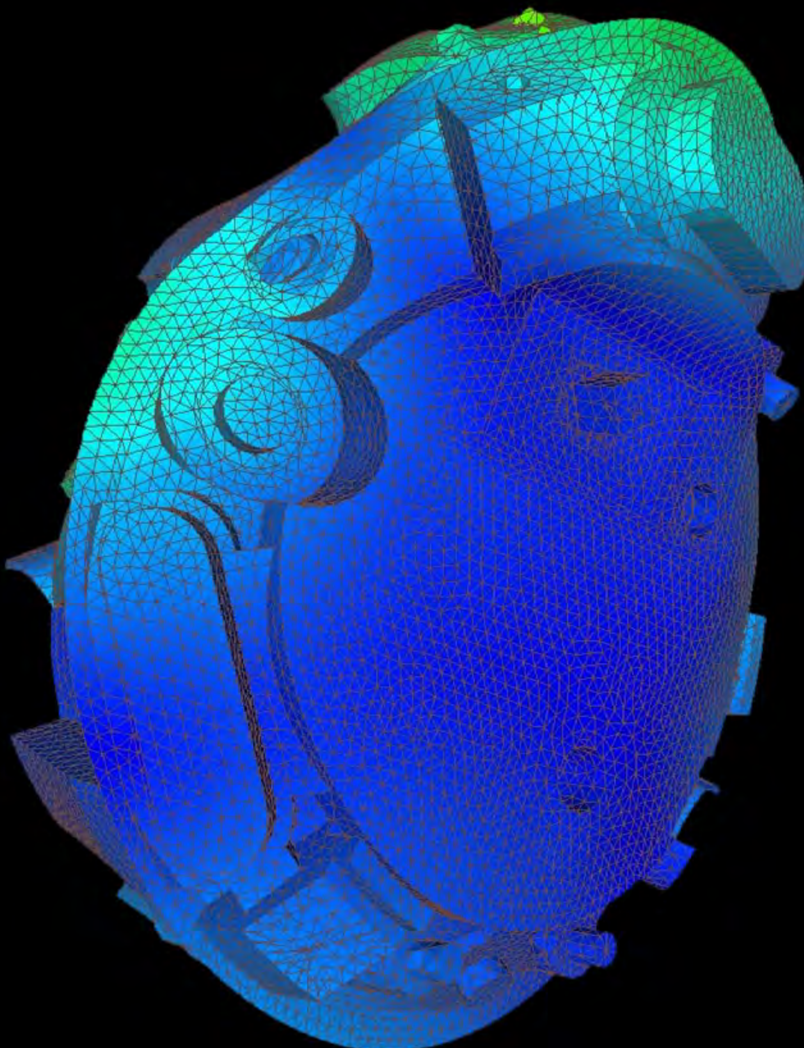
Front image: Computational model used for a Presto simulation of a B61-7 impact.

SAND 2006-6509P

Integrated Codes



Salinas Code Simulates Structural Response

During launch, reentry, and potential hostile nuclear countermeasures, a weapon system is subjected to tremendous mechanical and vibratory loads. The structural response to these loads and how loads applied to the exterior of the weapon are propagated to interior components must be understood. A significant constituent of predictive mechanical system modeling is the understanding of energy loss that occurs at joints and interfaces. The Salinas tool, in the SIERRA suite of codes, provides the capability to model the dynamics of these complex systems. Airborne noise may be very important during reentry, and recent additions to Salinas include nonlinear acoustics and structural mechanics in coupled models. To determine compliance with Stockpile-to-Target Sequence specifications, Salinas is used to study normal and hostile environments, including blast and impulse. Analyses on the W76-1 helped to steer early design architectures, and component-level specifications were developed based on them. All the functions required for the W76-1 will be required for the Reliable Replacement Warhead (RRW). These capabilities also need to be further generalized for microelectromechanical systems.

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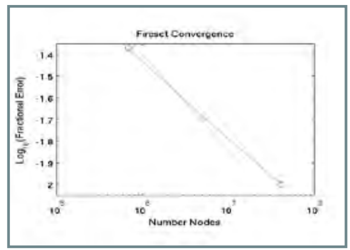
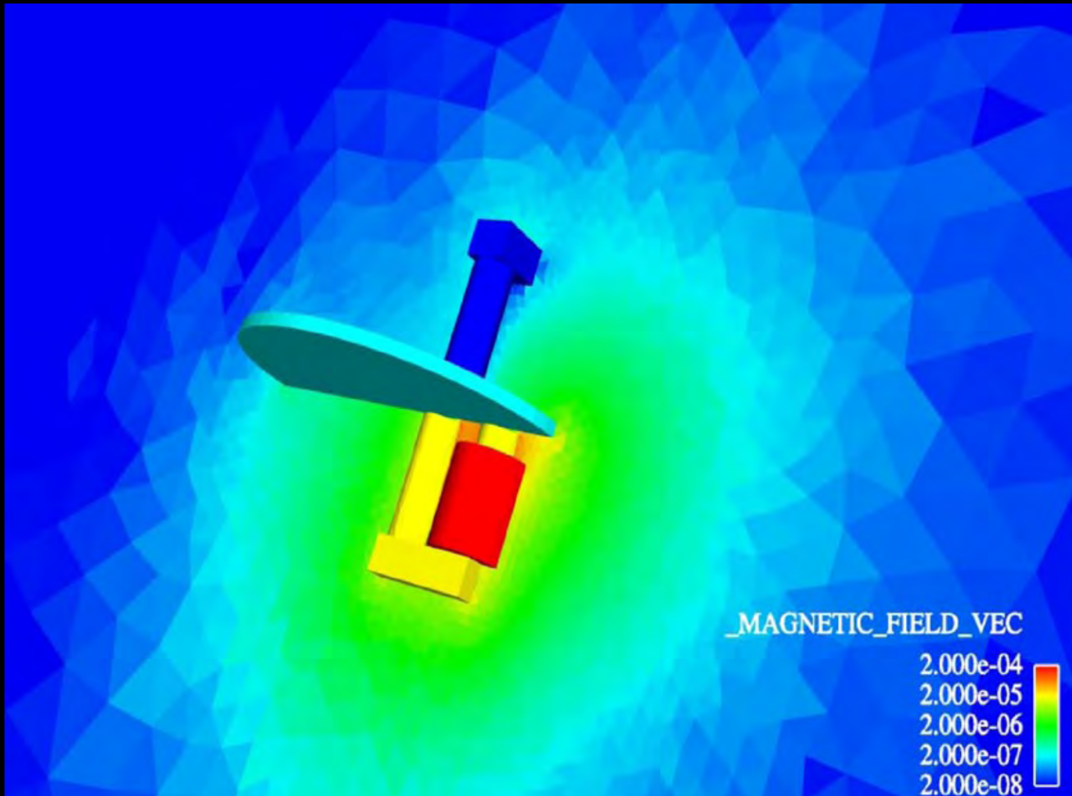


A verification and validation effort assesses predictive capabilities with complex models. As part of this work, and to determine the mesh adequacy required for predictive models, extensive mesh refinements have been performed. A coarse mesh of a portion of the model is shown (front) along with convergence information (back). The fine mesh has more than 130 million equations.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Integrated Codes

EMPHASIS Adresses SGEMP Simulations

Sandia's EMPHASIS code project is developing a set of general-purpose electromagnetic (EM) and plasma simulation capabilities for weapon-system applications. These applications include system response to cable, box, and cavity System Generated Electromagnetic Pulse (SGEMP), as well as modeling of the performance of weapon-system components. Component modeling and box-SGEMP response have challenging simulation issues because of geometric features that are very small compared to the wavelengths of the EM field, and several novel techniques have been developed to address these problems. EMPHASIS provides qualification evidence for box-SGEMP effects for the W76-1 life-extension program, where full-threat hostile environment testing is not possible. It will be used similarly in the Reliable Replacement Warhead (RRW) Program. EMPHASIS is also used to model crucial operational characteristics of safety components.

Intense x-ray environments produce SGEMP:

- The simplest of the SGEMP applications is cable-SGEMP, which is modeled using 2-D or 3-D periodic simulations coupled to radiation transport modules.
- The most difficult is cavity-SGEMP, which requires 3D-coupled EM, plasma and radiation transport.
- Box-SGEMP falls in between and is treated much like cable-SGEMP, but requires full 3-D modeling.

Component modeling with EMPHASIS addresses performance in a variety of different EM environments, including high-intensity radiofrequency fields and pulsed EM fields such as lightning.

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Front image: EMPHASIS simulation showing the magnitude of the magnetic field in a plane at one instance in time in a generic component with very small geometric features. The solid geometry of the component is overlaid and consists primarily of a conducting disk and magnetic materials. The component is energized by an electrical circuit.

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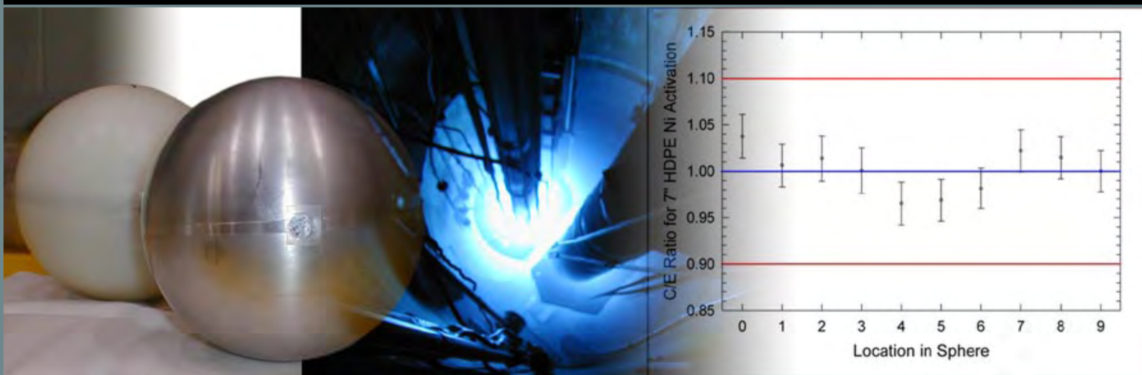

ASC

NuGET Enhances Radiation Modeling

The Neutron Gamma Energy Transport (NuGET) module of the RAMSES code models the neutron/gamma radiation environment in hostile and fratricide scenarios. Neutron/gamma radiation contours for component-level vulnerability modes can be generated, and the energy and time dependence of radiation environments can be modeled. NuGET has permitted Sandia to (1) improve the fidelity of component-level specification for internal components; (2) perform design trade-offs with calculations and save significant development and test costs; (3) select reactor test environments to support the qualification of DOE components; and (4) provide evidence to support the certification of DOE components to Stockpile-to-Target Sequence (STS) requirements. NuGET is an important link in the ASC series of codes that supports the certification of Sandia systems to radiation environments. The coherent environments provided by NuGET permit Sandia to be less conservative in the specification of experimental reactor test environments and in the development of damage/response matrix margins required to demonstrate compliance with the STS requirement. Development of a high-altitude uncontained fireball interface and the incorporation of features for debris electrons will be high future priorities.

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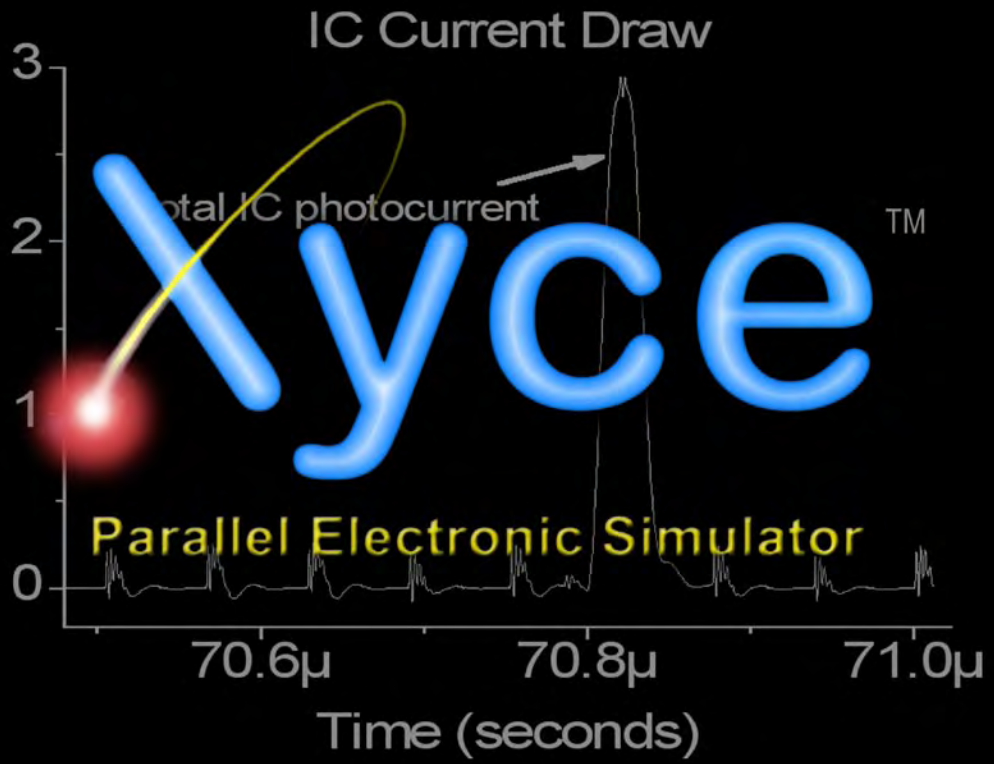
Front image: Various test items are used to validate the calculated radiation environment in reactor test environments. The center image shows Sandia's Annular Core Research Reactor with the central cavity. The left shows test spheres that contain many internal sensors used for validation. The right figure shows the calculated-to-measured agreement for the sensors as a function of their radial position within an aluminum test sphere. The red bounding lines indicate the RAMSES/NuGET acceptance metric, the central blue line indicates the position corresponding to complete agreement, while the ratios for the C/E values are given with associated uncertainty.


IC Current Draw
3
2
1
0
otal IC photocurrent
Xyce™
Parallel Electronic Simulator
70.6µ
70.8µ
71.0µ
Time (seconds)

Xyce™ Transforms Circuit Modeling

Dedicated to circuit simulation analysis, Xyce™ breaks the traditional approach to circuit modeling. Xyce™ code regularly models large-scale integrated electrical systems, including digital circuits, at the analog (transistor) level to credibly predict performance under a wide range of operating conditions and environments, including harsh environments associated with temperature extremes as well as prompt radiation effects. The unique capabilities of Xyce™ have been effectively used by the W76-1 Arming and Fuzing System team and the Qualification Alternatives to the Sandia Pulsed Reactor (QASPR), and by Sandia's Integrated Stockpile Evaluation (ISE) Program. Xyce™ continues to add new capabilities. These include advanced solution algorithms, world-leading device models, seamless integration of the DAKOTA suite within Xyce™, and the inclusion of microelectromechanical (MEMS) compact models to support larger integrated system-level simulations of electromechanical designs. Xyce™ plans call for a much broader set of capabilities to continue to meet Sandia's missions and help transform the design and qualification processes. For the B61 Alt, Xyce™ will add radiofrequency circuit analysis capabilites to support the tight time schedules needed to design and qualify new systems and subsystems.

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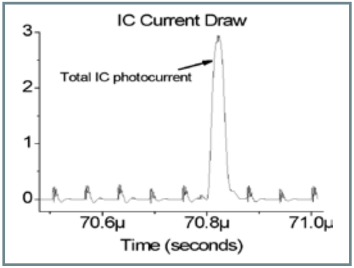
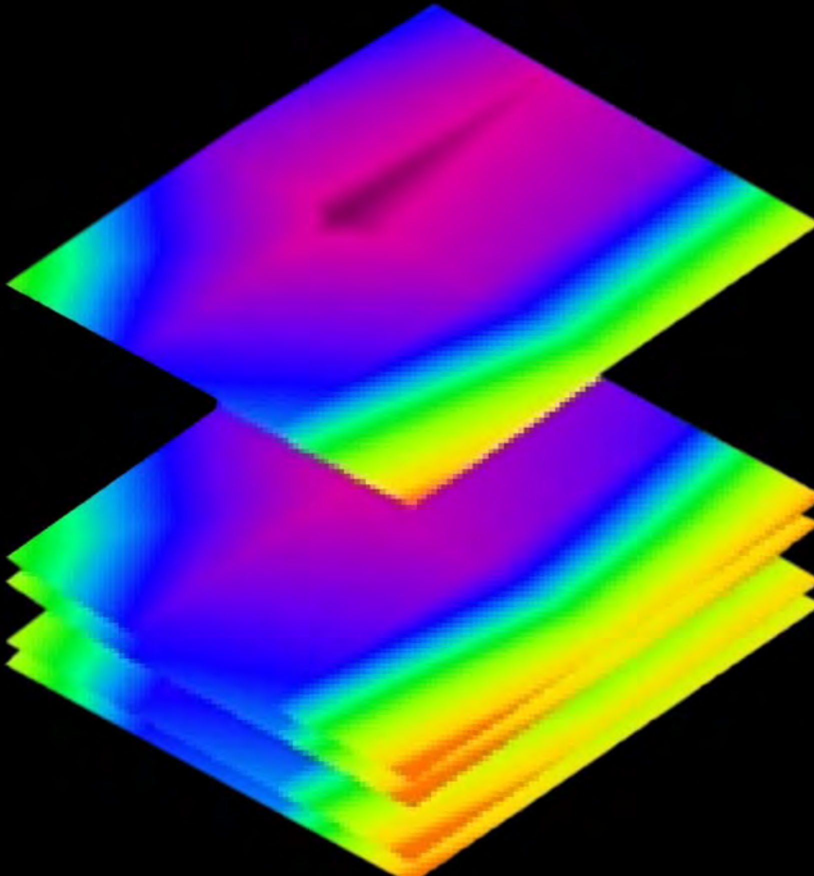


Predicted Integrated Circuit Current Draw under radiation conditions. This was the first time designers had a tool to predict performance response in an x-ray environment.

Integrated Codes



ITS and CEPTRE Codes Aid Weapons Design

The Integrated Tiger Series (ITS) and the Coupled Electron Photon Transport for Radiation Effects (CEPTRE) modules of the RAMSES code suite are used at Sandia to simulate the penetration and production of x-rays and electrons inside weapon systems from the radiation of hostile nuclear encounters and space environments. Calculations performed with these codes ensure that weapon components are designed to meet Stockpile-to-Target Sequence, hostile-radiation requirements. These radiation transport code modules can model the complex detail inherent in engineering CAD models and as-built geometries of weapon systems. The ITS code module of RAMSES has been used to predict dose and dose-rate levels in the W76-1 Arming, Fuzing, and Firing system and dose in the replacement neutron generator of the W78 to aid in qualification efforts of these components. The CEPTRE code has been used to predict charge deposition in cables in support of W76-1 qualification. Together, ITS and CEPTRE provide the initial conditions necessary for other ASC codes to support the qualification of Sandia systems and components to radiation environments. Improvements will target the evolving microelectronics and microelectromechanical systems technologies.

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Front image: Dose levels on circuit boards from hostile x-rays predicted with the ITS code module.

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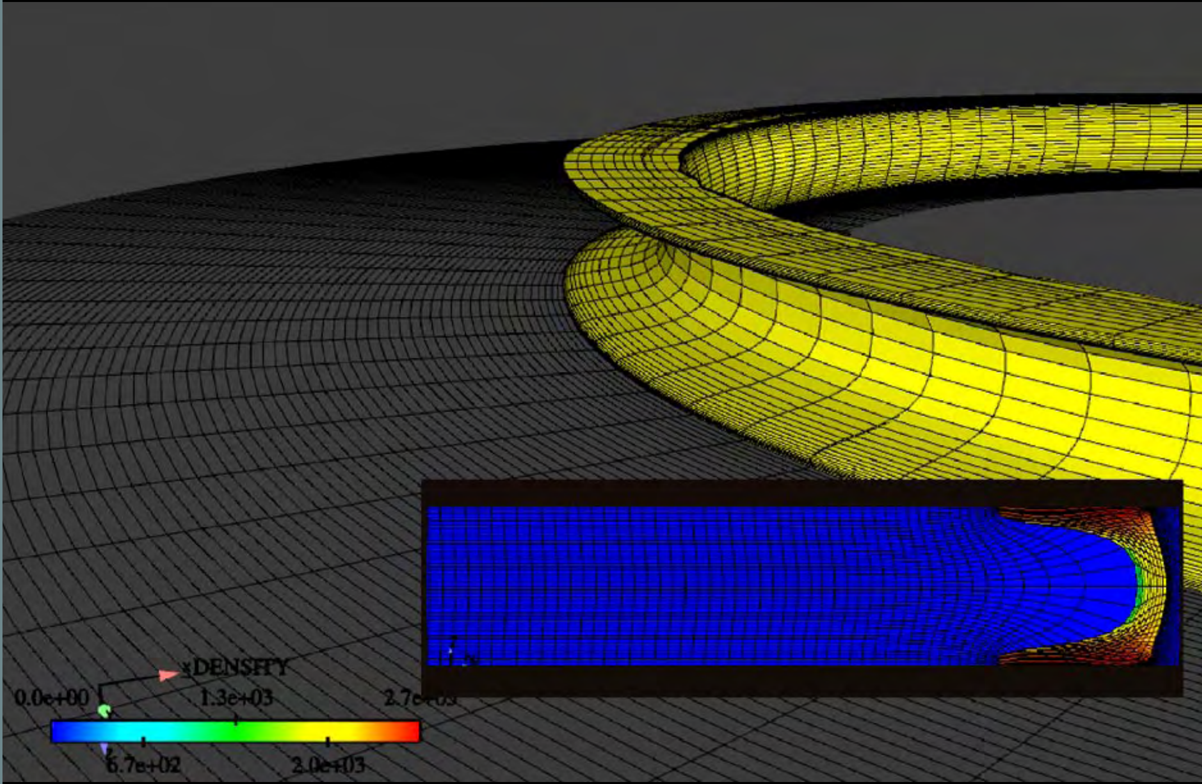

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ALEGRA-HEDP Code Suite Simulates HEDP Enviromnents

The Z machine, a pulsed-power capability within Sandia's High Energy Density Physics (HEDP) Program, is used for validating ASC codes, certifying the survivability of non-nuclear weapons components, and dealing with issues related to Significant Finding Investigations. The HEDP Program primarily contributes to science campaigns, including dynamic materials, secondary certification, nuclear survivability, and high-yield fusion. The long-term mission of developing a pulsed-power high-yield fusion capability also contributes to a growing national interest in inertial fusion energy. ASC has partnered with the HEDP Program in the development of ALEGRA-HEDP, a numerical modeling capability to simulate HEDP environments that solve resistive magnetohydrodynamics equations coupled with thermal conduction, radiation transport, two-temperature ion/electron physics, and an external circuit model. ALEGRA-HEDP contributes to the Stockpile Stewardship Program (SSP) through the design, fielding, and analysis of experiments in support of the dynamic materials program on the Z machine. ALEGRA-HEDP also contributes to the SSP through simulations of HEDP x-ray environments.

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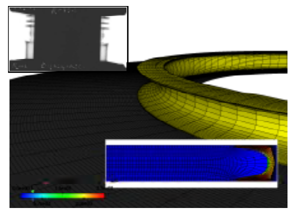

Three-dimensional ALEGRA-HEDP simulation utilizing Lagrangian boundaries and MESQUITE mesh smoothing during the ALE remesh step. Pegasus liner implosion experiments (LANL) are used to validate the technique (upper left radiograph), which previously was cost-prohibitive using a fully Eulerian simulation.

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The Computer Science Research Institute Enables Research Collaborations

Sandia's Computer Science Research Institute (CSRI) brings together researchers from universities and the national laboratories in an exciting and dynamic environment to address research problems in computer science, computational science, and mathematics and to develop new capabilities in modeling and simulation. Over the last two years, the CSRI has hosted more than 200 short-term visitors and more than 60 long-term visitors including summer faculty, sabbaticals, and student internships. These participants represented over 100 institutions, and participants are encouraged to develop long-term collaborative relationships with laboratory scientists and researchers. The CSRI is located in a new state-of-the-art facility immediately outside the Sandia security perimeter within the Sandia Science and Technology Research Park. CSRI sponsors collaborative research in a wide-range of technical areas including the following:

Computer Science - Next generation architectures; data-intensive computing; environments for scalable computing; parallel, scalable I/O; quantum computing.

Mathematics and Algorithms - Scalable solvers; optimization; multiscale methods; adaptivity and mesh refinement; solution of differential and integral equations; graph-based, discrete and combinatorial algorithms; uncertainty estimation and verification and validation.

Enabling Technologies - Mesh generation; data analysis and visualization.

The CSRI presents many opportunities for collaborations between university researchers and laboratory scientists.

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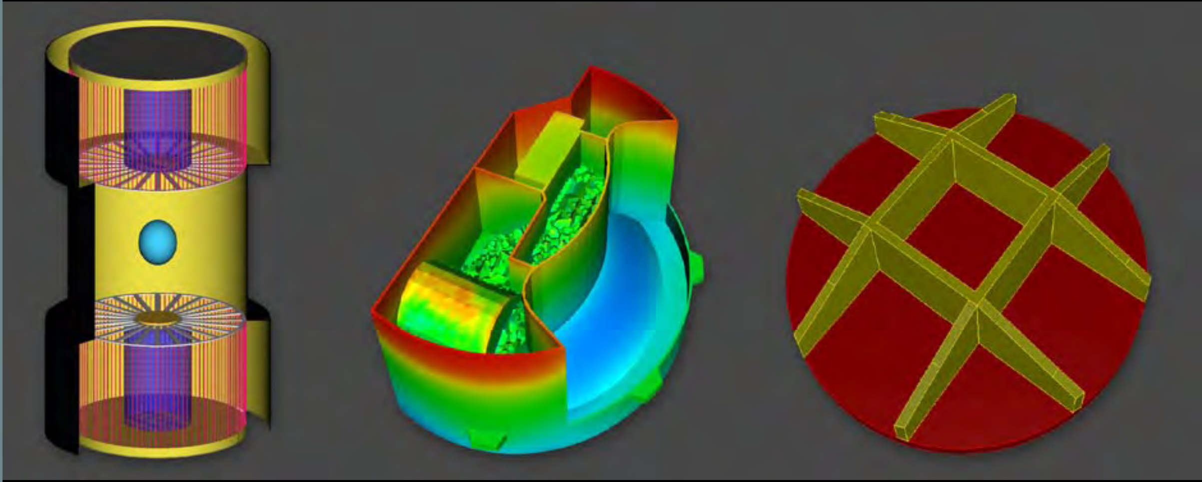

Examples of DAKOTA applications; (from left) IFC Capsule Robust Design, Fireset Thermal Surety, and Radar Support Structural Design.

DAKOTA Optimizes Applications

Design Analysis Kit for Optimization and Terascale Applications (DAKOTA) is a general-purpose software toolkit for performing systems analysis and design on high-performance computers. Sandia released DAKOTA, version 4.0, in FY06. DAKOTA is widely used within the Department of Energy, particularly for studies with ASC application codes at Sandia, Los Alamos, and Lawrence Livermore. As an open-source software framework, DAKOTA is also used in the broader community. DAKOTA provides a flexible and extensible interface between iterative systems-analysis capabilities and a broad variety of simulation codes used in the Stockpile Stewardship Program (SSP), including structural mechanics, heat transfer, fluid dynamics, shock physics, and many others. DAKOTA contributes to the SSP by providing algorithms for design optimization with gradient-based and nongradient-based methods; uncertainty quantification with sampling, reliability, and polynomial chaos methods; parameter estimation with nonlinear least squares methods; and sensitivity/variance analysis with design of experiments and parameter study capabilities. These capabilities may be used on their own or as building blocks within advanced strategies such as surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty. The DAKOTA simulation tools can be an enormous aid in understanding the complex physical systems they simulate.

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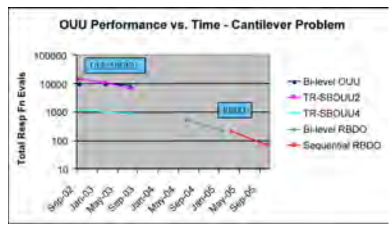
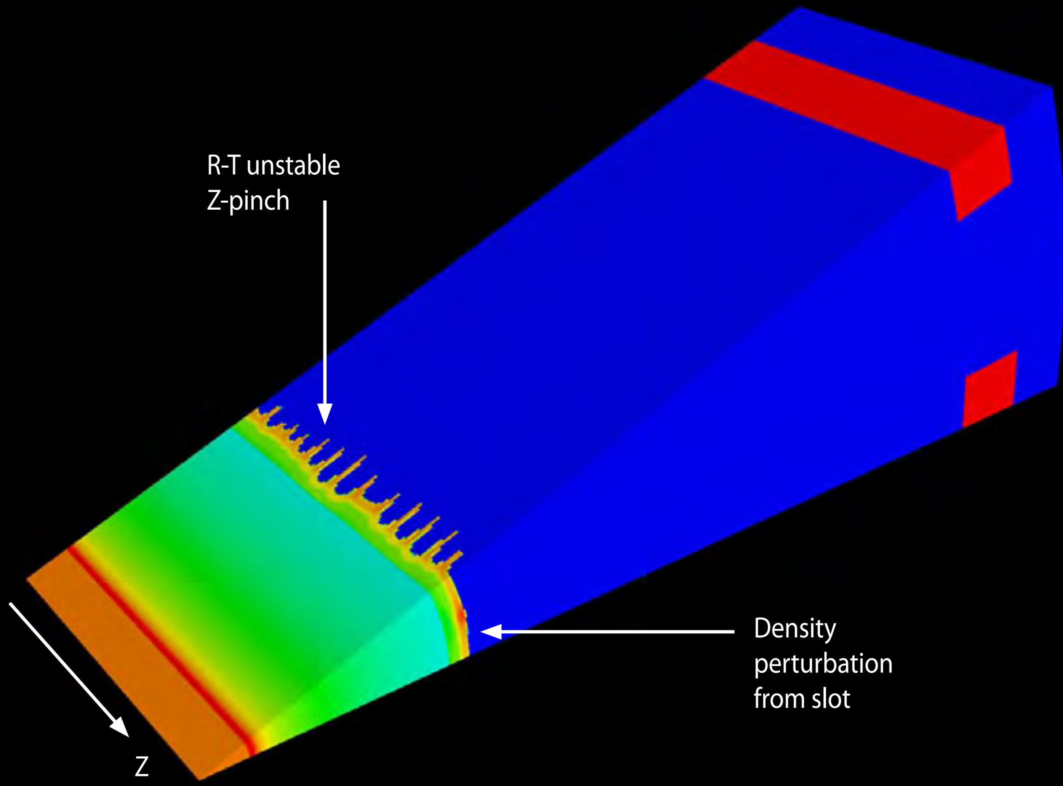


Progress in the efficiency of DAKOTA's optimization under uncertainty (OUU) algorithms over time. Relative to a standard nested approach to OUU, trust-region surrogate-based optimization under uncertainty (TR-SBOUU) algorithms reduced expense by two orders of magnitude.


R-T unstable
Z-pinch
Density
perturbation
from slot
Z

Trilinos Solver Excels at Parallel Solver Algorithms

Many of Sandia's scientific and engineering applications for computer modeling and simulation require the solution of large systems of equations. In many instances, an application's fidelity and efficiency are directly determined by how effectively the solvers work. The Trilinos project is an effort to develop and implement robust parallel solver algorithms using modern object-oriented software design and software engineering processes and tools, while still leveraging the value of established numerical libraries. Trilinos is now the largest single collection of solver capabilities and is expected to grow in the coming years. Trilinos has won several awards, including an R&D 100 award as one of the 100 best new products of 2004, and Trilinos is increasingly the preferred solver software framework for hundreds of application and solver developers throughout the world. At Sandia, Trilinos is the primary solver framework for all major applications including the SIERRA and NEVADA frameworks for computational mechanics and the Xyce™ framework for electrical modeling and simulation. Trilinos capabilities have enabled first-of-a-kind computations in numerous key problem areas for both defense and industrial problems. Continued work on solvers is extremely important for enabling new modeling and simulation capabilities.

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Front image: This visual depicts 1/18th (20 degree) periodic wedge simulation in 3-D of z-pinch liner implosion. Colors represent density. First-of-a-kind results in fidelity. Trilinos/ML's H(curl) multigrid magnetics solver is only viable solution method.

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ASAP Promotes Collaboration with Universities

In 1997, the ASC Program initiated the Academic Strategic Alliance Program (ASAP) by creating long-term strategic alliances with five U.S. universities (the Centers) to focus on high-fidelity, scalable, three-dimensional, multidisciplinary computational science problems. Sandia has been an active participant in this program. A multidisciplinary approach is essential to each Center's success because of the complexity of the problems requires integrating shared knowledge, computer codes, supporting infrastructure, and information across many areas of research. Although the ASAP computing problems do not involve nuclear weapons research, the computational science, computer science, and computational mathematics methodologies and tools developed provide benefits to the DOE Stockpile Stewardship Program, as well as to other national scientific, economic, and social needs. A major reason that the Centers were created was to demonstrate the power of verified and validated simulation, and tackling the issues surrounding verification and validation requires the Centers to develop new approaches to problems and possibly to expand their research in unexpected directions. The strategic focus of ASC and ASAP has currently shifted to improving the confidence in scientific and engineering prediction through simulations.

ASAP Centers

- Caltech Center for Simulating the Dynamic Response of Materials
- Stanford Center for Integrated Turbulence
- Center for Astrophysical Thermonuclear Flashes at the University of Chicago (FLASH Center)
- Center for Simulation of Advanced Rockets at the University of Illinois, Urbana/Champaign
- Center for the Simulation of Accidental Fires & Explosions (C-SAFE) at the University of Utah

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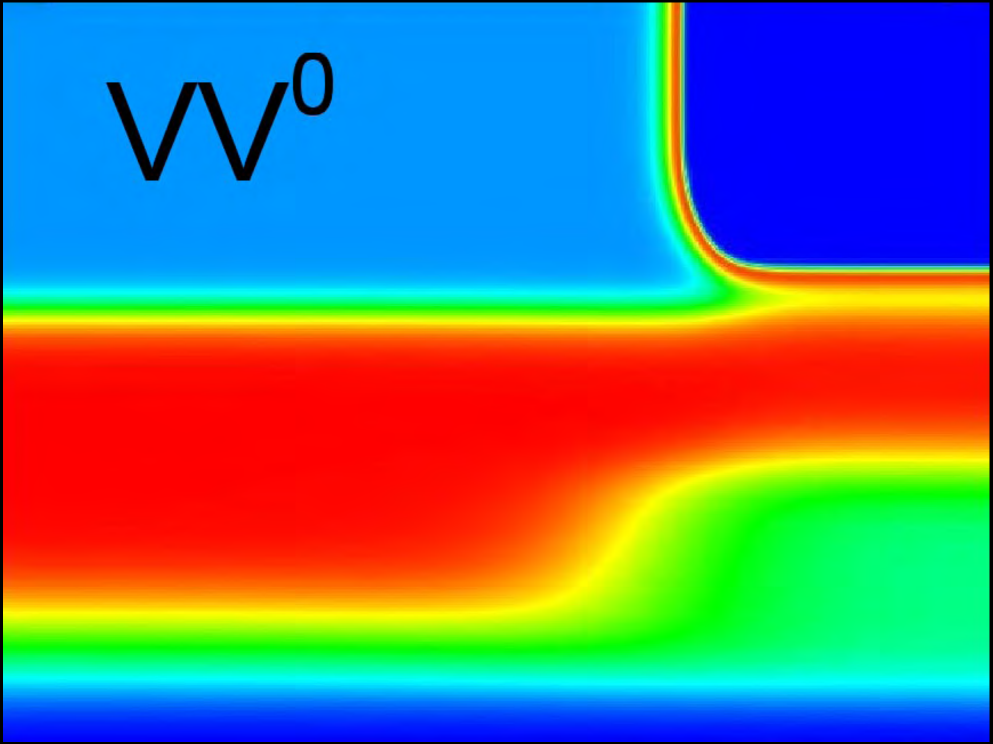
Front image: Chicago – Image of the flow in a column of sulfur hexafluoride 825 microseconds after the passage of a Mach 1.2 shock wave through it.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QASPAR Provides New Approach to Qualification of Weapon Systems

For security reasons, Sandia is developing a new approach to qualifying nuclear weapons systems without the use of the Sandia Pulsed Reactor (SPR). The Qualification Alternatives to the Sandia Pulsed Reactor (QASPR) is a major focus within Sandia's nuclear weapons program. It is a prime example of the utilization of radiation-hardening technologies, experimental tools, and validated models to support the design, qualification, and surveillance of nuclear weapons. The project has been undertaken to mitigate the reliance on high-fidelity sources of short-pulse neutrons utilizing special nuclear materials. Sandia will collect data at other facilities to supplement data from the SPR, to create and validate models describing the damage creation and annealing behavior, and to determine a best estimate with uncertainty for the response of the simple and complex prototype circuits irradiated in SPR. We will characterize the irradiation conditions at the radiation facilities and understand and model damage mechanisms at these facilities as the basis for damage equivalency determination within QASPR. The ASC work spans from the creation and exercise of new atomistic models to circuit-level simulation with quantified uncertainty. This approach will afford the Stockpile Stewardship Program a new tool to assess the performance of systems in abnormal environments and, for the first time, with quantified uncertainty.

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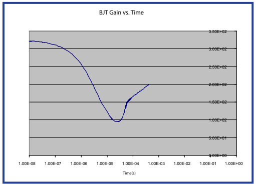
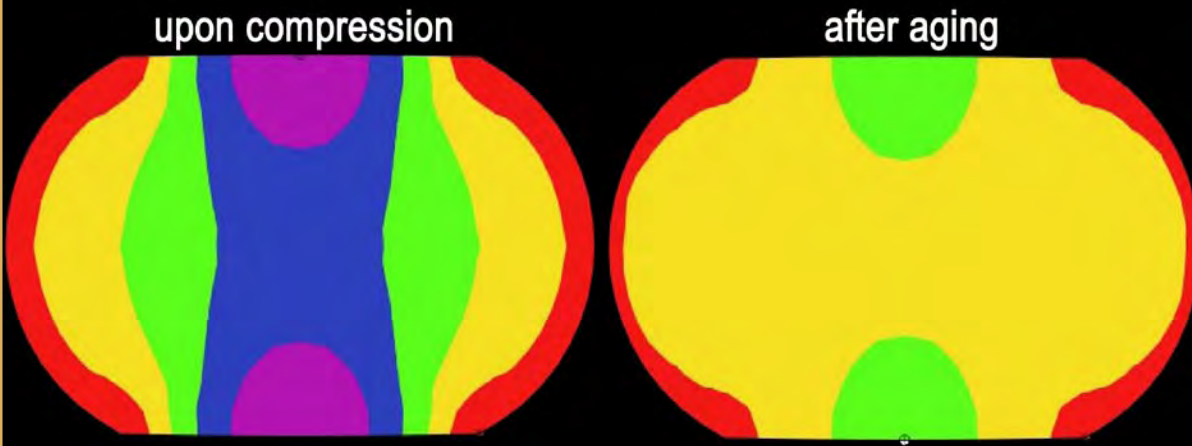


Front: Density profile of Si neutral divacancies in a 2-D model of a SiBJT.
Above: Variation of device gain following irradiation by a 50 ms neutron pulse with total dose of $3x10^{15}/cm^3$ simulated with the Charon code using more than 30 defect species and nearly 100 defect reactions.


upon compression
after aging

Understanding the Aging of Materials

Rubber is often used as a physical barrier to protect delicate components from oxygen, moisture, and other environmental contaminants. The goal of this project at Sandia is to develop a constitutive model to predict the loss of sealing force during chemical aging. The model also predicts permanent set, which is correlated with loss of sealing force and is more easily measured during field aging. Permanent set quantifies recovery toward original shape upon release of strain. A permanent set of 0% is complete return to original dimensions. A permanent set of 100% indicates remaining at the strained dimensions. Few rubber models are specifically designed to predict permanent set, so this is a novel effort. This model incorporates the effect of the coupling of strain and chemical reaction histories on the stress, and the multiscale nature of the problem complicates this task. Rubber seals and O-rings are used throughout the stockpile to protect delicate components against damage from moisture and other contaminants. Reliable predictions of the usable lifetime for these rubber items will help prevent inadvertent seal failure while allowing maximum time in service. The simulations will help elucidate reactions during aging, and the experiments will ensure that the model is validated for the new formulation.

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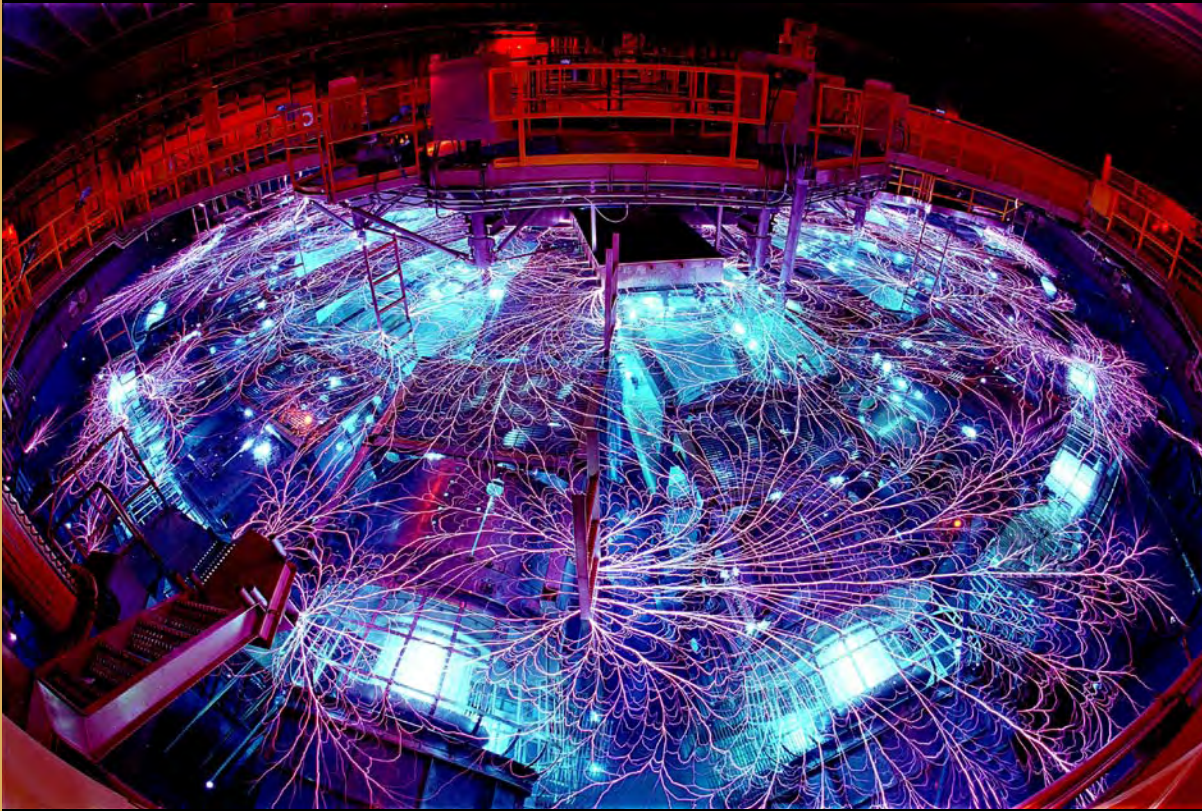
Front image: Illustration of O-ring under compression.
Left: Stress from the original network. Keeping the O-ring compressed during chemical aging results in scission of the original network and crosslinking of a second network. Right: O-ring after complete scission of the original network.



Sandia's Z machine

Understanding Melt Properties of Materials

The melt properties of materials under high pressure are generally poorly understood, but they are often of great significance to Sandia's high-energy-density physics programs. Certain materials, such as beryllium and diamond, have received much interest recently because of their potential role in ablator materials in inertial fusion capsules. The properties of materials under high pressure are of considerable interest to the stockpile stewardship programs. Of particular interest is the shock pressure at which proposed ablator materials such as beryllium melt under intense x-ray radiation pulses. Sandia conducted a computational study of the shock melting of beryllium using quantum molecular dynamics (QMD) to obtain the high-pressure melt curve, the shock Hugoniot, the liquid-metal coexistence region, and the bulk and longitudinal sound speeds. This project began just before beryllium shock-melting experiments on Sandia's Z machine, and results from the calculations were used to optimize the experimental search for the onset of melt.

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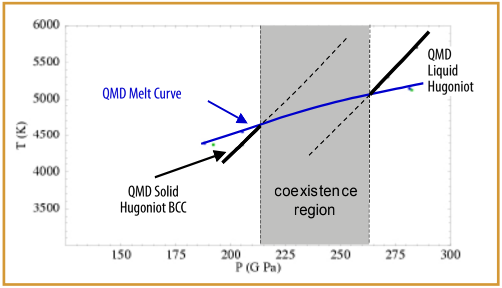
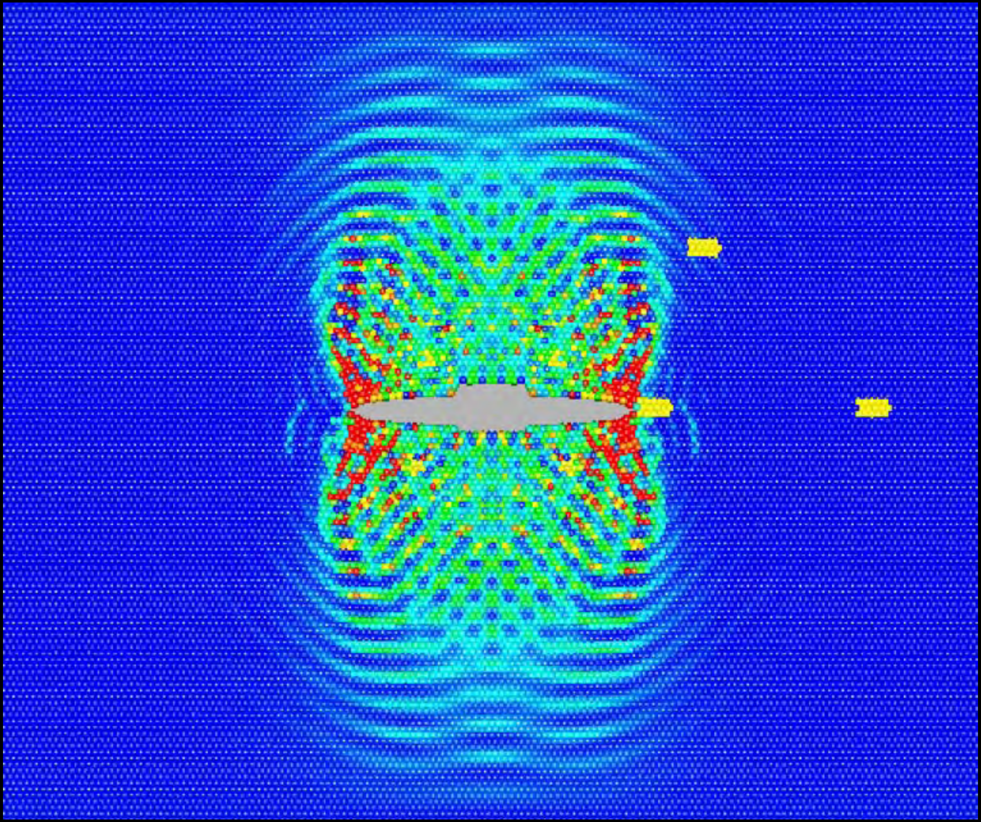


The calculated melt curve of beryllium (blue) at high pressure is shown as the melt temperature in Kelvins as a function of pressure in gigapascals (GPa). Also shown are the shock Hugoniot curves for solid beryllium (here in the BCC phase) below the melt curve and liquid beryllium above the melt curve (both in black). The coexistence region denotes the mixed phase region comprised of both solid and liquid phases.



Results of MD simulation of crack propagation.

Modeling Crack Initiation and Propagation

This project at Sandia provides a capability to model crack initiation and propagation in a ductile metal. Although both quasistatic and transient dynamics capabilities are being developed, the emphasis is on quasistatic behavior. In transient dynamics, inertia terms tend to dominate the solution. This makes the problem much simpler to solve, but also makes it much harder to evaluate subtleties of the crack-propagation process. While some limited-scope failure capabilities exist, a general-purpose, practical capability to model ductile crack initiation and propagation in a full-feature, finite element program in three dimensions for both quasistatic and transient dynamic loading rates will be unique. The preliminary capability developed has been used to model ductile failure in instances such as the B61 case tear during lay-down deployment, and more recently to help the redesign effort associated with the thermal pressurization of the W76 exclusion-region barrier.

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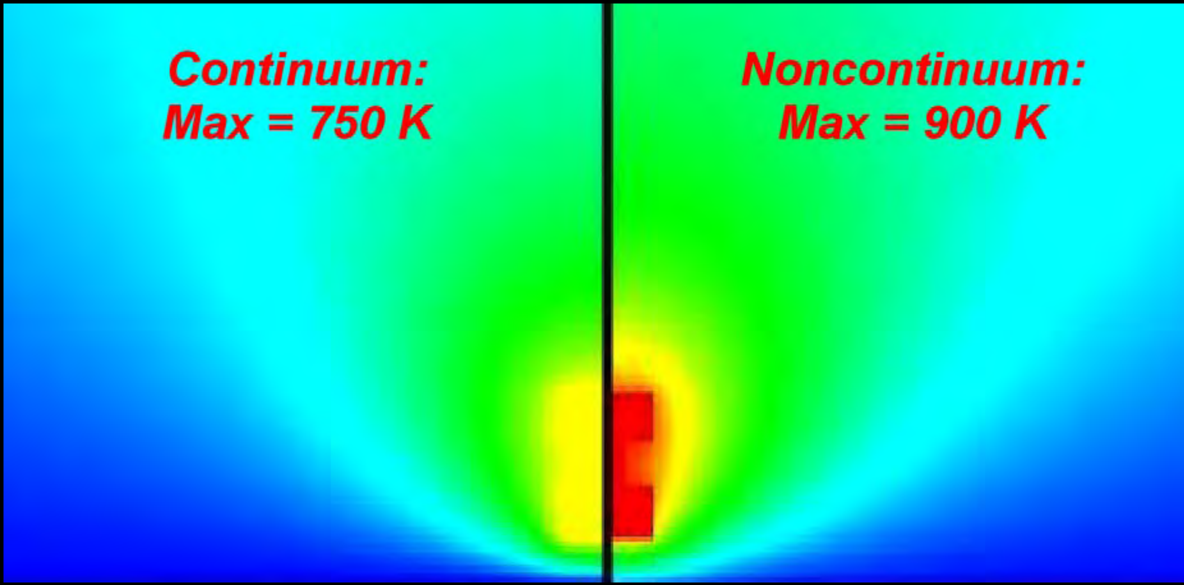
Predicting failure pressure and location as a function of temperature at the exclusion region barrier.


Continuum:
Max = 750 K
Noncontinuum:
Max = 900 K

Modeling Gas Damping and Heat Transport in MEMS

The microscopic scale of microelectromechanical systems (MEMS) devices presents new challenges to designers. In particular, as device length scales decrease into the microscopic domain, the continuum approximations typically used to model gas and solid heat transport and gas damping begin to break down. Sandia's new noncontinuum models will provide designers with the ASC simulation tools to predict gas stresses on moving parts or to manage thermal loads in this new class of devices. The compact models developed have been implemented in the continuum, finite-element code Calore and have been demonstrated to provide reliable simulations of microscale heat transfer in thermal actuators. Microscale devices are being considered for a broad set of future weapon-subsystem applications, including a variety of sensors and surety devices. Reliable, efficient computational tools are needed to provide designers with the predictive capability to design the next-generation MEMS parts that will play a key role in the future stockpile. The fundamental investigation of noncontinuum gas transport has earned Sandia a strong reputation in the Direct Simulation Monte Carlo technique modeling and rarefied-gas research communities.

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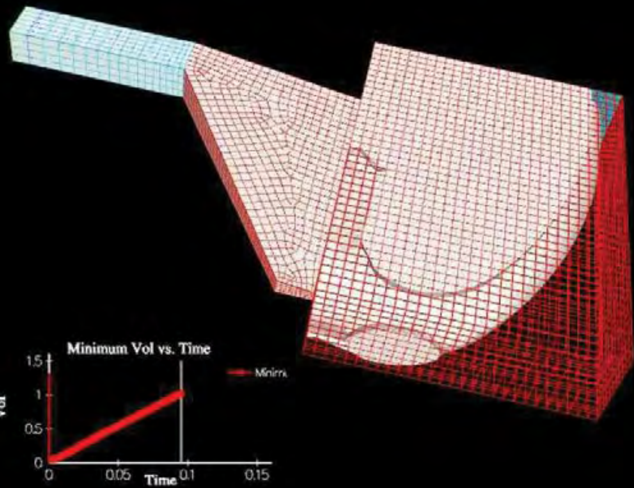
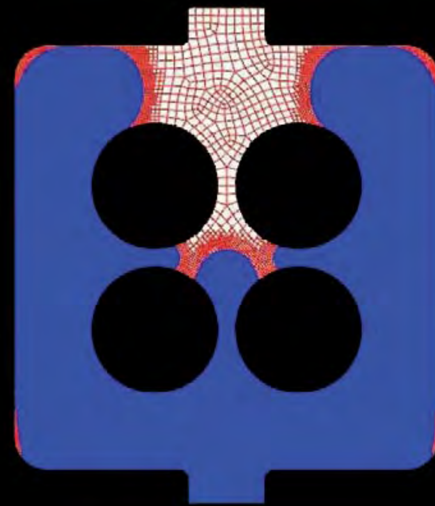
Front image: Calore calculations of temperature profiles for a heated microbeam separated from a room-temperature surface by a 2-micron air gap at ambient pressure.

Physics and Engineering Models





Engineering Sciences Research Foundation Encourages University Collaborations

This National Science Foundation (NSF)-leveraged Engineering Sciences for Modeling and Simulation Based Life-Cycle Engineering and Manufacturing Program creates direct collaborations and relationships between Sandia technical staff and the best university researchers in areas of critical importance to the Stockpile Stewardship Program. The objective is to fund research projects focused on science-based experimental, computational, and theoretical capabilities that enhance understanding of, and confidence in, the behavior of engineered systems at unprecedented multiple spatial and temporal scales. Sandia and the NSF evaluate proposals through the NSF review process, with rigorous peer review, and fund approximately 15 university projects for three-year durations. Research from previously funded work has provided insight into the behavior of microswitches, developed fundamental understanding of nonlinear structural joints, and provided innovative concepts to dramatically accelerate simulations of noncontinuum flows, among many others. Funded activities are always forward looking and are intended to provide technologies and capabilities to support future Defense Program needs in surety, safety, performance, and manufacturing.

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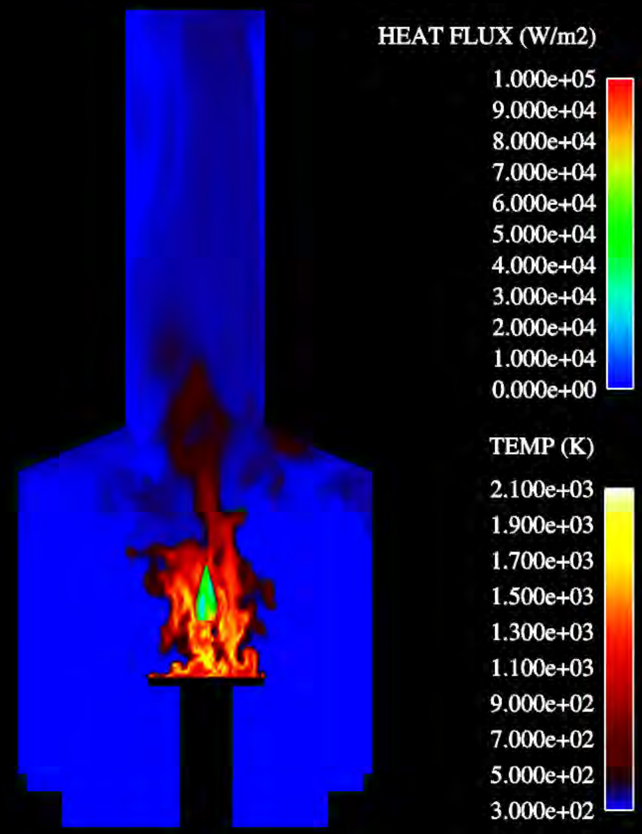
Front image: Mold Filling Application for laser welding, brazing, and encapsulation.


HEAT FLUX (W/m2)
1.000e+05
9.000e+04
8.000e+04
7.000e+04
6.000e+04
5.000e+04
4.000e+04
3.000e+04
2.000e+04
1.000e+04
0.000e+00
TEMP (K)
2.100e+03
1.900e+03
1.700e+03
1.500e+03
1.300e+03
1.100e+03
9.000e+02
7.000e+02
5.000e+02
3.000e+02

Validating Weapon Response Predictions in a Hydrocarbon Fuel Fire

Sandia validated coupled fire/thermal response predictions for a weapon-like calorimeter for a quiescent fire representative of a transportation accident scenario. Fire model predictions of heat flux from FUEGO were coupled with thermal response model predictions from CALORE to predict the transient internal temperature distribution of an object subjected to a fire as needed for determining weapon response. Three-dimensional, transient calculations were performed for fire conditions and object locations and compared with experimental data obtained in the FLAME facility. This was the first time that validation of the complete system (fire environment through thermal analysis) was performed for abnormal thermal environment qualification. W76-1 qualification tests will begin in the near term.

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Front image: Slice of a calculation of a weapon-like calorimeter in a fire. Fire temperatures (K) and heat flux (W/m^2) values on the calorimeter surface are displayed.

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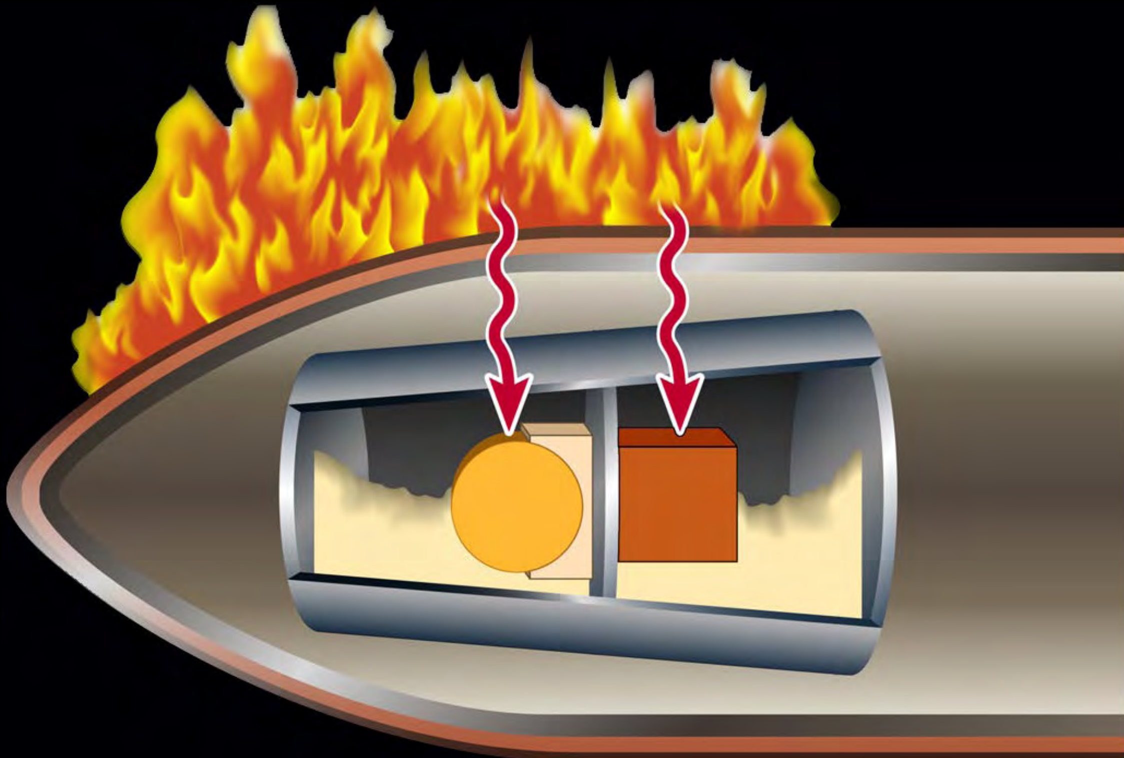
Validation and Verification



ASC™

Determining Weapon Safety

Sandia has developed new tools and procedures and integrated them with other tools to assemble a functional capability for quantifying margins and uncertainty (QMU) analysis that has enabled rational assessment of weapon safety in abnormal-thermal environments. An advanced approach to QMU applied to thermal stronglink/weaklink response in the W76-1 and W80-3 weapon systems has been demonstrated. If the stronglink does not maintain its normal operation at least until the weaklink is rendered inoperable (fails), then a Loss Of Assured Safety (LOAS) condition exists. Since the safety system is then indeterminate and can no longer positively insure against inadvertent detonation, it is considered to fail from a nuclear safety standpoint. Sandia's QMU analysis process attempts to quantify the largest margin of error in the models that can exist and still allow a positive assertion that the weapon qualifies to the safety requirement.

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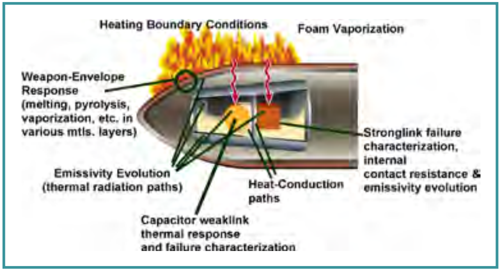
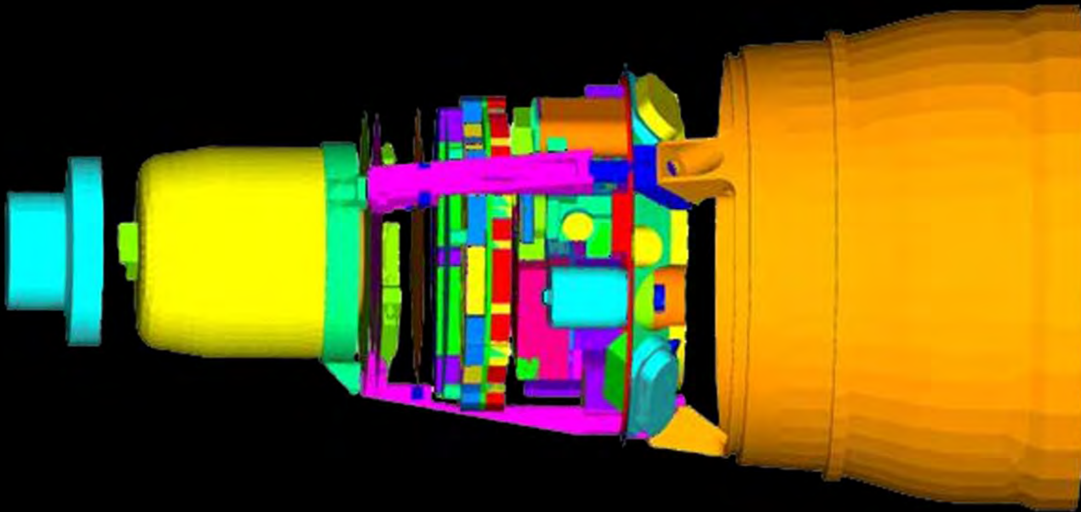


Important elements in Probability of Loss of Assured Safety (PLOAS) analysis of a simple stronglink/weaklink safety subsystem in a heating event.



Validating the W76-1

Validating Weapon Response Predictions

Sandia has developed a validation process for determining adequacy of arming, fuzing, and firing system (AF&F) response predictions in a full-system blast test for the W76-1, delivering advanced ASC physics and engineering simulation capabilities to support the W76-1 and W80 life extension/certification programs. The structural dynamics model of the W76-1 is complex and highly coupled. Tools and methods developed earlier provided valuable insight regarding model uncertainties and sensitivities. Current structural dynamics models are limited in capturing nonlinear response characteristics of systems under certain high-amplitude loading conditions. Sandia focused on inserting more refined constitutive models into a system-level structural dynamics model to provide more predictive modeling and simulation capabilities. The Sandia-developed, ASC structural dynamics simulation code, Salinas, was used with key nonlinear modeling features in a first-time system-level implementation. These simulations provided input to the Uncertainty Quantification (UQ) and sensitivity studies and were a credible framework for predictive system-level structural dynamics models.

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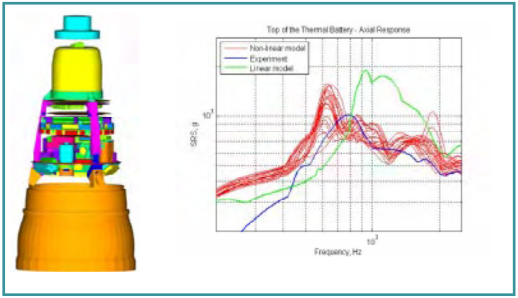
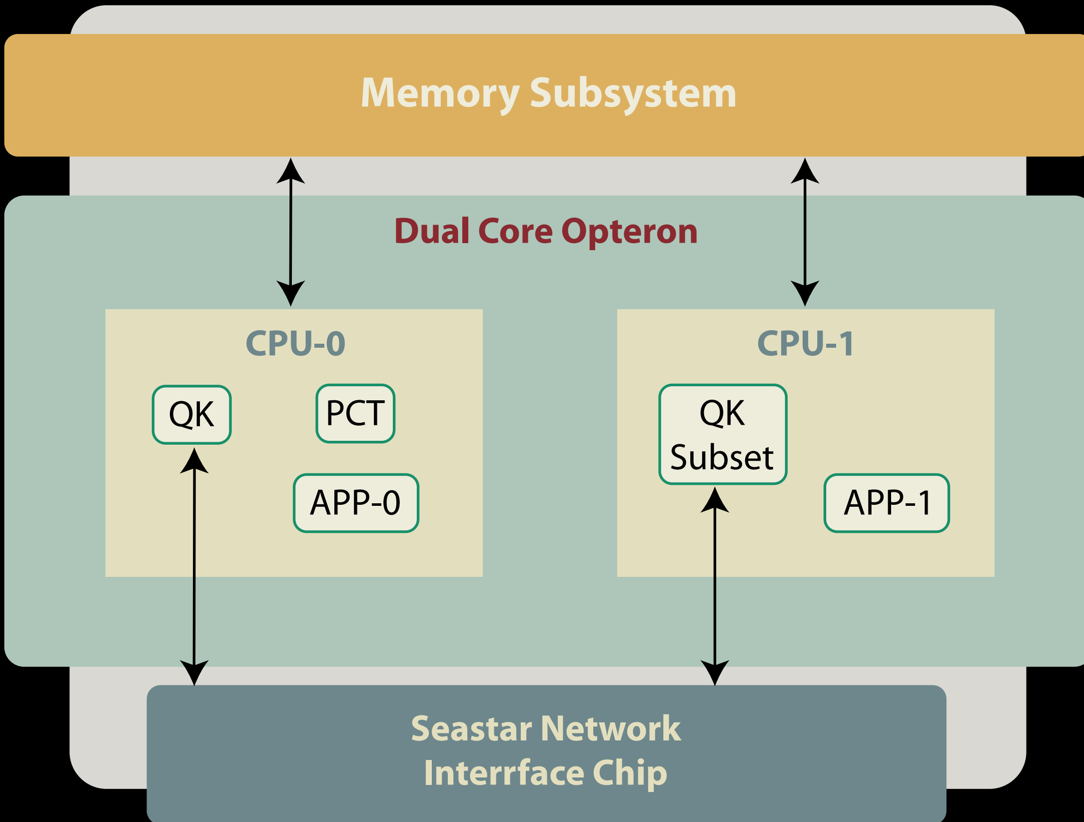


Improvements in hostile blast response predictions with addition of model physics.



Each CPU can run the application independently

Software Upgrades Maximize Red Storm Capability

Red Storm is a massively parallel processor computer system developed jointly by Sandia and Cray, Inc., for NNSA's ASC Program. The software architecture is based on one that Sandia has used successfully: node specialization. A small number of processors run Linux and provide services to the compute processors, which run a lightweight kernel (LWK) operating system called Catamount. There have been recent advances in commodity processors to support two central processing units in each processor socket. Red Storm processors can be swapped out, effectively doubling the raw processing power of the machine. No other hardware upgrades to the machine are required. The Catamount LWK operating system has been enhanced to make high-effective use of these new dual-core processors. The Catamount implementation to use both processors on a socket is called virtual node mode. Another enhancement to the Red Storm system software addresses the potential performance loss caused by the reduced network access per process. With these upgrades, ASC and Sandia have a valuable asset from which to solve important national security problems.

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Computational Systems and Software Environment

Red Storm

Red Storm Joins the Sandia Team

Red Storm is Sandia's newest NNSA/ASC capability computing platform. Developed through a partnership between Sandia and Cray, Inc., it is based on the successful ASCI Red architecture, with improvements that follow technology curves. In particular, Red Storm uses commodity AMD Opteron processors, a custom interconnect, a lightweight kernel on compute nodes, Linux on service and I/O nodes, and the Lustre file system. As initially configured, Red Storm provides over 10,000 compute nodes for massively parallel computations. Application teams from the three defense laboratories are successfully using Red Storm to provide computational result in support of various Level 1 and Level 2 milestones. Red Storm placed sixth on the Top 500 list (ASCI Red, which is now retired, was first on this list for many years). Red Storm placed first in the baseline High Performance Computing benchmarks that most severely test the communication network. In addition, Red Storm is faster than all its competitors at performing climate simulations. Other benchmarking studies are ongoing. Red Storm is now ready for general availability. A series of large runs (5,000 processors and more) has demonstrated the ability of nuclear weapons applications to effectively use the system.

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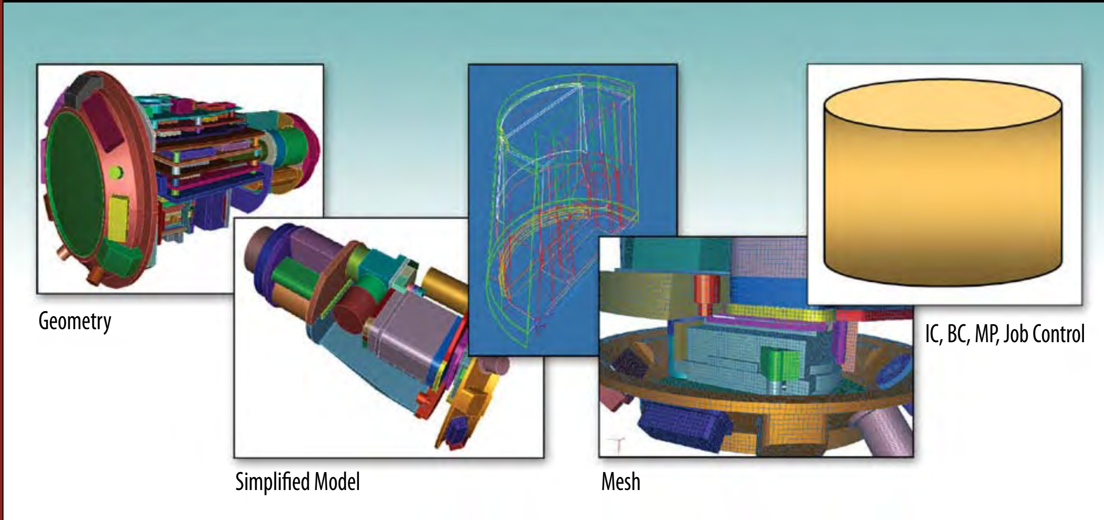

Five steps needed to define geometries for single element mesh

DART Speeds Analyses

The Sandia Design Through Analysis Realization Team (DART) system analysis in 2004 demonstrated that problem setup is a primary bottleneck for many ASC finite element engineering analyses. The study further concluded that one can reduce problem setup time by reducing the time spent on certain process steps, such as geometric editing and meshing, and by minimizing the iterative nature of the process. The DART environment, a federated collection of problem setup and simulation data management tools, addresses this problem. The environment has three primary objectives: reduce problem setup time, manage simulation data, and provide support for QMU methods. Recent DART pilot projects have demonstrated a significant reduction in system-level model creation time. By enabling simulation models to be created more quickly, the DART environment makes information available to weapon engineers earlier in the design process. Additionally, with less time spent creating models, more analyses can be performed in a given time, which provides more information and improves the engineers' understanding of their product.

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And

Mike Hardwick, Manager,
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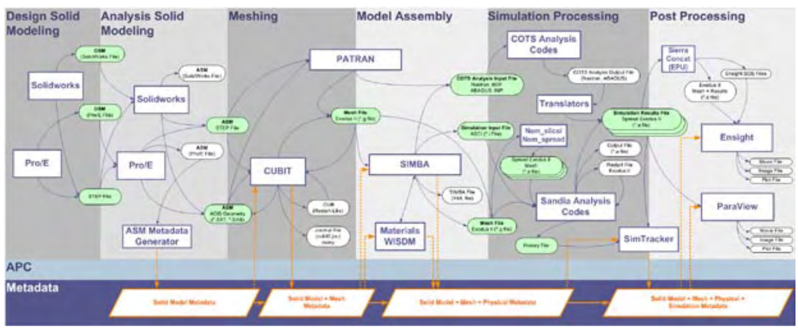

DTA Dataflow Model

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Computational Systems and Software Environment

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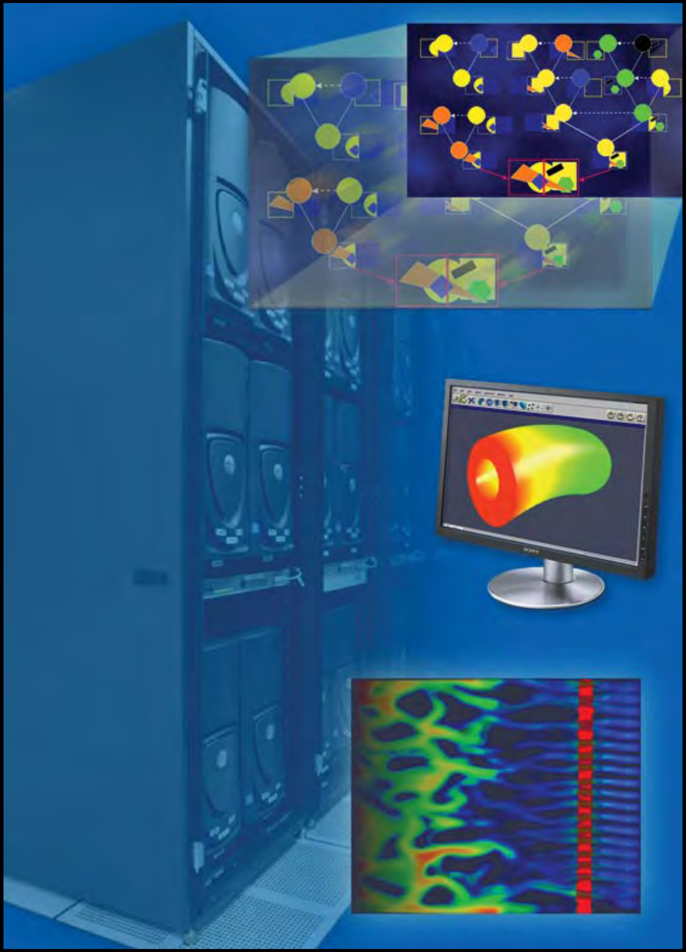

ParaView Supports Massive Visualizations

ParaView is an open-source scalable information visualization application that addresses many of ASC's large-data needs. The result of an NNSA/ASC Tri-Lab effort, ParaView is the world's most popular open-source visualization application—its binary distributions are downloaded 15,000 times a year, and it is used at more than sixty laboratories and universities around the world. ParaView's scalable infrastructure allows analysts to effectively explore data on a variety of platforms—from a laptop to massive supercomputers performing visualization and rendering in parallel. Sandia's ASC-funded contributions and collaborations with the open-source ParaView project have significantly impacted both the Tri-Lab visualization community and the visualization community at large. Advanced computation platforms such as Red Storm support computations of unprecedented size, requiring a scalable visualization solution that supports massive computations. ParaView also provides Sandia visualization researchers a platform to develop and deliver cutting-edge research in a parallel software architecture.

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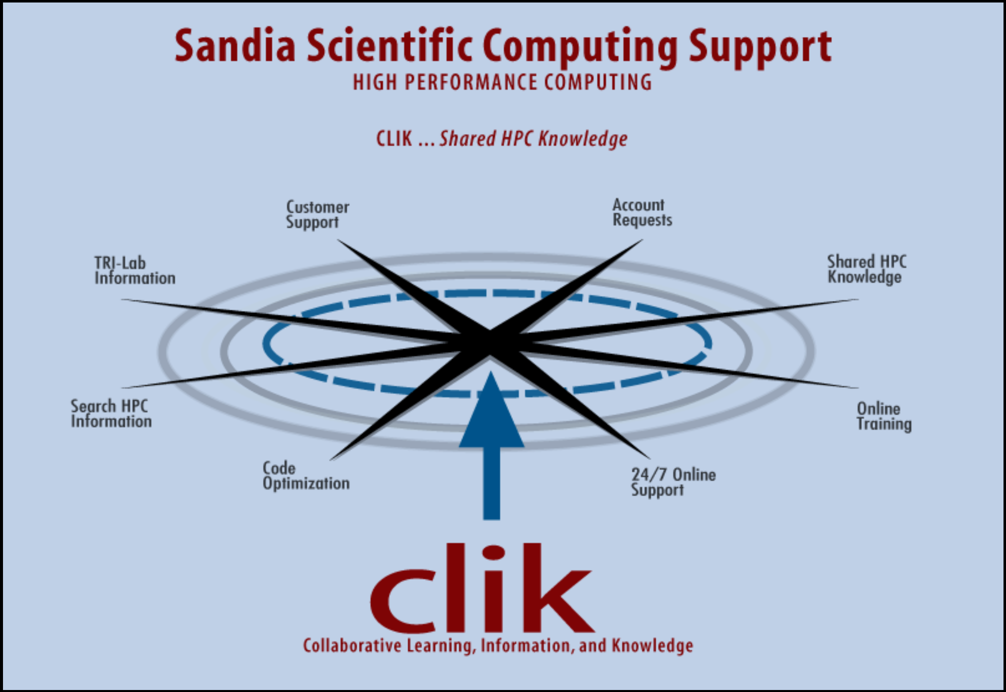
Front image: An illustration of ParaView technology. Sandia has enhanced ParaView with substantial capabilities such as a highly scalable tool that delivers multiplicative graphics power of visualization cluster machines.


Sandia Scientific Computing Support
HIGH PERFORMANCE COMPUTING
CLIK ... Shared HPC Knowledge
Customer Support
Account Requests
TRI-Lab Information
Shared HPC Knowledge
Search HPC Information
Online Training
Code Optimization
24/7 Online Support
clik
Collaborative Learning, Information, and Knowledge

Clik for Computer Support

Sandia's Scientific Computing Systems group provides High Performance Computing (HPC) support through the collaborative working environment most familiar to users of HPC systems. The group's capabilities are available to all users through electronic interface, regardless of their location. HPC support for Red Storm includes web-based training, email based technical assistance, and Google-powered knowledge base search capability. The Collaborative Learning, Information, and Knowledge (CLIK), allows sharing, through one tool, technical issues and solutions with users, vendors, other experts, and HELPDESKs at the other defense laboratories. The human support interface is provided directly from Red Storm system experts as well as other users of the system; thus, novice users and experts have access to individuals who are experienced with Red Storm.

The users for this system are both internal to Sandia and remote customers of the ASC HPC systems, including ASC university partners and any external support that might be required.

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Facility Operations and User Support

ASC Wide Area Network (WAN)

Increasing Distance Computing Capability

When it was installed, the ASC Wide Area Network (WAN) utilized the hardware and software available to obtain the best performance possible. It has been a key element in ensuring that ASC resources are shared among the three defense laboratories: Lawrence Livermor, Los Alamos, and Sandia. A new contract placed with Qwest provides two links between New Mexico and California, Los Alamos to Lawrence Livermore and Sandia/NM to Lawrence Livermore, at half the cost of the previous single link between Sandia/NM to Lawrence Livermore. Not only was the cost reduced, but the new links provided four times the speed of the old link, the use of a simpler technology made them easier to maintain, and they are configured to automatically back each other up, increasing network reliability. The performance increases obtained so far have improved the productivity of the code developers and analysts by reducing the time required to move data or visualization data from the remote computing asset to the local environment. This work demonstrates how the ASC WAN can be changed to meet evolving ASC needs and achieve high end-to-end performance without increasing cost to the program.

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