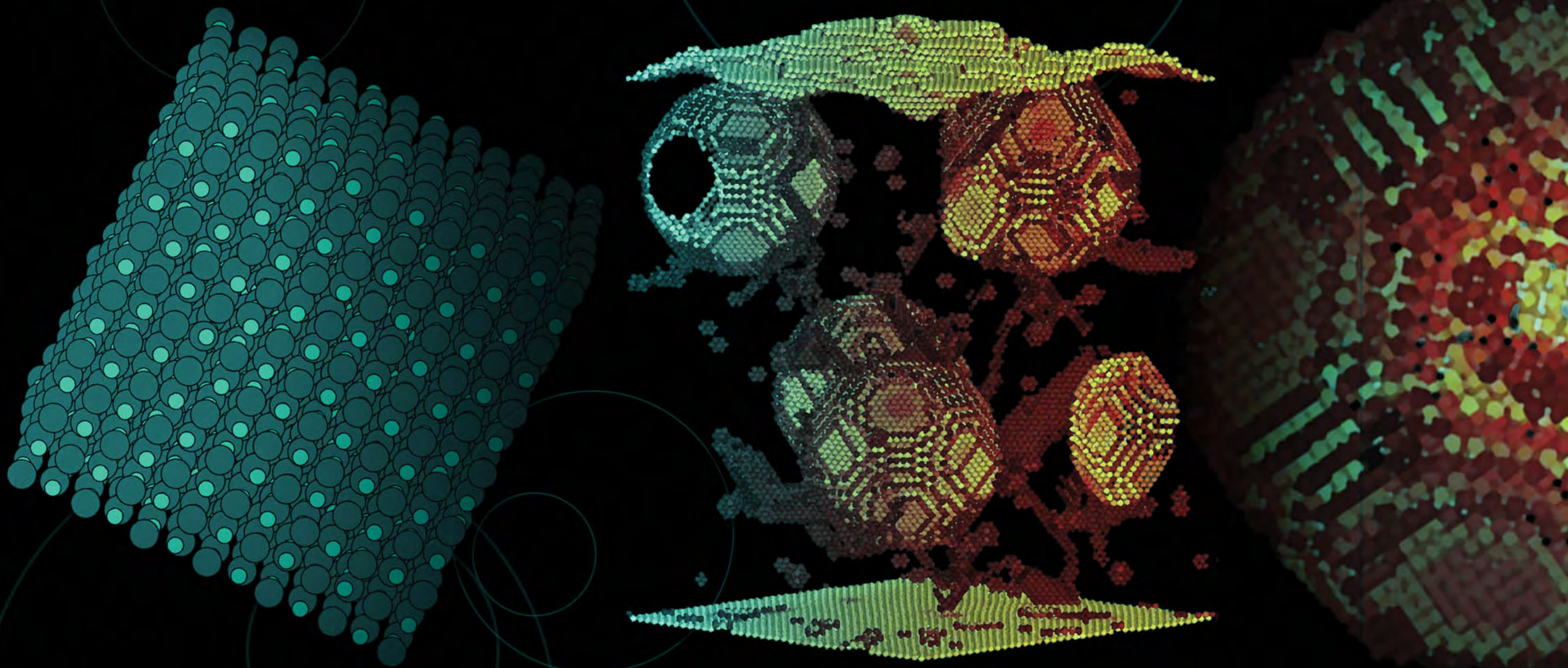
SANDIA NATIONAL LABORATORIES

ASC HIGHLIGHTS 2003



ADVANCED SIMULATION & COMPUTING™

Sandia National Laboratories

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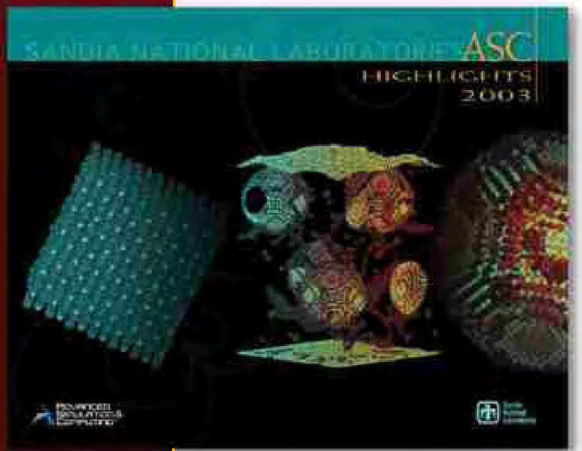
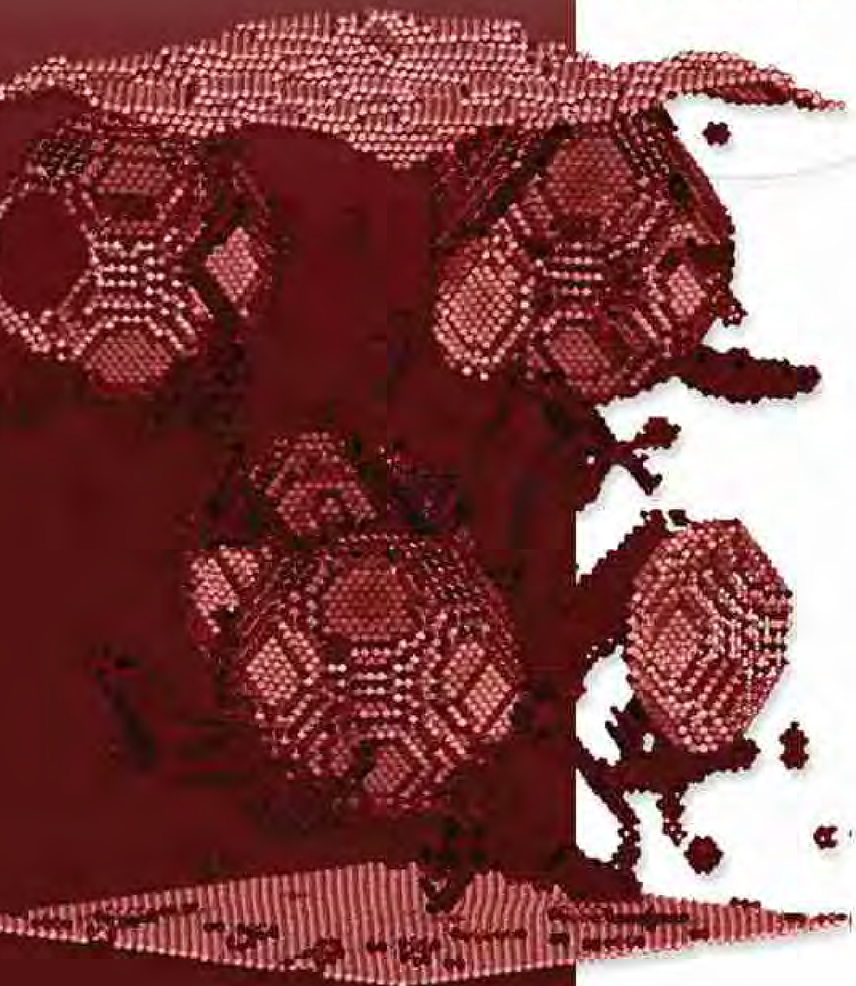


About the Cover

Material property degradation over time poses a potential weapons reliability problem. A project in the ASC's Aging and Reliability Program is developing a first principles models of the response of tritium components to intense radiation. The objective is to determine the mechanism responsible for accelerated release of helium (He) gas in metals, and to construct a continuum-scale for growth of He bubbles in metal hydrides that accounts for sub-scale phenomena such as initial defect content, stress-strain history, heat and radiation, and the interactions between bubbles.

Advanced Simulation & Computing (ASC) Highlights 2003



A publication of the
ASC Program at
Sandia National Laboratories

Acknowledgements

The effort represented in this document is a result of a variety of contributions that run the gamut of managerial support, NNSA guidance, multidisciplinary technical expertise, and skilled publishers.

We thus express our gratitude to our NNSA sponsors in NA 114 for their vision, direction and insights into the Advanced Simulation & Computing (ASC) program; to the Sandia ASC program element managers for their unfailing responsiveness to, and oversight of, programmatic challenges; and to Michael Vahle and Robert Thomas of the ASC Program Office for their skilled management of differing needs with unfailing patience. Most importantly, though, we applaud the work of our technical staff which appears within and which helps Sandia fulfill its mission of providing "...exceptional service in the national interest."

Many ASC projects are joint efforts of the three defense laboratories: Sandia, Los Alamos, and Lawrence Livermore. If these efforts are not clearly acknowledged in the highlights, we take this opportunity to thank both Los Alamos and Lawrence Livermore for contributing to the overall successes of these tri-lab projects.

This is the first report highlighting Sandia's successes in the ASC program. Its concept, written presentation and overall consistency of message is the work of Reeta Garber of the ASC Program Office. Doug Prout (Technically Write) is the graphic designer who has skillfully enhanced the written word through unusual and complementary design.
We thank them both.

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Foreword

Robert K. Thomas, Deputy Program Manager
Advanced Simulation and Computing

The ASC Program has made significant contributions to Sandia's nuclear weapons mission, particularly to the W76 and W80 refurbishments

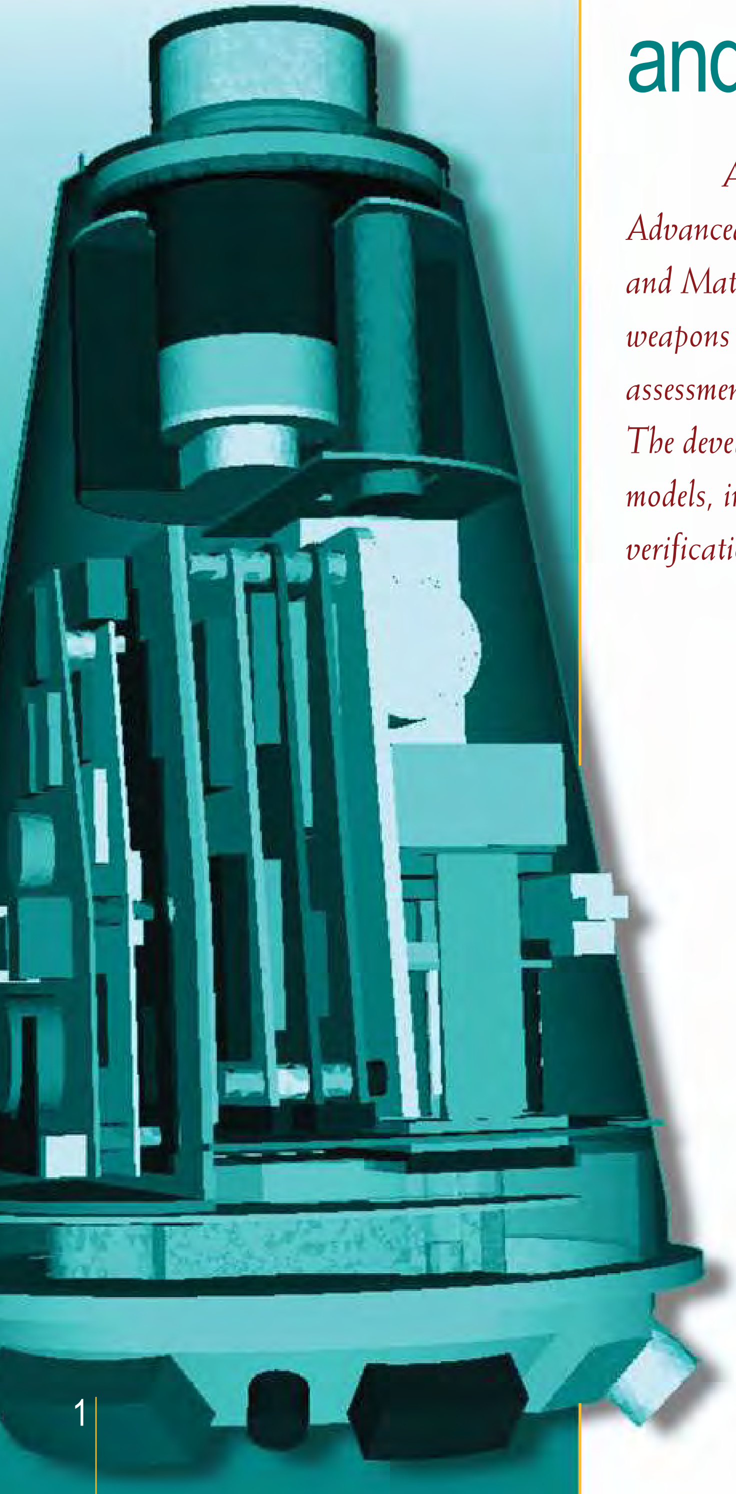
The Advanced Simulation and Computing (ASC) Program provides high-end simulation capabilities needed to meet Sandia's nuclear weapons stockpile mission. The program supports a broad spectrum of research and development activities spanning many core competencies across the laboratory within engineering sciences, computer sciences, and our Science & Technology programs. In FY03 the ASC Program supported over 325 engineers and scientists at the laboratory. Additionally, ASC funded the new Joint Computational Engineering Laboratory (JCEL) and the Supercomputing Annex, both at the NM site; as well as the Distributed Information Systems Laboratory (DISL) building at the CA site. Beyond the laboratory, ASC supports a number of university and industry partnerships in engineering and computer sciences. We are partnering with Cray, Inc, for the design and construction of Red Storm, a massively parallel supercomputer with a theoretical peak of 40 teraOPS, to be delivered to Sandia in the Fall of 2004. Red Storm will be one of largest supercomputers in the world when in full production mode, and will perform nuclear weapons simulations by all three NNSA defense laboratories - Sandia, Los Alamos and Lawrence Livermore.

The ASC Program has made significant contributions to Sandia's nuclear weapons mission, particularly to the W76 and W80 refurbishments. Our contributions, and progress, can be measured against the successful completion of recent milestones: we have delivered simulation capability for normal, abnormal, and hostile environments; we have stood up usage models and operating environments for the ASCI White computer at Lawrence Livermore and the Q computer at Los Alamos; we have partnered with Cray, Inc., to build Red Storm; and we have hired ten new staff members at the laboratory through our University Alliances Programs.

Validation of the materials and physics models in the ASC simulation codes are currently a high priority in the program. It is critical that ASC establish credibility in simulations which leads to confidence in the predictions for the nuclear weapons stockpile. Validation methodologies, and the underpinning science of understanding the materials and physics models, are being accelerated and are featured in current year milestones. Note that ASC also supports materials and physics modeling projects leading to stockpile simulations three to five years in the future – projects in microsystems, Z-pinch physics, and materials aging and reliability.

ASC is a tri-laboratory program. All three laboratories, Sandia, Los Alamos and Lawrence Livermore, collaborate with ASC's NNSA sponsors. In general, the program focuses on four major areas: (1) the development of three-dimensional physics-based codes for nuclear weapons applications; (2) the collaboration with the U.S. computer industry to create powerful high-end computing platforms to run the weapons simulations; (3) the building of a computing infrastructure and functional operating environments to make these capabilities accessible and usable, and (4) the collaborations with universities to accelerate simulation science and educate future weapon engineers and scientists at the laboratories. Since its inception in 1995, ASC has established aggressive performance goals, and has met every milestone.

This publication, the first of its kind, presents selected highlights from Sandia's ASC program during the past year—highlights that exemplify a broad spectrum of research and development activities within the laboratory. We hope that this ASC Highlights report will communicate, both within and outside the laboratory, the breadth and depth of the engineering and science projects within Sandia's ASC program.



Defense Applications and Modeling

ASC's Defense Applications and Modeling component is composed of four elements: Advanced Applications, Algorithms & Enabling Technologies, Verification & Validation, and Materials and Physics Models. This component develops and maintains all weapons codes used to support stockpile stewardship needs, including weapon design and assessments, accident analyses, certification issues, and manufacturing process studies. The development of high-fidelity, full-system codes requires new physics and materials models, improved algorithms, general code development, and a concerted effort in the verification of codes and their validation against experimental data.

Receiving the Gordon Bell Award for the Salinas Code

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Salinas won the prestigious 2002 Gordon Bell Award for special accomplishment in supercomputing based on innovation.

The Salinas Gordon Bell award certificate presented at Supercomputing 2002 conference.

Description

The Sandia-developed, ASC structural dynamics simulation code, Salinas, won the prestigious 2002 Gordon Bell Award for special accomplishment in supercomputing based on innovation. Salinas is a massively parallel code for modeling high-fidelity shock and vibration response of full-body weapons systems.

Technical Significance

Salinas sustained a performance of 1.16 teraOPS on 3375 processors of ASC White—an ASC supercomputer at Lawrence Livermore National Laboratory. This performance is about 30% of the possible peak rate for the number and type of processors used. The code also achieved unprecedented scalability for an implicit simulation code, demonstrating a constant solution time as the problem and computational resources were proportionally increased. Significantly, Salinas provided this performance as a general purpose code—a code that can be used to model and simulate a wide range of structural and mechanical systems, ranging from microElectroMechanical systems (MEMS) devices to aircraft carriers.

Contribution to the Stockpile Stewardship Program (SSP)

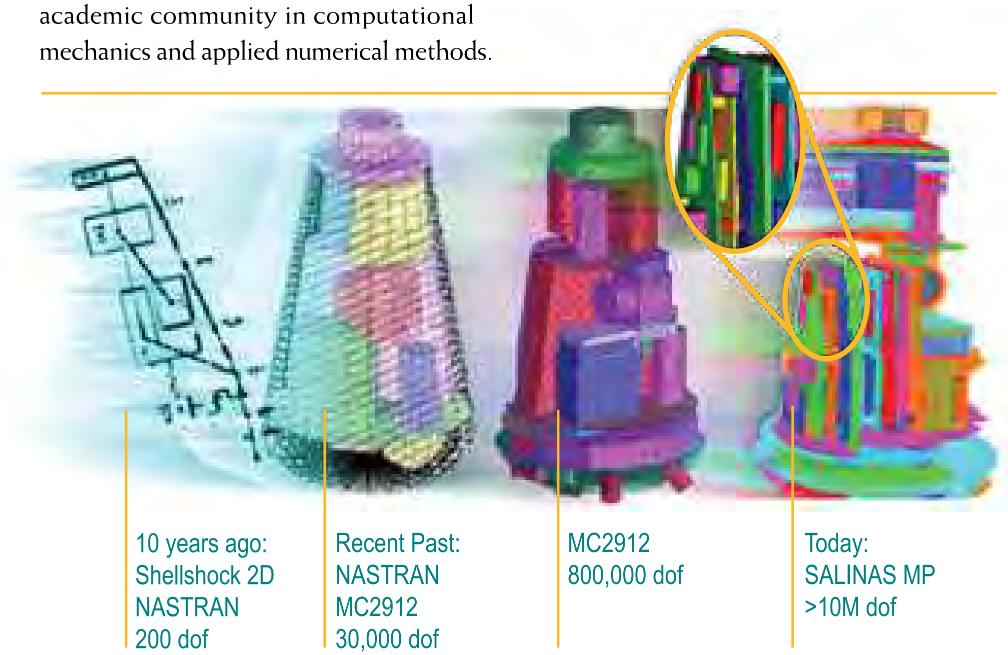
Salinas, which has just completed its first formal release to the Nuclear Weapons Complex, is already having a significant impact on modeling, simulation, and qualification activities for the Stockpile Stewardship Program. Specifically, Salinas is one of a suite of codes that address the system-level mechanical qualification issues for stockpile-to-target sequence (STS) hostile environments for the W76-1 life extension program, and STS normal environments for the W76-1 and W80 programs. Salinas is the only ASC code designed to address low-frequency shock and random vibration events, such as launch, re-entry induced vibration, and blast response.

Benefits to ASC and to Sandia

Salinas has established ASC and Sandia as leaders in the development of scalable and robust parallel solvers for engineering simulation, and as partners with the academic community in computational mechanics and applied numerical methods.

Future Developments

Salinas is currently focusing on a number of important development activities to extend its impact on the Stockpile Stewardship Program and the computational structural dynamics discipline in general. These activities include multi-physics coupling through the Sandia Integrated Environment for Research and Robust Analysis (SIERRA) mechanics framework, integration of contact capabilities in the parallel iterative solver, and the development and implementation of advanced methods in structural acoustics.



The Salinas code developed by ASC, together with the ASC-enabled explosion in computer hardware, allows more sophisticated structural dynamics modeling.

Developing Modeling Approaches for Penetrating Weapons

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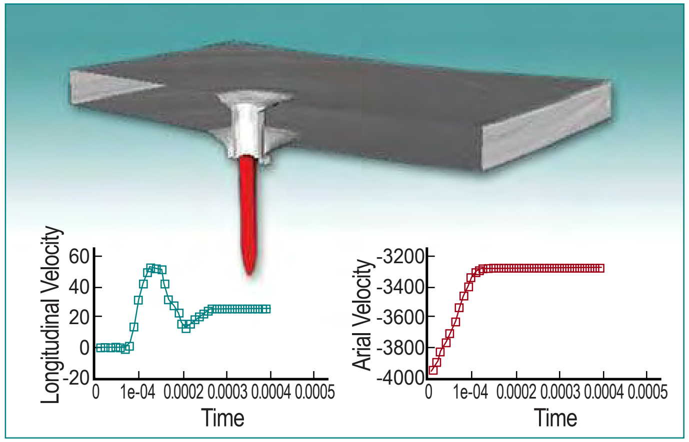
The penetration-simulation capabilities being developed are at the leading edge of computational mechanics and engineering simulation research.

On the right is an illustration of a Forrestal Plate Penetration using the Coupled Lagrangian/Eulerian Algorithm. This is a parallel simulation using the stress-based coupling for the Forrestal normal impact plate penetration simulation. In this simulation, a steel penetrator is shot through an aluminum plate.

Description

The ASC Applications program is developing the capability to simulate the performance of earth-penetrating weapons. To address this complicated problem, we have adopted three separate modeling approaches for penetration events. Each analytical method has benefits and drawbacks, but as a whole, they can cover many penetration scenarios. The following are the three modeling approaches.

1. A semi-analytic model, called Cavity Expansion (CE), models the penetrator with a Lagrangian finite element mesh. The target is represented with a boundary condition derived from opening a cavity in an infinite half-space. The CE boundary condition is maintained in a library shared by Alegra and Presto, the transient dynamics code, under SIERRA.
2. SHISM (Soft-Hard Interface Surface Mechanics) uses a Lagrangian penetrator and a geometrically conformal Arbitrary Lagrangian/Eulerian (ALE) target space. The SHISM model has been fully implemented and brought to production. Simulation results generally agreed well with experiment results, and mesh-convergence studies have been performed for the Warren experimental data set.
3. Alegra-EP (earth penetrator) uses a Lagrangian penetrator and an overlapping Eulerian mesh for the target region. This technology is loosely based on the Zapotec (legacy) code. We have implemented a Zapotec-like stress-based coupling algorithm in Alegra-EP. The capability is fully parallelized and has been demonstrated on several verification problems.



Technical Significance

Modeling penetration events is difficult because the target is "split" as the penetrator moves through it. This is difficult to model in a traditional Lagrangian framework because the path of the penetrator is not known *a priori*. A traditional Eulerian approach works well for the target (because *a priori* knowledge of the path is not needed), but it lacks the resolution and fidelity to capture all the necessary phenomena for the penetrator.

Contribution to the Stockpile Stewardship Program (SSP)

Penetration-simulation capabilities are beginning to influence penetrator system studies. The CE capability has been used extensively by the ASC Advanced Deployment (AD) penetration project and is meeting their analysis needs. The SHISM capability has been used by the Robust Nuclear Earth Penetrator (RNEP) development team and the ASC AD penetration project to assess the fidelity of the algorithm and to provide design information.

Benefits to ASC and to Sandia

The penetration-simulation capabilities being developed are at the leading edge of computational mechanics and engineering simulation research. These capabilities will also have a significant impact on other applications involving the interaction of large-deformation physics, including material failure, with small-deformation mechanics.

Future Developments

Because of deficiencies in the stress-based coupling algorithm used in Alegra-EP, we have begun developing a new coupling method that utilizes more information. Early testing indicates that it is more accurate and will become the preferred method. The basic framework is complete, so we can focus on improving the algorithms. The penetration-simulation capabilities will be demonstrated in an upcoming FY2005 Applications milestone.

Simulating Hostile Electrical Environments

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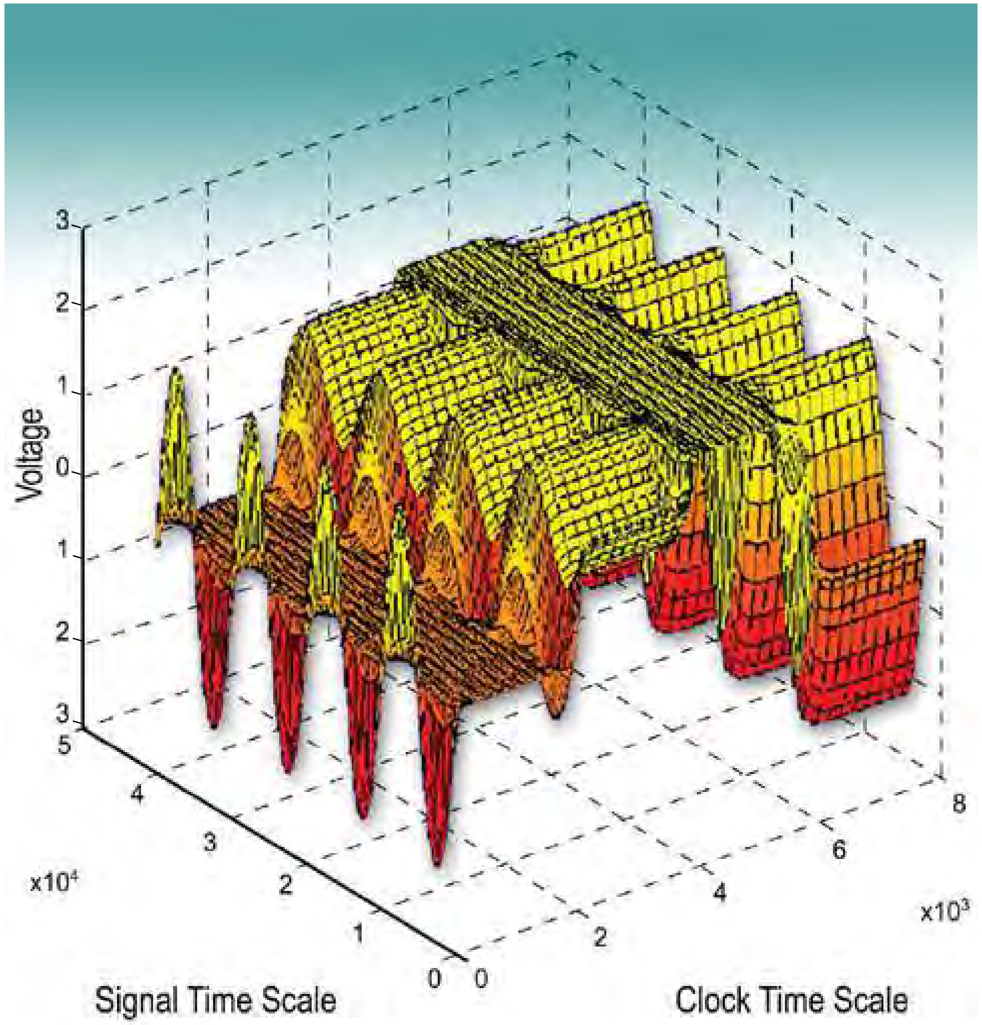
The better coupling between radiation-transport and circuit-analysis codes will also allow circuits and ASICs to be designed with significantly less margin, greater robustness, and reduced expense.

RIGHT: With the Xyce™ circuit code, novel methods are used to solve multiple-time partial differential equations, as shown here. At the milestone review in May 2003, the external review panel was "impressed with the work being done on time-parallel, multi-time partial differential equations within Xyce™."



Description

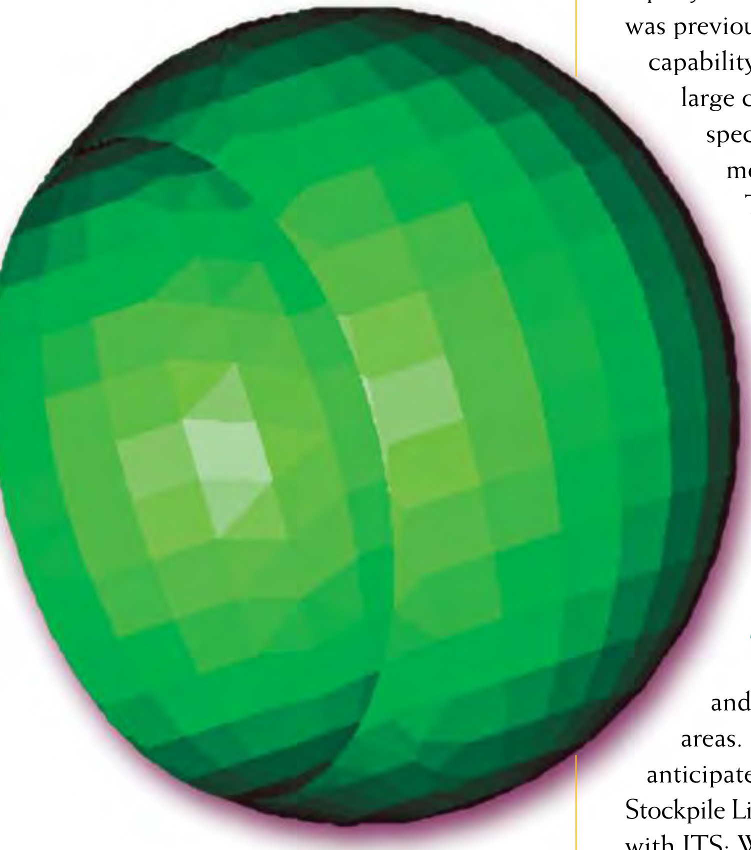
The completion of an FY03 ASC Level 1 Milestone, *"Stockpile-to-Target Sequence hostile environment simulation for cable SGEMP and electrical response to x-rays,"* demonstrated simulation capability for transient x-ray radiation response of electrical components, representative of weapon components in hostile environments. This new capability was demonstrated for a circuit of the replacement arming, fuzing, and firing (AF&F) unit for the W76-1. The Integrated-TIGER-Series (ITS) Monte Carlo code predicted dose rate for locations on circuit boards corresponding to the locations of radiation-sensitive semiconductor devices. Using the ITS dose-rate data, the Xyce™ circuit code predicted the response of the circuit under radiation.

On May 29, 2003, an external review panel concluded that the ITS team had successfully met its part of the FY03 milestone. The Xyce™ calculations were completed before the due date of September 30, 2003, and were reviewed by the external review panel on November 3 and 4, 2003.

Technical Significance

For this milestone, a new computer-aided-design (CAD)-based transport capability for Sandia's Monte Carlo radiation transport code, the ITS, was demonstrated. Before ASC, the legacy version of ITS required construction of a geometrical model specifically tailored for the radiation-transport code. This time-consuming method involved Boolean combinations of solid primitives. For complex weapon systems, more than a year of effort was required to assemble geometry models. For this milestone, the ITS radiation-transport modeling team demonstrated a new capability developed under ASC that allows radiation to be transported on a three-dimensional CAD model of a re-entry body. Thus, CAD models created by weapon designers can now be leveraged by radiation transport analysts.

The Xyce™ circuit calculations also showcased several new capabilities. The Xyce™ code is part of the ASC code-development effort of High Performance Electrical Modeling and Simulation (HPEMS) team. The development of new, predictive, radiation-aware device models and their integration into Xyce™ was



With the ITS radiation transport code, investigation of radiation transport to faceted surfaces, like the one shown here, is under way. At the milestone review in May 2003, the external review panel said that it "applauds the ITS team's effort to develop alternative geometry representation for ITS such as the faceted surfaces."

demonstrated. These photocurrent models for semiconductor devices can be more rapidly and less expensively created than was previously possible. Also, the new capability of Xyce™ to simulate very large circuits, including application-specific integrated circuit (ASIC) models, was demonstrated. Together, these two new capabilities allow Sandia circuit modelers to achieve unprecedented high fidelity in their circuit simulations, vastly surpassing the capabilities available from commercial software tools.

Contribution to the Stockpile Stewardship Program (SSP)

Both the ITS Monte Carlo and Xyce™ codes support SSP areas. Over the next two years, we anticipate supporting as many as five Stockpile Life Extension Programs (SLEPs) with ITS: W76-1 AF&F, W78 neutron generator (NG), W87 NG, W80, and B61. Such extensive support of the SSP would have been impossible without the new CAD capability of ITS. In FY04, we are performing calculations to assess the internal x-ray radiation in the W76-1 AF&F and the W78 NG. We anticipate doing the same for the W87 NG in the near future. Moreover, the ITS code (along with the Presto, Andante, and Salinas codes) is used to predict thermomechanical shock and structural effects in systems that need to be designed to cope with hostile radiation threats. We are also beginning simulations with ITS for the W80 and the B61 to predict a normal environment phenomenon, the internal radiation environment that occurs because of the intrinsic radiation from the nuclear explosives package. The Xyce™ circuit code is being used to analyze electrical systems for the W80, W76, and B61.

Benefits to ASC and to Sandia

The improved CAD version of ITS can be used to assess rapidly radiation-hardness design issues (the design-to-analysis process was reduced from a year to weeks with this CAD capability). This will allow more rapid, improved designs of radiation-hardened components for qualification. The better coupling between radiation-transport and circuit-analysis codes will also allow circuits and ASICs to be designed with significantly less margin, greater robustness, and reduced expense. Larger, more complex circuits can be simulated than ever before, so interface issues can be addressed without hardware fabrication. When functional blocks are simulated separately, design flaws or parasitic coupling (cross-talk) can be missed. If the flawed designs are fabricated, extra costs (hundreds of thousands of dollars) to the customer and inability to meet Department of Energy (DOE) / Department of Defense (DoD) production deadlines can result. Xyce™ can simulate large (>250K) transistor count circuits rapidly in days (not weeks) and aid the ASIC designers at Sandia.

Future Developments

The new ITS CAD capability will support the simulation of other phenomena that arise under hostile environments, including thermo-structural response and cavity system-generated electromagnetic pulse effects. Efforts are under way to improve the computational efficiency of CAD-based simulations, possibly through faceted representations of surfaces generated by the Cholla component of CUBIT. Improvements in ITS physical and numerical algorithms are also under way.

For the Xyce™ code, future work includes (1) the development of radiation-response models for ASICs and their inclusion in a complete circuit model, (2) more accurate determination of parasitic elements, and (3) enhanced linear solvers and preconditioning methods from the Trilinos library. Finally, we will continue to improve validation of both ITS and Xyce™ for radiation effects through our important links to Campaign 7 experimentation.

Analyzing Abnormal Environments Deformation and Thermal Race

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A deformed and damaged weapon system model, as calculated by Presto, could then be utilized to perform detailed weapon thermal analyses with Calore, which in turn can be directly linked with Fuego to provide a simulated fire thermal environment.

RIGHT: A series of figures from a W80 thermal analysis that demonstrates foam degradation under thermal loading.

Colors represent temperatures on the solid surfaces of the model from blue = 300 K to red = 1200 K.

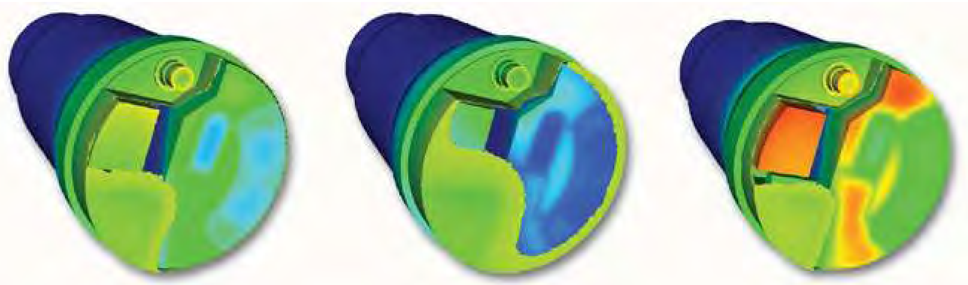
Description

The completion of an FY02 ASC Level 1 Milestone, *"Stockpile-to-Target Sequence abnormal environment prototype simulation for crash and burn events,"* demonstrated new SIERRA codes on the ASC White machine, an ASC supercomputer located at Lawrence Livermore National Laboratory. This milestone specifically aligns with the Nuclear Weapons program needs. To this end, two engineering mechanics codes of the SIERRA applications suite, Calore (a nonlinear conduction thermal code) and Presto (explicit transient dynamics code) were utilized to simulate weapons systems for abnormal stockpile to target sequence (STS) environments.

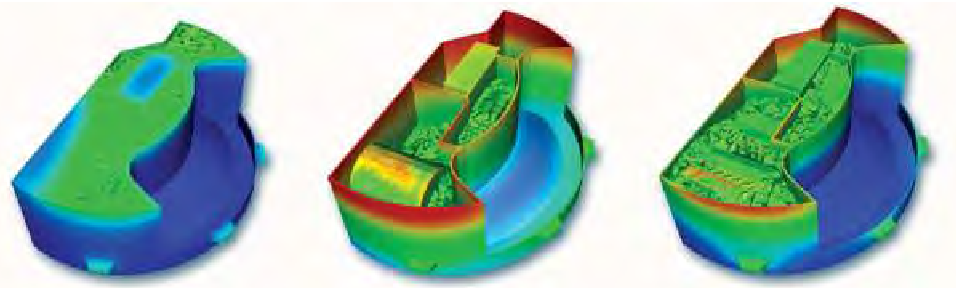
For Calore, a fully coupled simulation capability for a strong link/weak link thermal race was demonstrated, an analysis used for assessing weapon safety in abnormal environments from fires. For Presto, the STS abnormal mechanical environment of an accidental drop onto a hard, unyielding surface was assessed.

The milestone was completed on September 30, 2002. The external review panel met on October 28 and 29, 2002, assessed the evidence presented by the Calore and Presto teams and declared that the FY02 milestone was successfully met. Both Calore and Presto have been released for analysis of abnormal mechanical and thermal environments.

These achievements were recognized by the National Nuclear Security Administration (NNSA), which awarded the 2002 Defense Programs Award of Excellence to the Calore and Presto Milestone teams "for significant contributions to the Stockpile Stewardship Program."



Earlier: melting of the W80 WES cover, uncovering the interior components, including the fire set.



Later: top cover removed to reveal decomposing foam interface.

Technical Significance

Presto, together with the Calore thermal analysis code, is the first of a new generation of applications codes built upon the SIERRA advanced mechanics software framework. As with the other SIERRA codes, Presto is parallel and scalable, designed to run on the next generation of massively parallel supercomputers and engineered in accordance with a rigorous set of software quality practices. Presto has also advanced the state-of-the-art in computational mechanics in other areas, such as modular approaches to contact mechanics and cavity expansion, new failure modeling capabilities, and enhanced accuracy and robustness.

This milestone demonstrated several significant computational capabilities of the Calore code. An abnormal fire environment was simulated by directing an appropriate heat flux onto the Warhead Electrical System (WES) cover. Heat transfer within the warhead structures and components was simulated by two mechanisms—nonlinear conduction heat transfer and enclosure thermal radiation heat transfer. The conduction modeling used a very high degree of spatial resolution and employed several materials of differing thermal properties. The most striking simulation capability (a very significant achievement) was the addition of foam-decomposition modeling, which was based on foam chemistry models developed in the Materials and Physics Models (M&PM) program. The mechanical state of decomposing foam as a function of time and thermal conditions was modeled as causing the foam volume inside the firing

RIGHT: A series of figures from a W80 abnormal drop analysis using Presto.

Figure 1 shows the drop orientation prior to impact.

Figure 2 shows the detailed Von Mises stress state from blue = 0.0 to red = 415 MPa for the WES cover with two different resolutions of four and eight elements through the thickness of the housing.

Figure 3 shows a detailed view of a deformed corner with stress state indicated by color, again at two different resolutions of four and eight elements through the thickness.

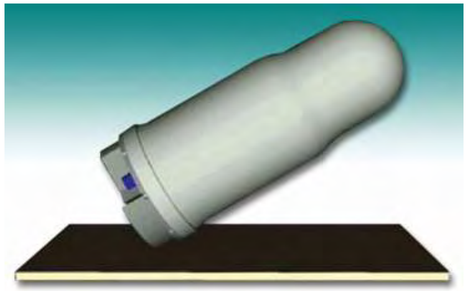


Figure 1. Initial geometry for a W80 warhead drop onto a hard unyielding target.

set to change over time, resulting in void spaces where foam had decomposed. Void spaces no longer have a foam-conduction heat-transfer path, but thermal radiation heat transfer then becomes a significant mechanism. The great difficulty introduced to the modeling is that the change of internal void volumes requires continuous recalculation of thermal-radiation view factors and the accurate computation of the thermal-radiation heat transfer within these spaces. This dynamic-enclosure radiation calculation to accommodate the temporal decomposition of foam was a significant computational feat. The combination of foam-decomposition modeling with dynamic radiation enclosures provides great improvement to the fidelity of thermal race analyses.

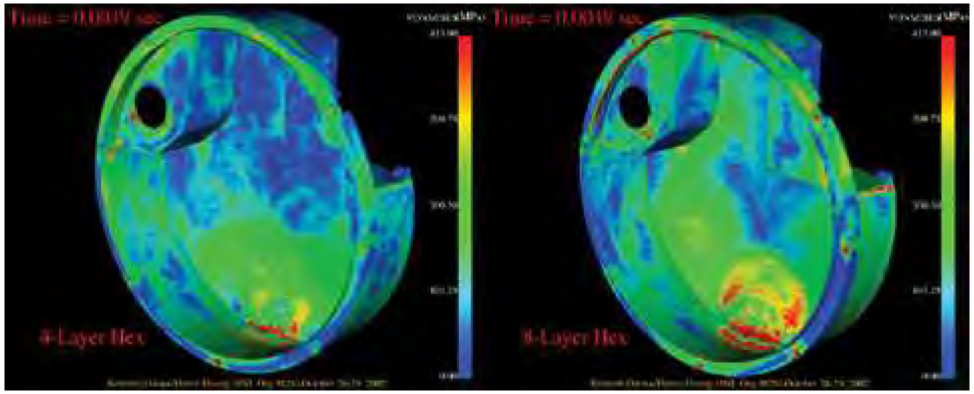


Figure 2. WES cover Von Mises stress state for two different discretizations.

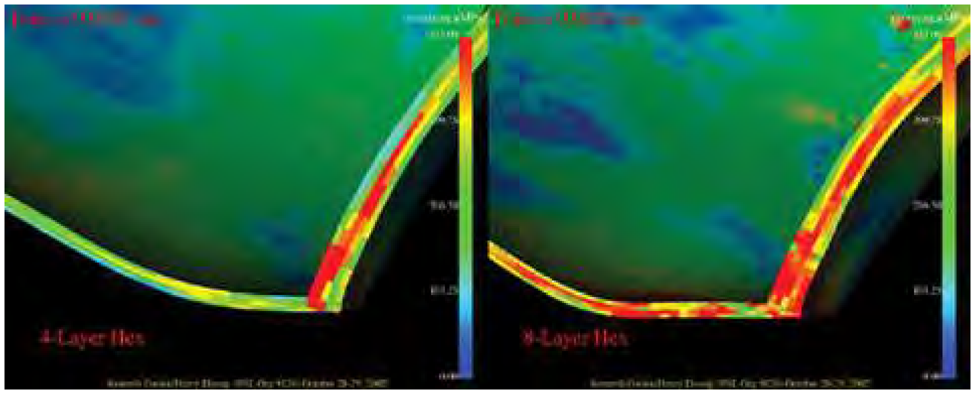


Figure 3. Close-up of the WES cover corner Von Mises stress state for two different discretizations.

Contribution to the Stockpile Stewardship Program (SSP)

Presto is used in STS abnormal and hostile mechanical analysis for the W76-1 program and is having a significant impact on most weapon-system programs, including the W80, W87, and B61, as well as projects and studies such as SGT, a transportation system, and Robust Nuclear Earth Penetrator (RNEP), an advanced concept robust penetration-weapon design. Presto permits analysis of mechanical environment scenarios involving high strain rates, large deformations, plasticity, contact, and material failure.

The capability to perform thermal safety analysis for both normal environments (e.g., thermal battery operation) and abnormal environments (e.g., fires) is a continuing need in weapons programs. Upcoming SLEPs for the W76 and W80 have required detailed thermal analyses to ensure acceptable margins for strong link/weak link thermal races under fire-induced boundary conditions. Virtually all weapons systems have portions of the STS—such as storage and transportation—in which abnormal thermal analyses are needed. The improved simulation methods afforded by including the significant physical phenomena resulting from decomposing foam lead to increased confidence in the assessed safety margins experienced in abnormal environments.

Benefits to ASC and to Sandia

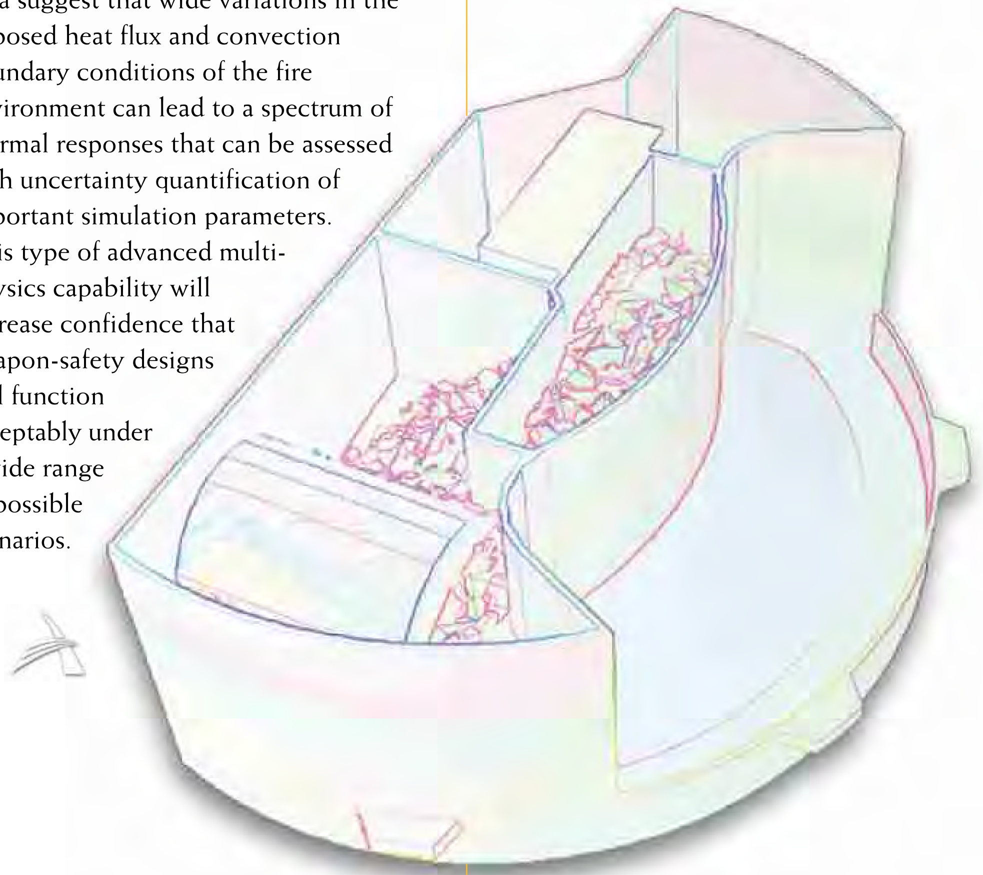
Presto permits analysis of mechanical environments of high strain rates, large material deformations, plasticity, general body-to-body contact mechanics, and material-failure modeling, all of this at very high spatial resolution. Presto utilizes the large machines that have been part of the ASC platform-acquisition strategy. The variety of applications for Presto would be hard to overstate. Many normal-, abnormal-, and hostile-environment weapon analyses lie in the realm of transient dynamics that Presto addresses.

Performing coupled calculations, including foam decompositions and dynamic radiation enclosures, has been a long-standing need in the weapons safety analysis community. The confidence in these critical safety calculations for stockpile systems has been greatly enhanced, and guidance during design with timely simulation can now be provided. Future studies for new and existing stockpile systems can include a greater variety of scenarios and off-design analyses, again leading to greater confidence in the soundness of safety designs. This detailed thermal-modeling capability is also increasingly used as part of the coupled electro-thermal mechanical modeling of MEMS devices.

Future Developments

In the future, detailed weapon-system performance analyses can be fully coupled with all relevant mechanics through the SIERRA code framework. For the classic crash-and-burn weapon-safety scenario, a coupling and handoff from Presto to Calore, Fuego, and Andante can be envisioned. Fuego is a fire simulation code, and Andante is a quasistatic mechanics code also under the SIERRA code framework applications suite. A deformed and damaged weapon system model, as calculated by Presto, could then be utilized to perform detailed weapon thermal analyses with Calore, which in turn can be directly linked with Fuego to provide a simulated fire thermal environment. Finally, Andante could be used to assess the effect of internal pressurization on failing an exclusion region within a firing set.

Advanced coupled physics simulations will enable calculation of interactions such as those of the weapon system on the fire environment as well as the fire environment on the weapon. Experimental data suggest that wide variations in the imposed heat flux and convection boundary conditions of the fire environment can lead to a spectrum of thermal responses that can be assessed with uncertainty quantification of important simulation parameters. This type of advanced multi-physics capability will increase confidence that weapon-safety designs will function acceptably under a wide range of possible scenarios.



Assessing Software Quality Internally

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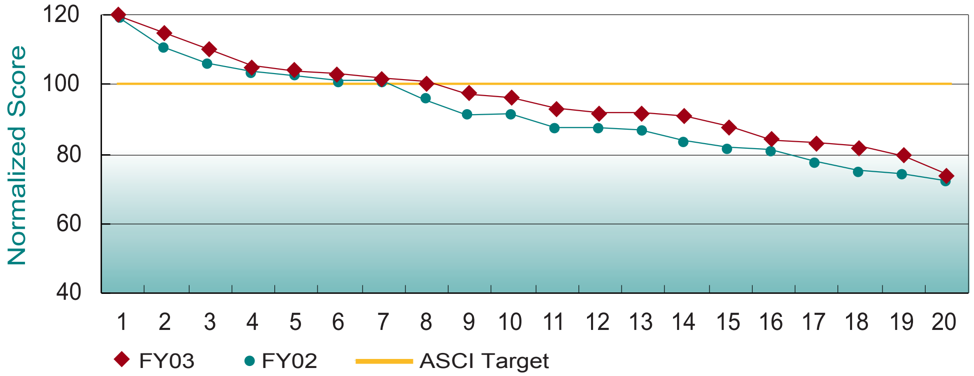
This assessment provided a uniform examination of software practices across the Advanced Applications program.

Description

The Advanced Applications program conducted an internal assessment of the software quality practices used by the 20 code development projects supporting design and qualification of nuclear weapons. Ten assessors from departments outside the code development groups trained in software quality and conducted the assessment over four months. They followed the practices documented in Sandia's ASC Applications Software Quality Engineering Practices, Version 2.0, SAND2003-0962. The assessment team will publish their results in an unlimited-distribution SAND Report, *SNL ASC Applications Software Quality Engineering Assessment Report*. This is part of the ASC program's strategy of improving software practices and software quality assurance.

Technical Significance

This assessment provided a uniform examination of software practices across the Advanced Applications program. It identified best practices and practices that can be improved. This is a precursor to revising the software quality practices document, SAND2003-0962. We revised the software quality practices following an FY02 internal assessment.



FY02 and FY03 sorted total scores for the 20 software packages.

Contribution to the Stockpile Stewardship Program (SSP)

This assessment is a key component of our software quality assurance activities. It provides objective evidence of the status of our software quality practices.

Benefits to ASC and to Sandia

Improved software practices will result in lower lifetime costs and fewer defects in the software used for design and qualification of the stockpile. We are disseminating lessons learned and best practices through conferences, documents, and sharing between code development teams to improve the software practices throughout the Nuclear Weapons Complex.

Future Developments

We will update our software quality practices document in accordance with the recommendations of the assessment team and continue to improve our software practices.

Developing the Trilinos Framework for Solvers

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Trilinos solvers greatly shorten the development cycle and improve the computational efficiency of modeling and simulation codes.

Description

Researchers at Sandia have developed the Trilinos framework to facilitate the design, development, integration, and ongoing support of mathematical software libraries in support of modeling and simulation in the Stockpile Stewardship Program (SSP). In particular, the goal is to develop parallel solver algorithms and libraries within an object-oriented software framework for the solution of large-scale, complex multiphysics engineering and scientific applications. The emphasis is on developing robust, scalable algorithms in a software framework, using abstract interfaces for flexible interoperability of components while providing a full-featured set of concrete classes that implement all abstract interfaces. Figure 1 (next page) shows the structure of Trilinos, including the major packages and capabilities that are available.

Technical Significance

Trilinos uses a two-level software structure designed around collections of packages. A Trilinos package is an integral unit usually developed by a small team of experts in a particular algorithms area such as algebraic preconditioners, nonlinear solvers, etc. Packages exist underneath the Trilinos top level, which provides a common look-and-feel, including configuration, documentation, licensing, and bug-tracking.

Trilinos packages are primarily written in C++, but provide some C and Fortran user interface support. We provide an open architecture that allows easy integration with other solver packages, and we deliver our software to the outside community via the Gnu Lesser General Public License (LGPL).

Two packages distributed within the Trilinos framework merit special attention. The first is Epetra, which takes its name from the Greek word for foundation. Epetra is a collection of concrete classes that supports the construction and use of vectors, sparse graphs, and dense and sparse matrices. It provides serial, parallel, and distributed memory capabilities. It uses the BLAS and LAPACK where possible, and as a result has good performance characteristics.

The second package is TSF. TSF is a collection of abstract classes that provides an application programmer interface (API) to perform the most common solver operations. It can provide a single interface to many different solvers. Furthermore, TSFExtended has powerful compositional mechanisms that support the lightweight construction of composite objects from a set of existing objects. As a result, TSF users gain easy access to many solvers and can bring multiple solvers to bear on a single problem.

Contribution to the Stockpile Stewardship Program (SSP)

Because Trilinos is applicable to many modeling and simulation activities in the SSP, it provides many advantages to algorithm and library developers. All Trilinos packages, including the Epetra and TSF packages, are available to developers as well as to applications. These greatly shorten the development cycle and improve the computational efficiency of the final product. New packages have moved from conception to distribution in three months.

Benefits to ASC and Sandia

Trilinos provides an infrastructure supporting established software quality engineering practices within the ASC program. This infrastructure includes configuration management, regression testing, automatic testing, bug tracking, code repository and distribution tools.

The Trilinos solver framework, now in its third version, has had a major impact on Sandia's modeling and simulation capabilities during the past several years by providing access to accurate, robust and efficient solvers and tools. In addition, Trilinos is being released publicly under the LGPL in September 2003.

Future Developments

Trilinos development continues with the addition of new solver packages and improvements in overall algorithms performance.

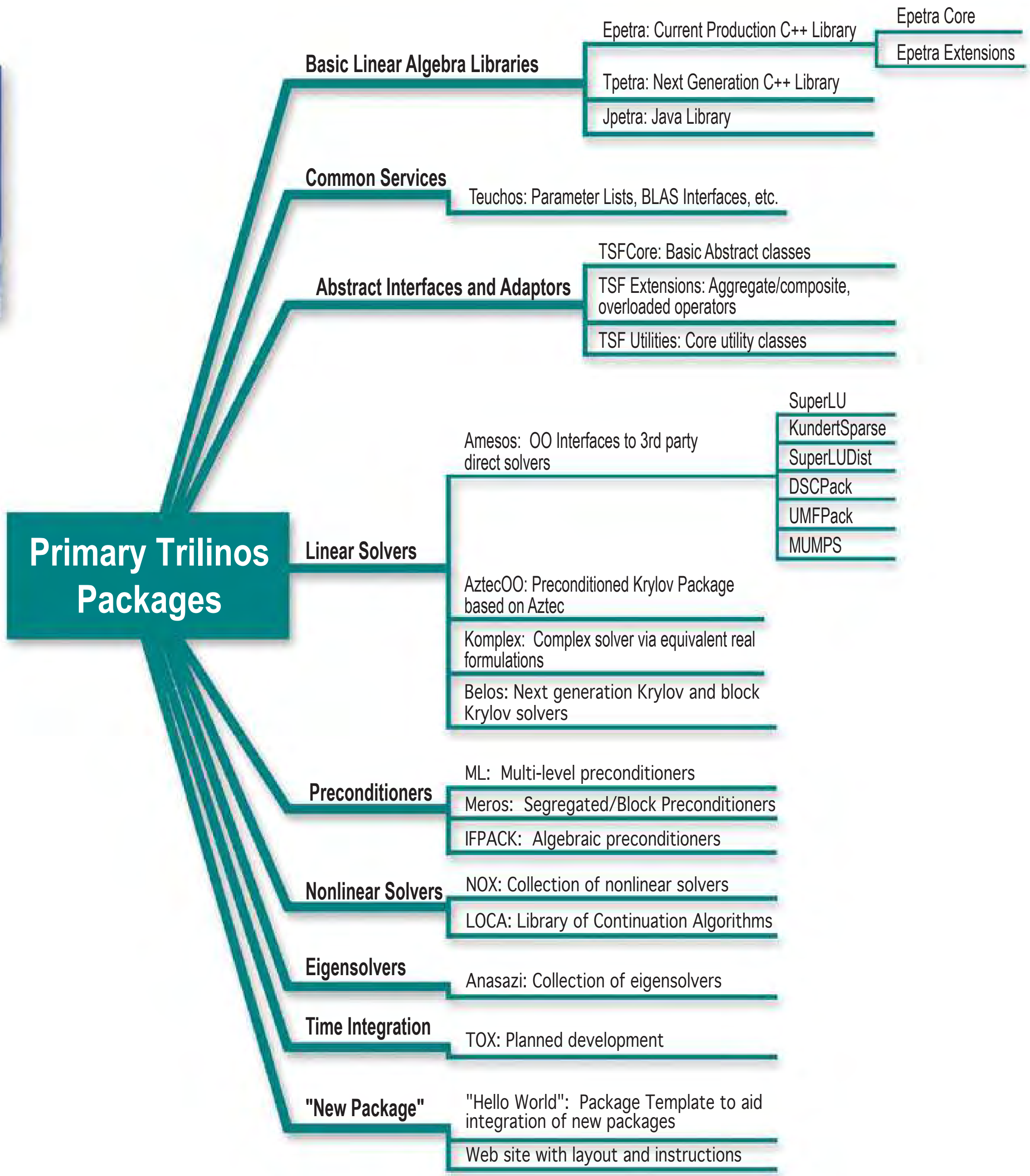

Figure 1. The Trilinos framework provides access to the wide range of solver capabilities shown above.

Developing the DAKOTA Framework for ASC-Scale Optimization and Uncertainty Quantification

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DAKOTA allows "Sandia analysts to address directly the fundamental issues of foremost importance to our programs, such as computing optimal designs, identifying worst-case surety, and assessing the predictive accuracy of computational models."

Description

DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) is a general-purpose software toolkit for performing systems analysis and design on high-performance computers. As an open source software framework, DAKOTA is widely used within DOE, the federal government, universities, and industries. Its use is supported with ASC application codes at Sandia, Los Alamos, and Lawrence Livermore. Within the broader community, over 1,300 external download registrations have occurred since December 2001.

Technical Significance

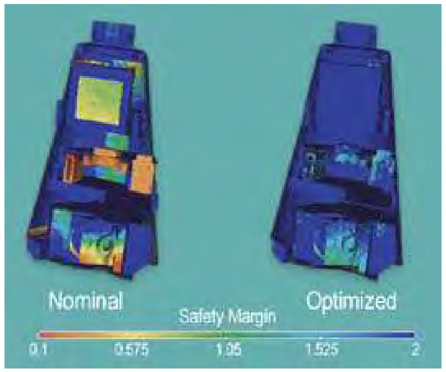
DAKOTA provides a flexible and extensible interface between iterative systems analysis capabilities and a broad variety of simulation codes used in the SSP, including structural mechanics, heat transfer, fluid dynamics, shock physics, and many others. These simulation tools can be an enormous aid in understanding the complex physical systems they simulate.

DAKOTA provides generic simulation interfacing facilities that allow the use of a variety of engineering and physics simulation codes as "function evaluations" within an iterative loop. This interface may be completely *non-intrusive* or "black box," which allows for rapid interface development and turn-around in time-critical systems studies; *semi-intrusive*, which allows for elimination of repeated overhead and streamlined execution on massively parallel architectures; or *fully intrusive*, which seeks maximal computational efficiency through the tightly coupled "all-at-once" solution of optimization, uncertainty quantification, and simulation conditions. The *non-intrusive* interfaces provide general-purpose support for arbitrary applications, whereas the *semi-intrusive* and *fully intrusive* interfaces target highly leveraged Sandia simulation frameworks such as SIERRA and NEVADA.

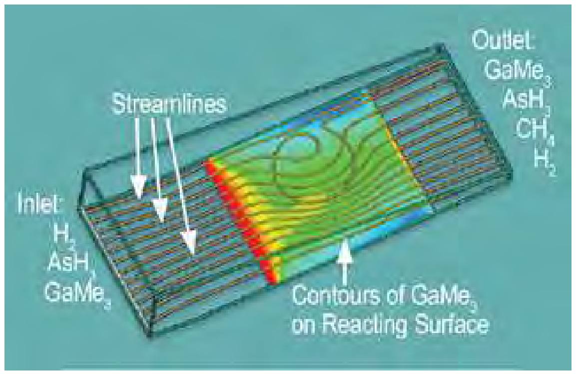
Parallelism is an essential component of the DAKOTA framework. Particular emphasis has been given to simultaneously exploiting parallelism at a variety of levels in order to achieve near-linear scaling on massively parallel computers. DAKOTA manages the complexities of its analysis and optimization capabilities through the use of object-oriented abstraction, class hierarchies, and polymorphism. The flexibility of the framework allows for easy incorporation of the latest external and internal algorithmic developments.

Contribution to the Stockpile Stewardship Program (SSP)

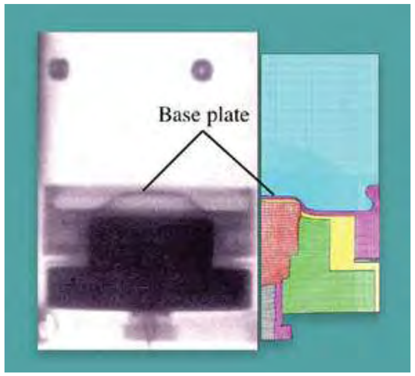
DAKOTA has contributed to the SSP by providing algorithms for design optimization with gradient-based and nongradient-based methods; uncertainty quantification with sampling, reliability, and stochastic finite element methods; parameter estimation with nonlinear least squares methods; and sensitivity/main effects analysis with design of experiments and parameter study capabilities. These capabilities may be used on their own or as building blocks within advanced



AF&F Structural Design



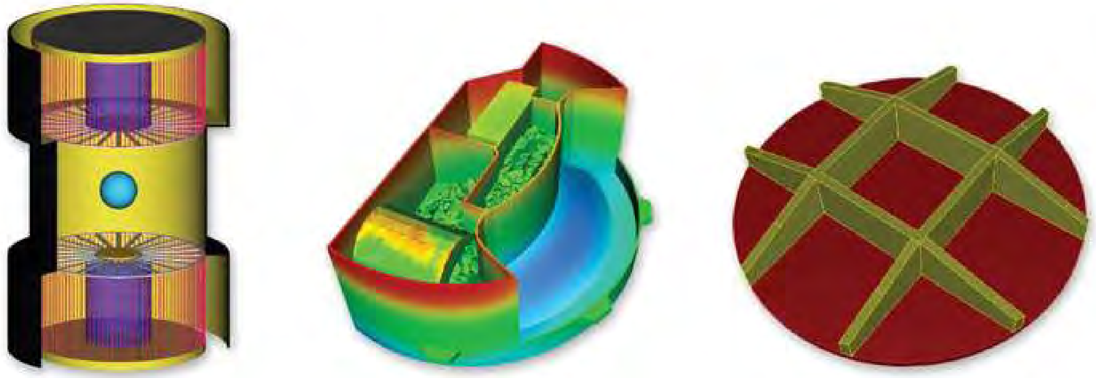
CVD Reactor Design



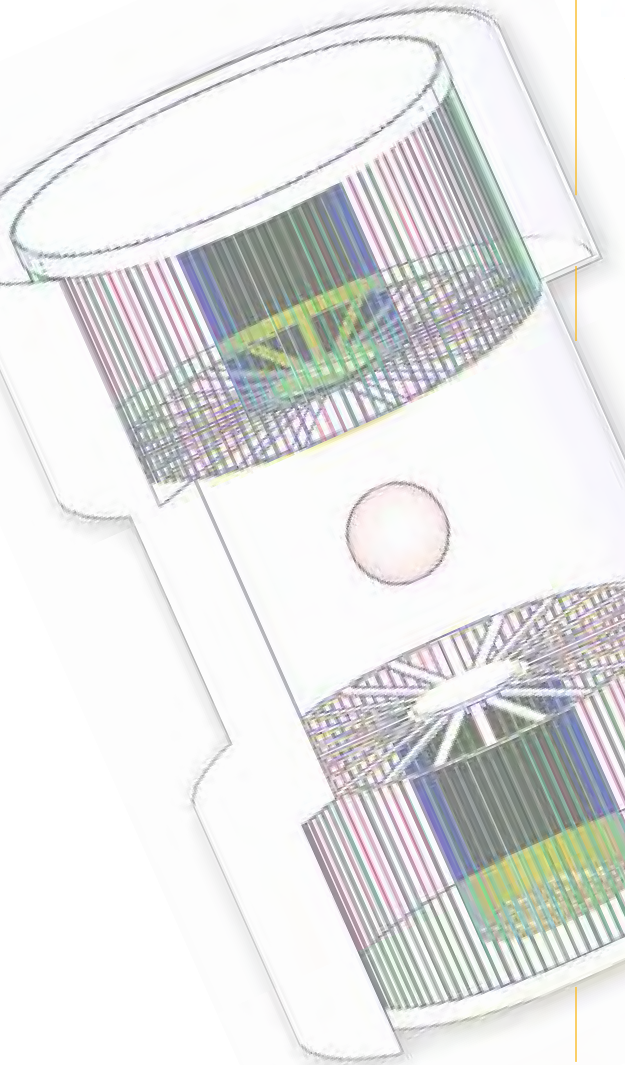
Neutron Generator Model Calibration

Figure 1. Examples of DAKOTA applications.

Figure 1 continued. Examples of DAKOTA applications.



IFC Capsule Robust Design — Fireset Thermal Surety — Radar Support Structural Design



strategies such as surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty.

Benefits to ASC and to Sandia

With the addition of automated design tools through DAKOTA, simulations may be used for more than just single-point predictions and can serve as virtual prototypes for automated assessment and improvement of system performance throughout the product life cycle. This allows Sandia analysts to address directly the fundamental issues of foremost importance to our programs, such as computing optimal designs that satisfy operational requirements, identifying worst-case surety, and assessing the predictive accuracy of computational models.

Future Developments

Highlights for FY03 include the DAKOTA Version 3.1 major release, an initial integration of DAKOTA within SIERRA, and research and development of new trust-region surrogate-based optimization under uncertainty algorithms for robust and reliability-based design. Figure 1 displays several example DAKOTA applications from within the Sandia user base. Research and development continues in the area of simultaneous analysis and design (SAND) and in the area of uncertainty quantification, with a particular emphasis on its use in model validation. In addition, closely affiliated projects will provide new optimization and uncertainty quantification algorithms through the SGOPT, COLINY, PICO, OPT++, APPS, MOOCHO, and DDACE libraries available through DAKOTA.

Modeling MEMS

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MEMS accomplishments "... extend the operational space of the ASC analysis codes to address microsystems issues associated with microsystems design, development, and qualification for the nuclear weapons stockpile."

Description

Microsystems promise to be a significant part of Sandia's security mission, including an alliance of ASC, the Microsystems and Engineering Science Applications (MESA) project, and the Microsystems Engineering Program (MEP). This alliance of programs is developing the computer codes to be used to design and qualify weapon systems incorporating MEMS. MEP is exercising the codes on MEMS applications of interest to the DSW program.

Technical Significance

The accomplishments described below extend the operational space of the ASC analysis codes to address micro-systems issues associated with micro-systems design, development, and qualification for the nuclear weapons stockpile.

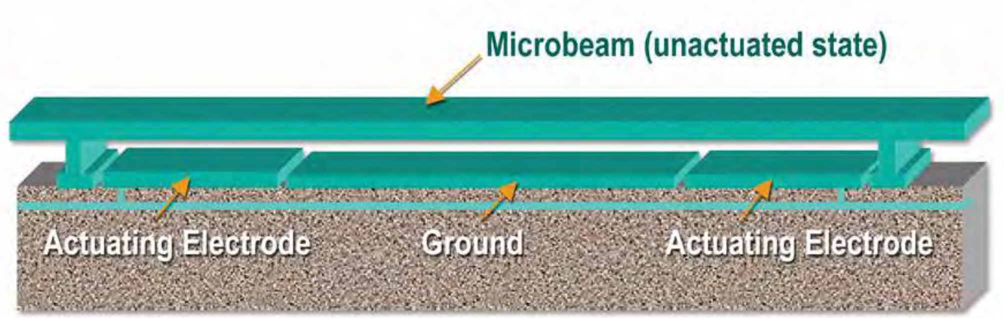
Because of the small size of micro-systems, the ratio of the surface area to the volume is much larger; consequently, surface phenomena, such as electrostatic forces, are more important than body forces such as gravity. As a result, electrostatic forces that are negligible at macro-scales generate significant motion in microsystems and are the basis of the most commonly used methods to generate motion in microsystems, such as comb-drives and torsional-ratcheting actuators (TRAs).

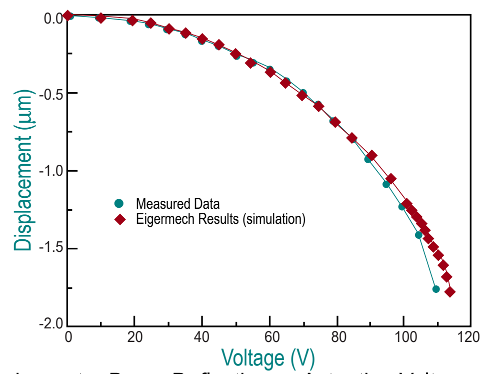
Similarly, thermal expansion of a material is negligible at macro-scales, but a few microns of expansion is a large motion in a micro-system. As a result, thermal expansion is the basis for a new actuator technology that provides significantly larger forces than do electrostatic actuators.

The fundamental feature of both electrostatic and thermal actuators is that system performance depends on coupled phenomena, which is also a focus of the SIERRA Framework being developed in the ASC Advanced Applications program at Sandia. The framework will provide all the computer-science services so that analysis code teams can focus on algorithms and computational mechanics. Another focus of the SIERRA Framework is to facilitate the coupling of analysis codes. Thus, the common focal point for ASC code development and microsystems development is coupled phenomena, which is the focus of the accomplishments discussed here.

First, we considered electrostatic actuators (Figure 1). A coupled electrostatic and quasi-static solid mechanics simulation capability was developed to evaluate the motion of electrostatic actuators. The quasistatic nonlinear solid mechanics code Adagio (which was developed in the SIERRA Framework) was coupled with the electrostatic code Eiger_S (a standalone boundary element code). Figure 1 shows an electrostatically actuated microbeam. By applying a voltage difference across regions on the substrate and the beam, an electrostatic force was applied to the beam causing it to deflect. The deflection of the center of the beam was shown in terms of experimental data and simulated results. The good comparison indicated that the initial coupling of the two codes provides accurate results.

The second example of coupled code capabilities described the motion of a thermal actuator prototype (Figure 2). The thermal actuator was a microbeam that was electrically heated, causing it to expand, which is the basis for initiating motion of the microbeam. Since the surface area was large relative to the volume of the beam,





Polychromator Beam Deflection vs Actuating Voltage
(500 μm beam length with 80 μm electrode length)

Figure 1. Electrostatically actuated microbeam. Electrostatic forces obtained by applying voltage difference between the microbeam and the actuating substrate. The simulated and measured deflections are for the midpoint of the microbeam.

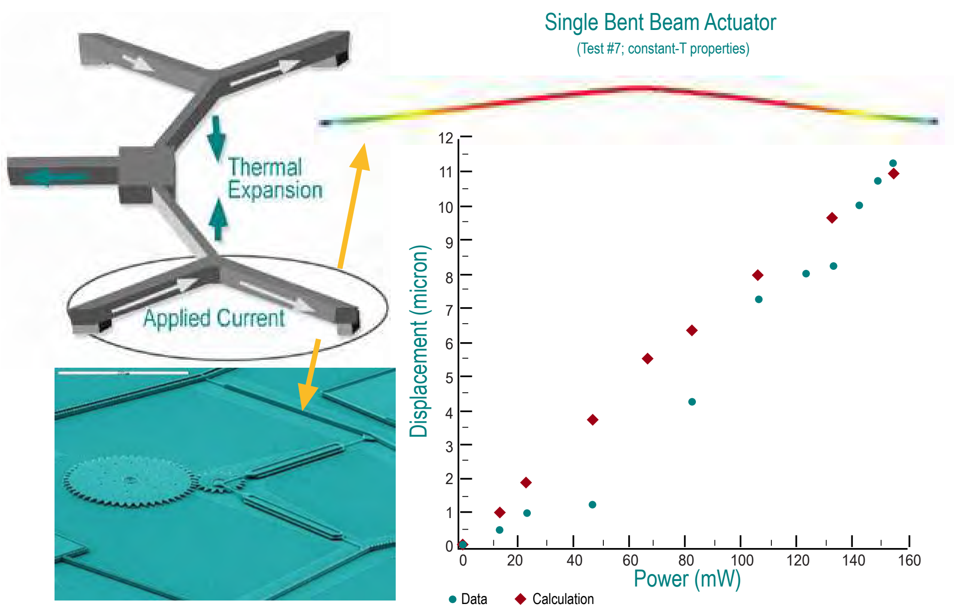


Figure 2. Prototype microsystem thermal actuator which is electrically heated, causing the polysilicon microbeam to expand (deflect). The calculated and measured deflections are shown to be in reasonably good agreement. For the calculations, the ohmic heat generation rate is assumed to be uniform, which might not be valid, and is being addressed by coupling a simulation of the electrical phenomena with the thermal and mechanical coupled codes.

heat transfer to the surrounding gas and thermal radiation was very rapid, allowing the actuator to expand (upon heating) and retract (upon cooling) at kilohertz frequencies.

To simulate the performance of the thermal actuator, the thermal analysis code Calore and the quasistatic nonlinear solid mechanics code Adagio, both of which were developed within the SIERRA Framework, were also coupled within the SIERRA Framework. The calculated deflections shown in Figure 2 were based on the assumption of a spatially uniform ohmic heat generation rate, which was a good first step but might not be within engineering tolerances. Comparison of calculated and measured deflections shown in Figure 2 are in reasonably good agreement. Better agreement is needed, though, to make plausible the use of simulations to evaluate future prototypes with confidence. Thus, in FY04, electrical phenomena are being coupled with the thermal-mechanical capability, to calculate the spatial distribution of the ohmic heat-generation rate.

As in the electromechanical code capability, the thermal-electrical-mechanical code capability has the ultimate goal of confidently eliminating conceptual designs using simulation, thereby avoiding long fabrication times. Confidence in the simulation capabilities is being developed with cooperative efforts among ASC, MESA, MEP, and Laboratory Directed Research and Development programs at Sandia.

Contribution to the Stockpile Stewardship Program (SSP)

The objective of using microsystems is not simply to provide smaller-sized components with the same functionality as existing components (although that is an important first step); rather, micro-systems will provide increased functionality that benefits our national-security mission, in the same way that semiconductors and integrated circuits provide increased functionality over macro-scale resistor/inductor/capacitor circuits and vacuum tubes.

The ultimate goal for this capability is to gain sufficient confidence in the simulation capability through combined experimental and computational studies to use the simulation capability to evaluate conceptual designs. If some designs can be confidently eliminated without having to be fabricated, years in development time could be saved, and fabrication of prototypes could be focused on workable designs.

Benefits to ASC and to Sandia

By incorporating simulation into the development of microsystems, Sandia plans to accelerate the maturation of microsystems for commercial and nuclear weapons use. Thus, there is a natural synergy between ASC and MESA. This work extends the operational space of the ASC analysis codes into the micro and noncontinuum scales.

Future Developments

FY04 work to develop electrostatic actuators will include enhancing the electromechanical coupling capability in two areas:

- Development of micro-scale constitutive models to account for the fact that polysilicon grain sizes (~ 1 micron) are a significant fraction of the overall length of the device, such that the continuum assumption is not obviously valid.
- Improved stability and efficiency of the coupling between electrostatic and quasistatic codes.

FY04 work to develop thermal actuators will include development of thermal-electrical-mechanical coupled-code capability. An important feature of the coupling is the temperature dependence of the electrical resistivity, which strongly couples the thermal and electrical analysis codes.

Modeling PMMA Chemistry in LIGA Processing

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Since LIGA is being considered, commercially, as a fabrication route for such devices as microscale valves, motors, solenoid actuators, and gear trains, remaining at the forefront of this technology should be of great value.

Description

This project formulates and solves physically based models for the exposure and development steps of the LIGA process. LIGA (an acronym from the German for lithography, electroforming, and molding) is an emerging process for the fabrication of high-aspect-ratio microstructures. The lithography involves two tasks:

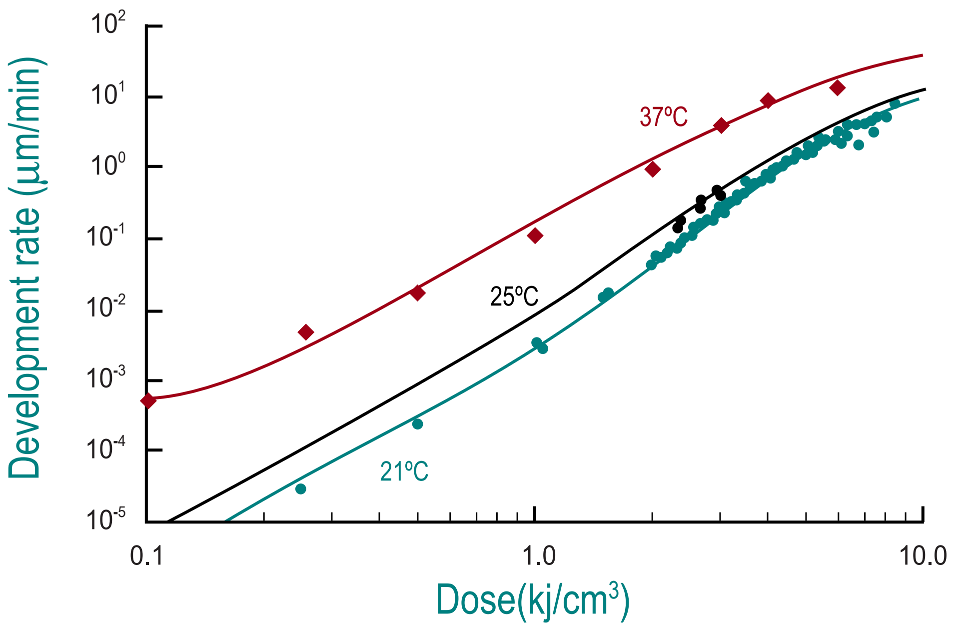
1. A thick film of polymethyl methacrylate (PMMA) resist material is exposed to x-rays through a patterned absorber mask.
2. The exposed areas are then dissolved by immersion in an organic developer solution. The resulting trenches are then filled with a suitable metal or alloy by electro-deposition, the remaining PMMA is dissolved in a strong solvent, and the finished metal part is used as a template for mass production.

LIGA has great promise for the efficient fabrication of microparts, but it requires much process improvement and optimization. Progress has been achieved through experimentation and empiricism, and it is desirable to have a more fundamental understanding of the physics and chemistry involved.

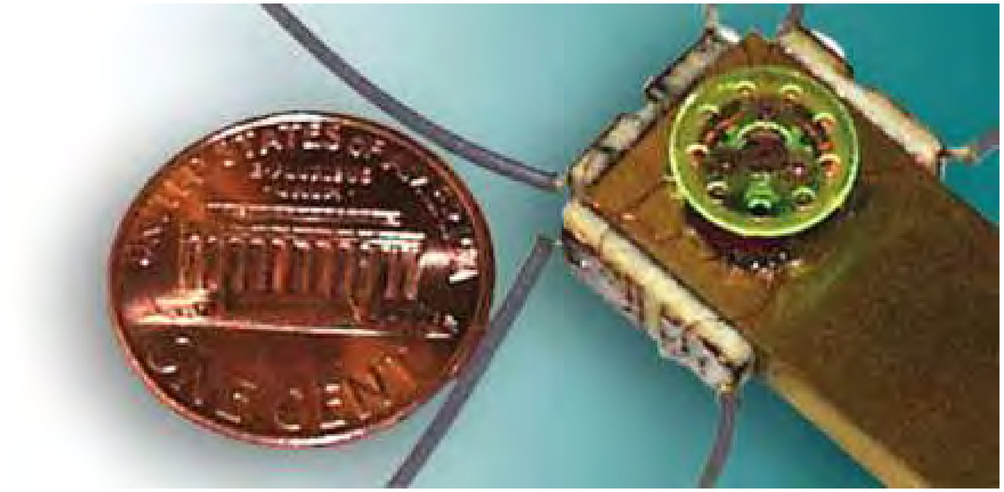
Technical Significance

The usefulness of LIGA in fabricating microparts for Defense Programs applications will depend on achieving tight dimensional tolerances. Since the dimensions of the finished part are largely determined by the geometry of the PMMA mold produced in the lithography step, predicting the dissolution rate as a function of position within the exposed resist is crucial. The variation of the deposited radiation dose with position can be computed accurately via Sandia's LEX-D code; therefore, the remaining challenge is to predict the dependence of the dissolution rate on the absorbed dose (as well as the development temperature). We have achieved this through the formulation of physically based mathematical models for both the photochemistry and the dissolution kinetics of the PMMA.

The exposure model uses a simple three-step chemical mechanism to account for both side-chain and main-chain scissions of the PMMA molecules, and it expresses the average molecular weight in terms of the absorbed x-ray dose. The development model incorporates a postulated second-order chemical reaction between the exposed polymer and the developer. Using the Stefan-Maxwell equations for multi-component diffusion and the Flory-Huggins formulas for polymer-solution thermodynamics, the model describes the conversion of PMMA molecules to a more soluble form, the transport of these molecules across an interfacial gel layer, and finally their dissolution into the solvent phase. The model's equations have been solved for various combinations of values of the key system parameters (e.g., the second-order reaction-rate constant). The results, when combined with those from the exposure model, give rise to an overall expression for the dissolution rate as a function of the development temperature and the absorbed x-ray dose. This formula has successfully been fitted to an extensive experimental data base generated at Sandia. The graph illustrates these results. Among other things, the model plausibly explains the observed variation of the activation energy for development with the x-ray



Fitting of the combined exposure-dissolution model to experimental rates from the Sandia data base.



Millimotor containing components fabricated by LIGA.

dose. The new result is well suited to supplement the semi-empirical formulas in the LEX-D code.

Contribution to the Stockpile Stewardship Program (SSP)

This project is one of several aimed at improving the fidelity and versatility of the LIGA process at Sandia. As the ability to fabricate parts with completely predictable dimensions and material properties improves, potential applications will increase. This is especially relevant to the SSP, which offers many opportunities to replace aging components with smaller, lighter, more robust counterparts. Replacement components being developed are low-g accelerometers, environmental sensing devices, millimotors, and other strong-link parts. For many such devices, LIGA is the only practical means of production. The photograph above shows a miniature electromagnetic motor containing 20 LIGA-fabricated parts.

Benefits to ASC and to Sandia

In addition to direct Defense Programs applications, progress in the optimization of LIGA has several less tangible but still important benefits to Sandia. Sandia is already recognized as a world leader in the development of this technology, from both experimental and modeling standpoints, and this project will reinforce that status. Since LIGA is being considered commercially as a fabrication route for such devices as microscale valves, motors, solenoid actuators, and gear trains, remaining at the forefront of this technology should be of great value.

Future Developments

While this work has been successful in reproducing the observed dissolution behavior in the data base, several areas for exploration remain. First, it should be verified that the constants used in fitting the data are not significantly affected by the energy spectrum of the x-ray source. The behavior of initially cross-linked PMMA should also be examined as a potential avenue to process improvement. Finally, an experimental program to confirm the existence of the chemical effects postulated here would be very enlightening.

Modeling Geological Materials for Earth Penetrating Weapons and Hard and Deeply Buried Targets

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The ability to model rock response is significant in the analysis of loads on a penetrating weapon, the analysis of ground-shock propagation, and, ultimately, the analysis of shock-structure interaction for HDBT defeat scenarios.

Description

High-fidelity predictive simulations require material models that include all the physical processes that have an impact on a solution. For earth-penetrating weapons, these materials include the materials comprising a weapon system and the materials comprising the target system. A stockpile-to-target sequence (STS) Normal project addresses how material models for the target system are developed.

This Hard and Deeply Buried Target (HDBT) material-model development project provides a library of material models for earth-penetrator analysis that describe the geological material behavior from the vicinity of the penetrating weapon site to the materials surrounding deeply buried targets. This library results from a comprehensive program of laboratory experimentation (not funded by ASC), parameter estimation, verification and regression testing, validation, documentation, and quality assurance activities.

Technical Significance

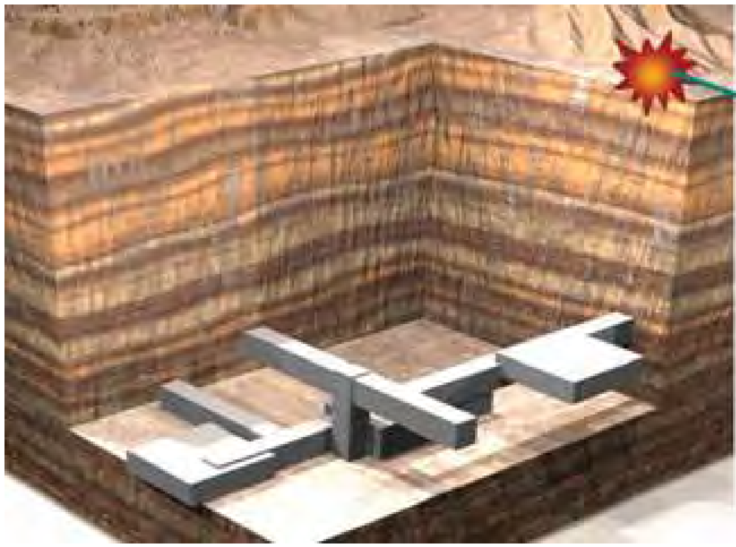
This project develops and implements, in large-scale massively parallel computer codes, material models that capture multi-physics phenomena in jointed rocks to provide high-fidelity predictive simulation for design and qualification of weapons systems. The ability to model rock response is significant in the analysis of loads on a penetrating weapon, the analysis of ground-shock propagation, and, ultimately, the analysis of shock-structure interaction for HDBT defeat scenarios. New penetrator designs rely heavily on numerical models to predict deceleration-time profiles, stresses in the penetrator, and weapon penetration depth in various hard-rock targets for different angles of attack and penetrator striking velocities.

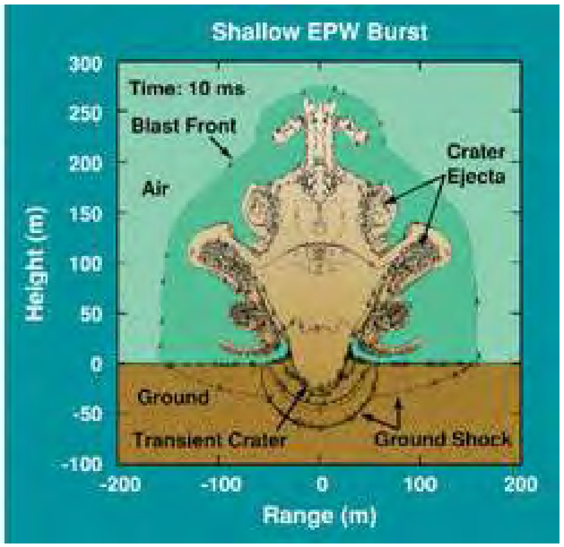
Contribution to the Stockpile Stewardship Program (SSP)

This project aligns directly with DSW deliverables. It ensures that the ASC codes have the material models necessary for STS Normal design and qualification simulations for the B61, RNEP, and other penetrators, and weapon effects on hard and deeply buried targets.

Benefits to ASC and to Sandia

This project supports the goals of ASC's and Sandia's Materials and Physics Models (M&PM) program to develop and implement models for multi-physics phenomena commensurate with length scales at which the physics predominates.





Material models are being developed for earth-penetrator analysis that describe the geological material behavior from the vicinity of the penetrating weapon site to the materials surrounding deeply buried targets.

Porous-rock material models developed under the ASC M&PM program are used in the SIERRA codes to make large-scale three-dimensional finite-element reservoir simulations during production to assist oil companies in formulating well-management procedures.

The capability to perform earth-penetrator analyses directly enhances Sandia's ability to support design and qualification issues through high-fidelity, predictive simulations. Development of these porous-rock material models has benefited from leveraging projects from the fossil-energy field—Sandia provides technical expertise to oil companies. The illustration above shows a mechanical oil-field model containing 260,000 finite elements used to model pore-pressure drawdown during oil production. Where appropriate, knowledge developed in the project will be transferred to projects unrelated to weapons work.

Future Developments

In addition to increasing the library of hard-target material models, efforts will be made to quantify material-model uncertainties, including point-wise and spatially varying quantities. Material parameter sets will be maintained in a materials data base and on a Web fileshare system. Improvements will continue to be made to address advection issues and computational efficiency. Scale effects will continue to be an important topic for future development, as will fracture processes that require treating discontinua.

Modeling Removable Epoxy Foam to Support the W76 and W80

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This work demonstrates how ASC can conduct leading-edge research while developing useful models to solve today's problems.

Description

Both the W76 and W80 AF&F use a Removable Epoxy Foam (REF) for encapsulation. Safety concerns and design guidance necessitate the

1. Development of a decomposition chemistry and response model to predict this response and an
2. Understanding of the thermal, chemical, and mechanical response of REF to abnormal thermal environments, such as fire.

A Simplified Removable Epoxy Foam (SREF) chemistry model has been developed to describe decomposition of polymeric foam exposed to high heat fluxes. The SREF model considers polymer fragments that subsequently evolve into the gas-phase based on vapor-liquid-equilibrium constraints. Percolation theory is used to describe the fragment distribution. The SREF chemistry model was implemented into the ASCI code Calore to describe the macroscopic response of the foam. Figure 1a shows calculations done with Calore. Calore is a thermal/chemistry code that uses element death and dynamic radiation enclosures to describe the developing enclosure. Calore does not solve the momentum transfer and therefore material relocation due to flow. The flow simulations include chemical kinetics, phase transitions, and material flow based on the developing viscosity. The coupled-physics model is solved using a multi-physics, finite-element code Goma capable of tracking moving liquid-vapor and solid-liquid interfaces. Figure 1b shows a 2-D snapshot of foam degradation when heated on the side.

Technical Significance

Modeling flow of decomposing foam including phase transitions is challenging. In this work, the model is further complicated by several factors: complex polymeric materials, radiation heat source, gravity-induced flow, and pressurization. In the past, liquefaction of the foam was considered negligible for modeling unconfined decomposition of polyurethane foam. This was not adequate for REF100, especially when the decomposition products were confined, since liquid formation was significant. Solid material dissolves at elevated temperatures ($T > 300$ °C) partially because of the rigid polymeric network becoming soluble by its own lightweight decomposition fragments. The complex physics associated with flow of decomposed foam has not been addressed in detail in the published literature.

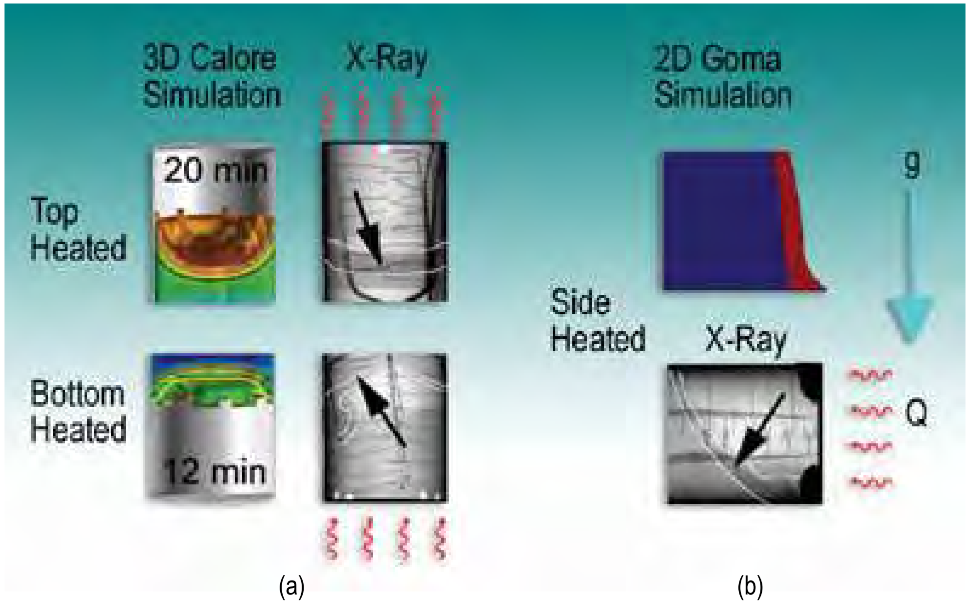
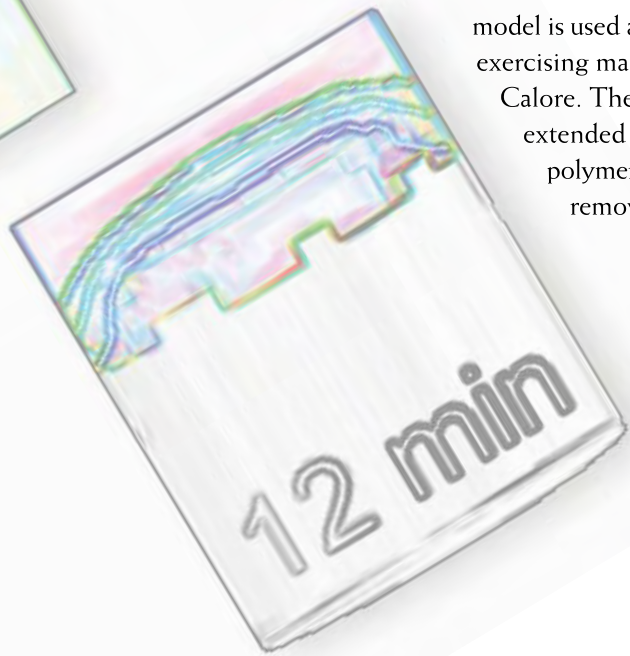


Figure 1. Comparison of REF in a 9-cm-diameter can exposed to fire-like heat fluxes at various orientations. Three-dimensional Calore modeling results and their corresponding x-ray images are shown on (a) while 2-D Goma modeling results are shown on (b). The decomposition front location is highlighted in the x-rays, using a thick black arrow. White lines indicate estimates of phase interfaces by visual judgment. Significant flow effects are observed for the bottom- and side-heated experiments.



Contribution to the Stockpile Stewardship Program (SSP)

REF encapsulates thermally and mechanically sensitive components within the firing set of the W76-1 and W80-3 systems. These systems are designed to be safe (less than 1 in 1,000,000 chance of inadvertent detonation) in a fire environment. This is accomplished by designing specific components to fail at known temperatures and times, and it requires an accurate understanding of the fire-induced response of various polymeric materials. The polymer response includes the decomposition front velocity/location, pressurization of sealed systems, formation of liquids, relocation of polymeric liquids, etc.

Benefits to ASC and to Sandia

This work demonstrates how ASC can conduct leading-edge research while developing useful models to solve today's problems. Fire-induced liquefaction of materials is not limited to foam. This work will benefit future modeling of multi-phase, multi-physics flow problems. The SREF model has proved extremely useful and pushes the limits of the ASC computational resources, especially when the model is used at full grid resolution, while exercising many of the capabilities of Calore. The methodology can be extended to other decomposing polymers of interest to Sandia (e.g., removable syntactic foams).

Future Developments

The near-term goal of the REF model research is to address pressurized systems that may have different modes of decomposition. In the long term, this analytical capability (software and engineering knowledge) is expected to apply to safety studies of all polymeric-based foam candidates. Results of the SREF model will be compared to real-time x-rays of foam in a can exposed to fire-like heat fluxes. Pressurization of sealed systems will also be considered. The model will be extended to syntactic removable foam, which is expected to behave similarly except for the substitution of glass microballoons for bubbles created using the blowing agent.

Developing Physics-Based Models of Radiation Effects on Micro-Electronic Devices

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This project demonstrates our ability to first understand difficult atomistic-scale phenomena using modeling, and then to develop component-scale models that replicate the atomistic-scale phenomena.

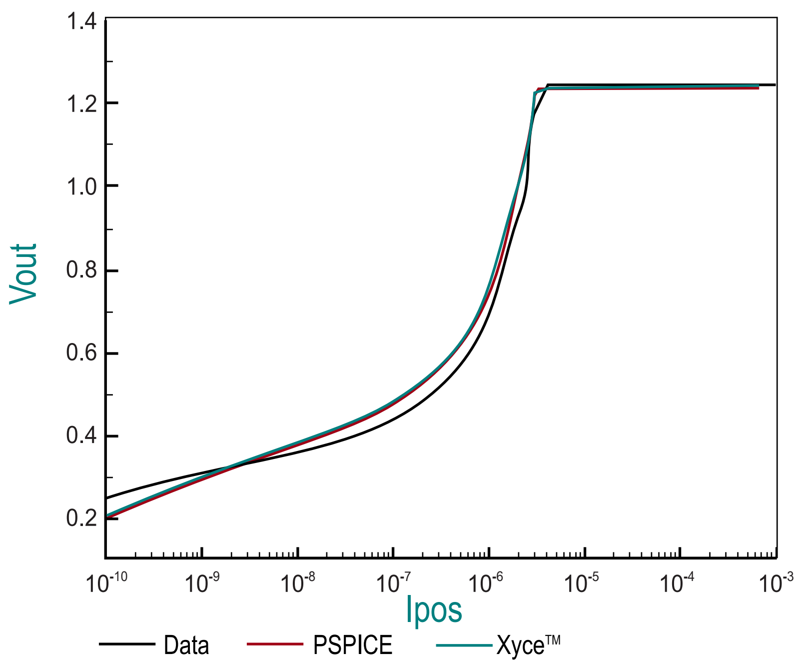
Description

The overall goal of this project is to develop physics-based models of radiation effects on microelectronic devices in the stockpile. The initial focus was established by stockpile aging studies showing that certain devices have radiation damage that depends on the dose rate of the testing. This phenomenon is called Enhanced Low Dose Rate Sensitivity (ELDRS). These results raised the concern about vulnerability of stockpile devices to the low dose-rate intrinsic radiation encountered in storage.

The specific goal of this project is to develop a computational model to be used in Xyce™ circuit simulations of the effects of low dose rate radiation at the very low dose rates expected during storage. Another goal is to develop a scientific understanding of the problem to eliminate it in future stockpile refurbishments and to avoid technical surprises. One important consideration was the absence of modeling capability for the effects of radiation on microelectronics in the stockpile. Furthermore, some of the scientific issues concerning the effects of ionizing radiation have not been resolved in the scientific literature. Given the lack of previous research and modeling, the approach taken involves a blend of scientific and engineering emphasis. This multi-scale approach uses atomistic, continuum, device and circuit simulations. In addition, a strong collaboration with experimenters was initiated early in the project.

Technical Significance

The development of the ELDRS model is based on the bimolecular recombination mechanism developed to explain ELDRS. The essence of the explanation can be obtained from the following simplified discussion of the effects of ionizing radiation on bipolar transistor devices. Such radiation releases hydrogen atoms from source sites within the silicon oxide layer surrounding the most vulnerable portion of such transistors, the base-emitter junction. This hydrogen reacts with silicon dangling bonds thereby creating interface traps that reduce the transistor gain. As part of processing, each of these dangling bonds has been "passivated" by bonding with a hydrogen atom. In the radiolysis reaction, another hydrogen atom reacts with the passivated atom to recreate the trap. In the bimolecular theory, the dose rate dependence arises because the hydrogen released by radiation reacts with other hydrogen instead of the passivated interface trap. This reduces the radiation



This figure shows the reference voltage of an unirradiated LM185 in a standard test circuit. These measurements are compared with Xyce™ simulations. They are also compared with simulations using the ELDRS model in PSPICE, another circuit simulator. As the current rises, the voltage rises and then saturates to the value 1.25 V, the reference voltage for this device. By inspection, the PSPICE and Xyce™ implementations of the ELDRS model are both in good agreement with the data.

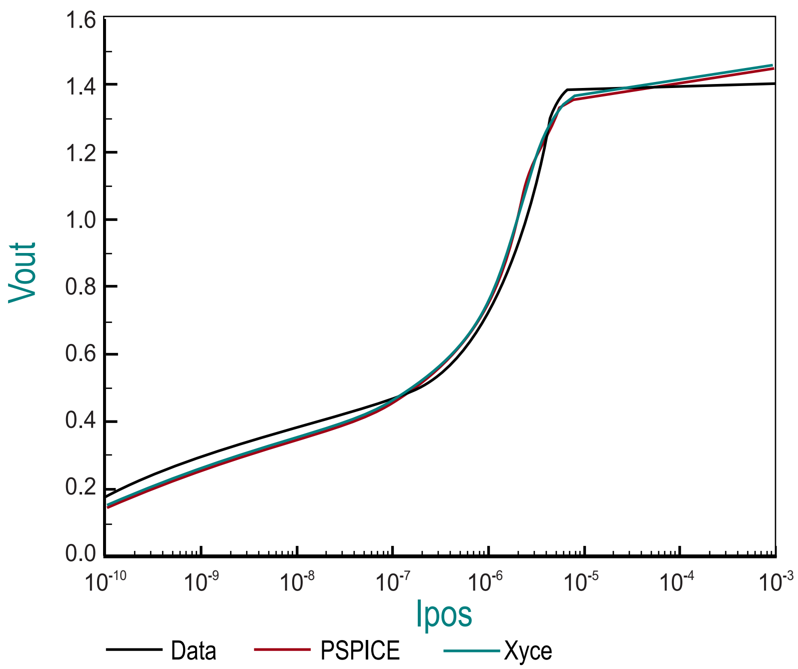
damage. Other portions of the bimolecular mechanism have a similar effect. The main consideration is that these phenomena at high dose rates reduce and obscure the true radiation softness of the device.

At low dose rates, the physical phenomena and the model both become simple. The model depends on only one parameter, the efficiency. This parameter represents the probability that the ionizing radiation will produce an interface trap. This simplified, one-parameter theory was incorporated into a model for bipolar transistors.

The new modeling capability was successfully applied to LM185 integrated circuits (ICs) used as voltage references. The effect of radiation on several of the 13 transistors in this IC was measured at several dose rates. The measurements at the lowest dose rates were used to derive an empirical value for the efficiency parameter, approximately 0.01. This parameter was then used in semiconductor device simulations for the other transistors to obtain Xyce™ models for these transistors also.

Contribution to the Stockpile Stewardship Program (SSP)

The capability to model the effects of low dose rate radiation will enable simulations to estimate the lifetime of stockpile microelectronics. Furthermore, the collaborative work has guided our approach to Enhanced Surveillance Campaign (ESC) studies of the effects of ionizing radiation on stockpile components. Also, the project led to photocurrent modeling used to verify and validate the model used for the milestone Xyce™ calculation. Presently the project is leading to a coordinated approach to physics-based models for radiation effects including low dose rate, total dose, photocurrent and neutrons.



This graph shows a similar comparison for an LM185 that has received 50 K rad of ionizing radiation during low dose rate testing. The irradiation has degraded the performance of this LM185. For example, the regulation voltage has shifted to approximately 1.4 V. The PSPICE and Xyce™ implementations are both in good agreement with these data also.

Benefits to ASC and to Sandia

This project demonstrates our ability to first understand difficult atomistic-scale phenomena using modeling, and then to develop component-scale models that replicate the atomistic-scale phenomena. This study strengthens Sandia's physics-based understanding of a puzzling material-science phenomenon that is important to the reliability of the stockpile. This work has national-scale impact because the work is applicable to the radiation effects of microelectronics in satellites.

Future Developments

An initial time-independent model has been developed for the LM185. This model will be tested by comparing the predictions of the full model to additional experiments in progress. In addition, similar models will be developed for other stockpile devices.

Simulating Thermomechanical Fatigue in Stockpile Components

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In this project, we developed a new, experimentally validated constitutive model and applied it to simulate the thermo-mechanical fatigue failure of solder in stockpile components.

Description

Failure of solder joints in weapons electronics is difficult to detect because failures cannot be observed during extended electrical inactivity. Therefore, aging solder joints in electronic systems pose a potential weapons reliability problem. Although no analysis was performed to characterize the failure mode, thermomechanical fatigue (TMF) has been identified as the prominent solder-degradation and interconnect-failure mechanism in the lead-tin solders that predominate in the current stockpile.

The goal of the Thermomechanical Fatigue of Solder Joints project is to develop coupled micro and macroscopic models that utilize state-of-the-art, high-performance computing technology to predict the degradation and lifespan of lead-tin solder joints in weapon electronics. Integrated, multi-level models enable scientists and engineers to predict the properties and lifetime of solder joints. This capability, in turn, allows both informed design decisions and early identification of reliability problems so that preventive actions can be implemented effectively.

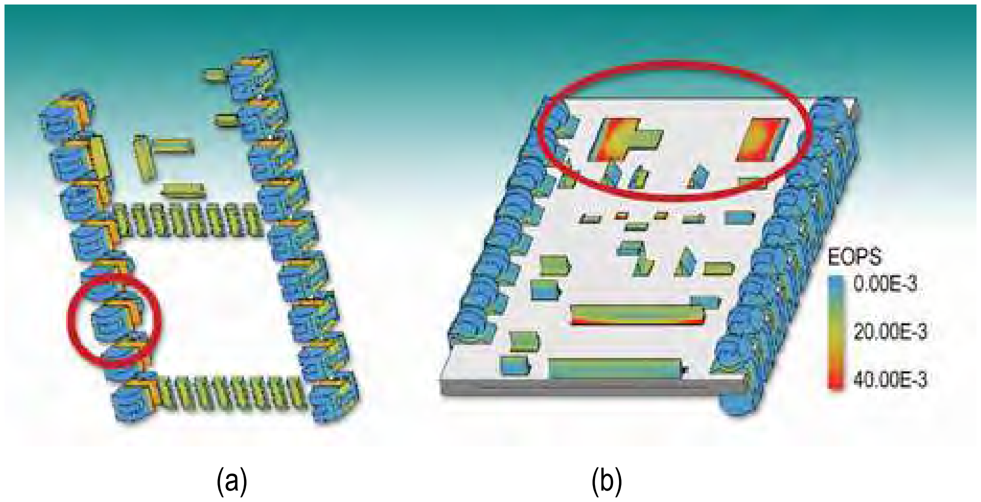
Technical Significance

Thermomechanical fatigue in solder entails a feedback loop between microstructural evolution and mechanical response. As local strain increases, the microstructure coarsens, which in turn weakens the material locally, driving strain up farther. Because of this microstructurally mediated change in mechanical response, conventional constitutive models are not adequate to capture the TMF behavior of lead-tin solders. Furthermore, localized microstructural changes govern the failure event in these materials but are not generally included in failure models. In this project, we developed a new, experimentally validated constitutive model and applied it to simulate the thermomechanical fatigue failure of solder in stockpile components.

Contribution to the Stockpile Stewardship Program (SSP)

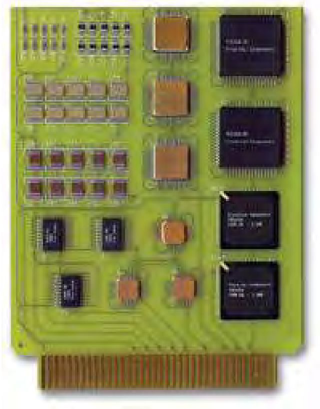
The viscoplastic continuum damage (VCD) constitutive model, developed for lead-tin solder, has been applied to analyze solder-joint failure in several weapon components. For example, in the MC4226M clock module, the VCD model predicted a greater likelihood of failure in the potted module than in the unpotted module as shown below. This application aids identification of reliability problems for the stockpile steward.

In addition, the VCD model has been applied to a range of solder-joint configurations in test vehicle circuit boards as shown above. The studies of the results suggest good-practice design rules for the weapons engineer, and a simplified VCD-based design code is being developed for use across the Complex.

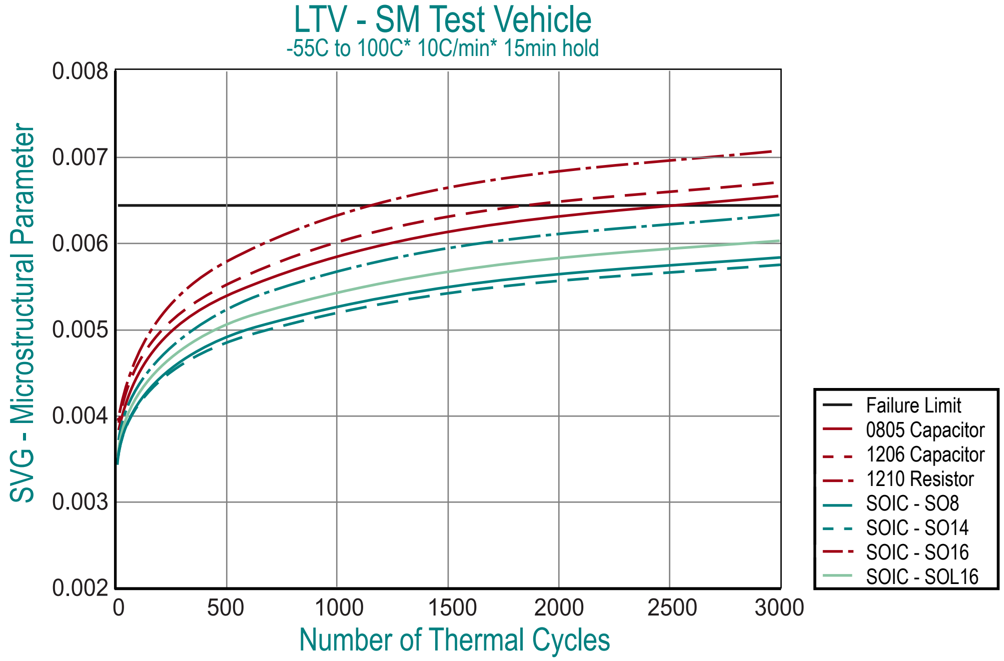


Viscoplastic continuum damage model reliability simulations of thermomechanical fatigue of solder joints in the MC4226M clock module. (a) The unpotted module fails at the edge clips (circled) after 4200 thermal cycles. (b) The potted module fails at the largest internal component (circled) after only 358 thermal cycles. The color scale shows equivalent plastic strain.

Viscoplastic continuum damage model reliability simulations of thermomechanical fatigue of solder joints in the LTV-SM circuit board test vehicle. (a) The test vehicle contains a variety of components and solder joint configurations. (b) Simulations show that some solder joints fail long before others, providing design guidance.



(a)



(b)

Benefits to ASC and to Sandia

Development and application of the VCD model has driven important extensions to ASC production codes, including JAS3D and ADAGIO/SIERRA. The results of VCD-based design and reliability simulations have contributed to Sandia's stockpile stewardship mission.

Future Developments

The VCD model will be utilized as a production-analysis tool for predicting failure in stockpile components. Furthermore, it will be incorporated in a desktop circuit board design application. Most significantly, the model will be extended to lead-free solder materials that will replace lead-tin solders in future component designs and in replacements and retrofits.

Modeling Multi-Length Scales

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A multi-length-scale theoretical framework, under which coupled multi-length-scale boundary value problems can be solved, has been completed for future implementation in the Adagio multi-level framework.

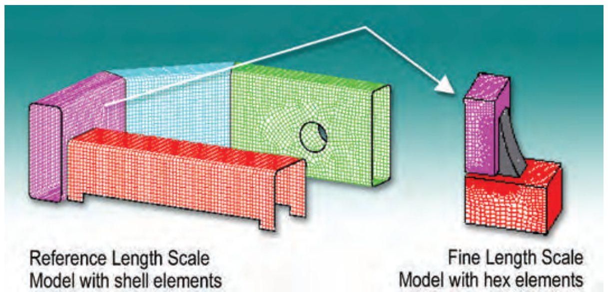

Figure 1. Failure of a welded bumper.

Description

Failure prediction is inherently a multi-length-scale phenomenon, involving a physically based failure model and an analytical capability that provides input. Traditional multi-scale global/local analytical capability provides no coupling between the two length scales. Can this coupling be incorporated as a solution strategy?

Technical Significance

Multi-length scale modeling is an analytical capability that solves multiple coupled-boundary-value problems. To provide this coupling, two continuum mechanical arguments need to be addressed. The first is a boundary constraint such that the boundary between the length scales described by two separate discretizations, Γ^{rls} and Γ^{fls}, deform consistently. The other is an interior constraint such that the material described by both length scales, within an element e^{rls}, deforms consistently.

Multi-length scale modeling should be applicable to problems using hexahedral elements and shell elements. Therefore, the boundary constraint must be developed for surface-to-volume (hex face to hex element) and surface-to-membrane (hex face to membrane element) interfaces. The interior constraint must be developed for volume-in-volume (hex element to hex element) and volume-in-surface (hex element to quad membrane). This capability is expected to be viable for quasistatic and dynamic applications.

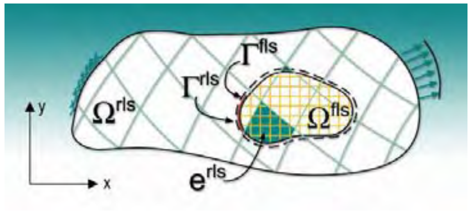

Figure 2. Discretization of reference length scale domain Ω^{rls} and Fine length scale domain Ω^{fls}, showing interfaces Γ^{rls} and Γ^{fls} and overlapping material in element e^{rls}.

Contribution to the Stockpile Stewardship Program (SSP)

A multi-length-scale theoretical framework, under which coupled multi-length-scale boundary value problems can be solved, has been completed for future implementation in the Adagio multi-level framework. The boundary constraint providing consistent deformation of the boundary between hexes and between hexes and shells is complete. As shown in Figure 3, the accuracy of the boundary constraint applies to the general interface problem of tying together meshes with dissimilar discretizations. This general capability allows separate mesh components of a larger model to be joined in a consistent, accurate manner.

A specific application of this multi-length scale analysis capability is in analyzing stress concentrations, fracture, etc., in abnormal environment drops or normal environment nose crush/tail slap. Another application is in analyzing the integrity of welds in the abnormal crash of the SGT. These applications are unique in their requirements for an explicit transient dynamics event that depends crucially on the integrity of material at stress concentrations and in joints and welds.

Benefits to ASC and to Sandia

The ability to "freely insert" a fine-length scale mesh requires a solution of a coupled boundary value problem. We anticipate that, for many applications, this ability will determine how well failure can be predicted (e.g., predicting joint failure in a laydown simulation).

Future Developments

The multi-length-scale analysis capability requires the fine-length scale model to be fully embodied in the reference scale model from the beginning of the analysis. Because the analysis of an abnormal event (crash) might proceed some time before failure at a stress concentration is imminent, inserting midway into the simulation a fine-length-scale model would be desirable for a more efficient use of computing resources.

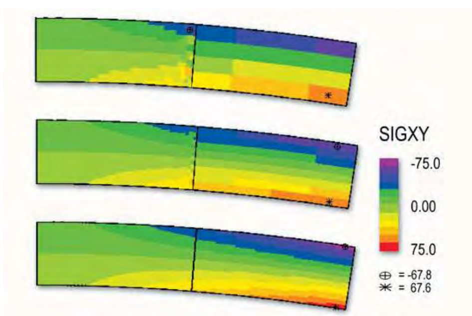

Figure 3. A mesh convergence study for consistent mesh tying. Consistent mesh tying is boundary constraint, which passes the patch test for the general case of curved interfaces.

Contributing to Risk-Informed Decisions

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In FY03, we articulated a position on risk-informed decisions, emphasizing the importance and impact of computational uncertainty quantification and validation-based credibility.

Description

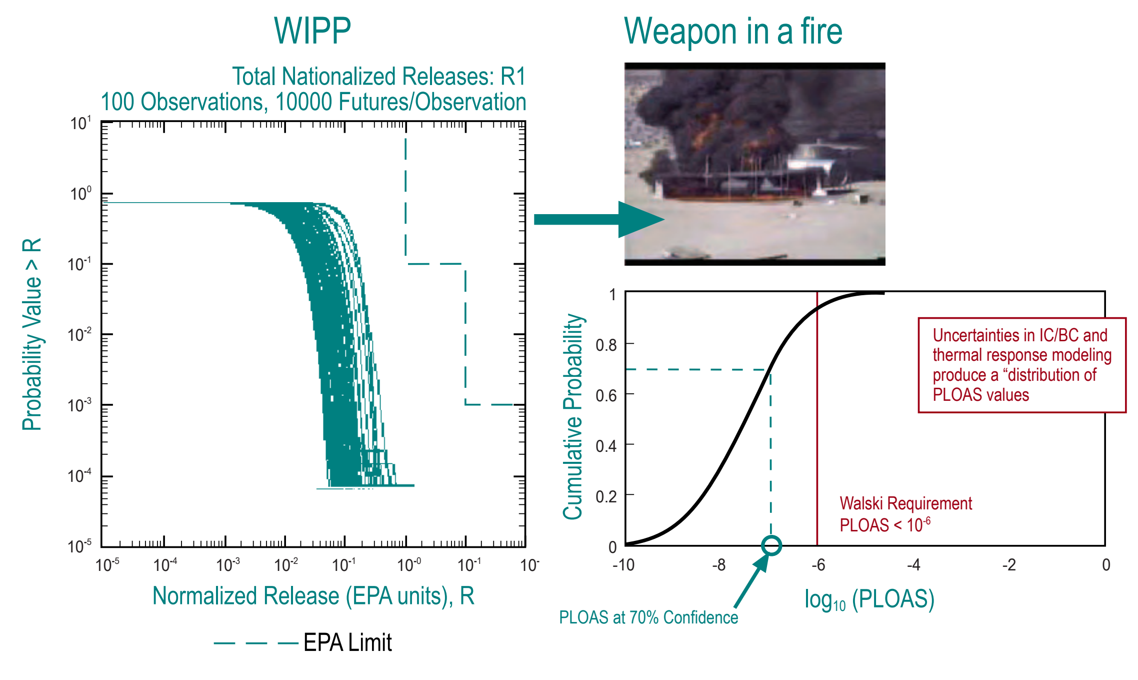
In FY03, the Verification and Validation (V&V) program began to address the NNSA specification Quantifying Margins and Uncertainty (QMU) through a series of future Level 1 milestones for specific stockpile systems. The goal of V&V was to define a technical basis for understanding QMU in computational DSW projects at Sandia, particularly in the context of risk-informed decision making and develop guidance for future V&V work focused on QMU. In FY03, we articulated a position on risk-informed decisions, emphasizing the importance and impact of computational uncertainty quantification and validation-based credibility. We systematically presented our position to Defense Programs managers at Sandia during the year. In FY04, we will build on this experience by writing a document that specifies the important technical concepts underlying risk-informed decisions using modeling and simulation and anticipated processes for appropriate application to DSW problems.

Technical Significance

Risk-informed decisions and the broad problem of QMU lie at the intersection of three important technical problems for DSW modeling and simulation: (1) suitable uncertainty quantification technologies, including deployed tools appropriate for DSW computation, are required; (2) the quantified basis for credibility in ASC codes that emerges from validation activities must be identified; and (3) a technical foundation for decisions that rely upon high-consequence modeling must be provided. Our task takes advantage of the fact that the Sandia V&V program has had a broad and integrated view of these three issues for several years and sees the need for scientific progress in all three to use ASC computational capabilities optimally to support DSW at Sandia.

Sandia has historically relied upon progress in these three areas in its technical work supporting nuclear-reactor safety analyses, the licensing of the WIPP waste-disposal site, and currently the licensing process for the proposed Yucca Mountain waste-disposal site. From this perspective, our task is not isolated technical work in the ASC program, but rather a somewhat logical extension of past Sandia experience in managing high-consequence and high-risk decisions of importance to the nation.

A key technical underpinning for our ongoing work is to build appropriately upon the past work, with due acknowledgement of the differences in problems posed by Sandia DSW and modeling capabilities provided by the ASC program. The figure at left suggests our expectations in this regard.



Historically, nuclear reactor safety and the Environmental Protection Agency-driven waste repository assessments have created methodologies for usefully quantifying uncertainties and defining margins for use in risk-informed decisions. Our task is to successfully merge past experience, ongoing technical work in validation, uncertainty quantification and ASC code development, and proper characterization of DSW problems to successfully manage risk-informed decisions for the U.S. nuclear stockpile.

Contribution to the Stockpile Stewardship Program (SSP)

Several NNSA Level 1 milestones use the language "Complete certification of a [stockpile system] with Quantified Design Margins and Uncertainties." This creates an imperative for our current task and guarantees its impact. More generally, our task confronts the increasing importance of modeling and simulation to the SSP. Risk-informed decisions are historically and currently common to the SSP. Development of a definitive scientific methodology for successfully blending computational modeling and simulation into the SSP decision framework with due accounting for uncertainties and limitations is a necessary element of managing the U.S. nuclear stockpile in the future.

Benefits to ASC and to Sandia

Our focused effort to develop an appropriate framework and implementation strategy for QMU and risk-informed decisions in the context of large-scale computational modeling directly supports the ASC program and its impact on Sandia's DSW.

Future Developments

In FY04, we will complete a technical specification of risk-informed decision principles and QMU appropriate for Sandia DSW, ASC, and the V&V program. Beyond FY04, the emphasis will be on implementing this specification for the ongoing DSW modeling activities and SSP related milestones, such as LEP schedules. We stress, however, that we perceive our future steps to be evolutionary, not revolutionary, at least from the perspective of the V&V program. The ultimate goal to support risk-informed decisions has been built into the V&V program at Sandia from the beginning and is an important basis for our intense desire to link ongoing V&V activities to important DSW work at Sandia. During FY04 and beyond, we see an ever-increasing focus on this need.

Meeting ASC's Validation Milestones on Non-Nuclear Environments

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Validation milestones are critical to the Sandia Verification & Validation (V&V) program. They emphasize our most important V&V methodologies and processes and prototype their application to DSW activities.

Description

Milestones subject to external review by the Non-Nuclear Environments Simulation review panel have been defined and are progressing. In FY03, progress toward the Verification and Validation (V&V) Level 1 milestone, *"Initial Validation of STS Abnormal Environments,"* (VV-4.1) due by the close of the second quarter of FY04, was particularly noteworthy. The milestone was precisely specified, and progress toward delivery was presented during the May 2003 external panel review. Final specification of this milestone was a key issue because concrete specification of additional validation milestones now mirrors VV-4.1, particularly the specification of Level 1 milestone *"Initial Validation of STS Hostile Environment Blast and Impulse Simulation,"* (VV-5.1) due by the close of the first quarter of FY05.

Validation milestones are critical to Sandia's V&V program. They emphasize our most important V&V methodologies and processes and prototype their application to DSW activities. These milestones have been carefully aligned with ongoing LEP efforts, which increase their weapon-program impact as well as associated risks for delivery on the milestone schedule.

Technical Significance

The Sandia V&V program has developed and documented themes and methodologies for establishing the credibility of ASC codes for stockpile applications. The programmatic Level 2 milestones provide a critical demonstration of these methodologies for DSW problems of importance. Progress on VV-4.1 in FY03 directly supports Sandia LEP activities for the W80-3.

Key technical components of VV-4.1 are directed at predictive credibility for application of the Calore code (thermal modeling) and Presto code (mechanics modeling) to abnormal environments. Work in FY03 emphasized code verification, validation calculation accuracy assessment through convergence studies and error-estimation techniques, execution of dedicated and coordinated validation experiments (provided by Campaign 6) responding to documented validation plans, uncertainty quantification of experimental-computational validation comparisons, and analysis of predictive credibility of Calore and Presto resulting from completed validation activities. Progress in all these areas was presented at the May 2003 Non-Nuclear milestone review. The written comments of the review panel stated that VV-4.1 would likely be achieved on schedule, although risks were identified. The risks of concern primarily centered on (1) close linkage of the milestone to W80-3 LEP schedules that are not controlled by the V&V program and (2) milestone dependence on successful research and development (R&D) in the science of credibility quantification, an ongoing activity in the Sandia program.

The milestones use a hierarchical approach to validation (see next page) for abnormal mechanical environments. The hierarchy starts with material and constitutive law characterization, builds on experiments of increasing geometric and physics complexity, and culminates in an integral system test. In the absence of the lower elements, analyses of the system test will be conducted with many unconstrained "knobs." The most that can be hoped for is a calibrated model rather than a predictive model; consequently, inclusion of hierarchical elements significantly increases the predictive capabilities of a model by ensuring that we get the right answer for the right reason. Do we then need a system test, given the investment in the lower element of the hierarchy? We argue that at least one system test is desirable to disclose any unknowns. This hierarchical approach to validation, along with the process elements noted above, provides evidence of "due diligence" for high-consequence decisions.

Contribution to the Stockpile Stewardship Program (SSP)

VV-4.1 expresses the most important underlying principle of the Sandia V&V program—that validation must be strongly linked to an intended application of the subject code(s). VV-4.1 is very tightly correlated with W80-3 DSW work, which guarantees significant SSP impact for even partial milestone success. The problems VV-4.1 addresses are not *related* to stockpile issues. Rather, these problems *are* stockpile issues.

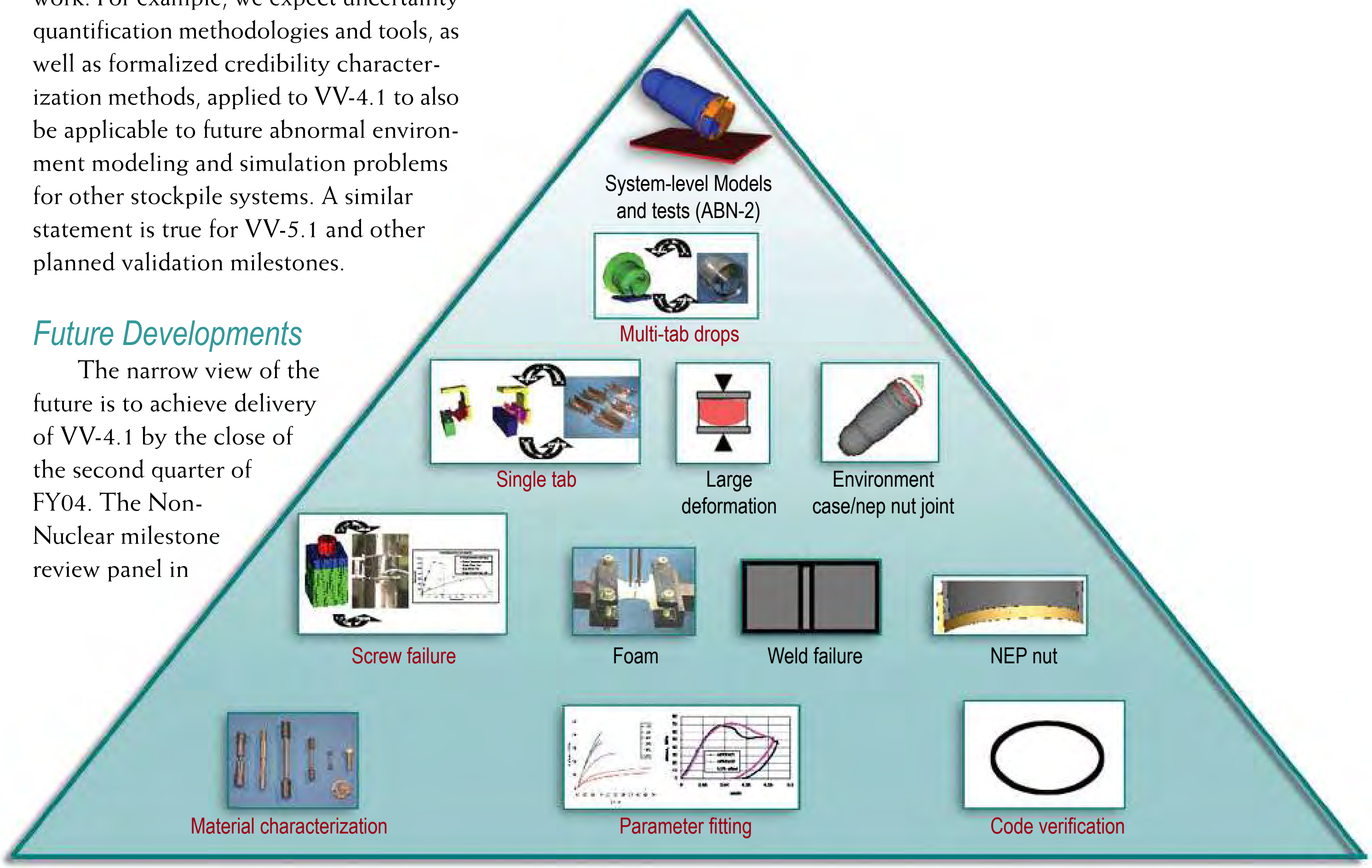
Benefits to ASC and to Sandia

VV-4.1 implements general methodologies and processes that the Sandia V&V program advocates for all V&V work supporting computational DSW activities at Sandia. Future milestones are specified similarly. Because the methodological demands and constraints of these milestones are equally applicable to the broad scope of computational DSW work at Sandia, progress and success on VV-4.1 and other milestones can easily be leveraged for future non-milestone-centric weapons work. For example, we expect uncertainty quantification methodologies and tools, as well as formalized credibility characterization methods, applied to VV-4.1 to also be applicable to future abnormal environment modeling and simulation problems for other stockpile systems. A similar statement is true for VV-5.1 and other planned validation milestones.

Future Developments

The narrow view of the future is to achieve delivery of VV-4.1 by the close of the second quarter of FY04. The Non-Nuclear milestone review panel in the May 2003 review identified some issues that must be dealt with to achieve this goal. These include further code verification for Presto, progress on solution accuracy estimation methods, and particular validation issues associated with thermal analysis. We are addressing these issues and others, and progress was reviewed again in November 2003.

More broadly, the future is dominated by the impact of our V&V milestone work on DSW at Sandia, in particular the W80-3 LEP for milestone VV-4.1. We will continue to measure our success by our ultimate impact on DSW. What we accomplish in V&V is a necessary condition for application of Sandia ASC codes to DSW problems.



Hierarchical approach to validation for abnormal mechanical environments.

Supporting Experimentation on the Z Pinch Machine

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The long-term mission of developing a pulsed power high-yield fusion capability also contributes to a growing national interest in inertial fusion energy.

Description

The Z Machine is a valuable NNSA facility for obtaining data from Sandia's High Energy Density Physics (HEDP) Program for use in validating ASC codes, certifying the survivability of non-nuclear weapons components, and dealing with issues related to Significant Finding Investigations (SFIs). The HEDP program primarily contributes through participation in the science campaigns, including: dynamic materials (C-2), secondary certification (C-4), nuclear survivability (C-7), and high-yield fusion (C-10). The long-term mission of developing a pulsed power high-yield fusion capability also contributes to a growing national interest in inertial fusion energy.

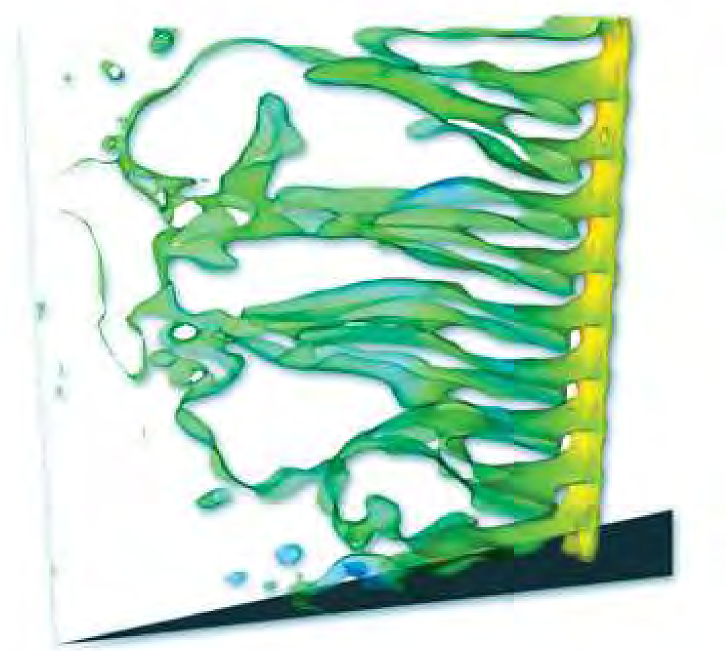
Technical Significance

Effective use of the Z experimental facility requires a predictive design capability for creating HEDP environments and applying them to the needs of the Stockpile Stewardship Program (SSP). ASC has partnered with the HEDP Program in the development of ALEGRA-HEDP, a numerical modeling capability used to simulate HEDP environments that solves the resistive magnetohydrodynamic equations coupled with thermal conduction, radiation transport, two-temperature physics, and an external circuit model. Since the fidelity of a simulation is only as good as the underlying equation-of-state (EOS), opacity and conductivity models, a variety of such models have been implemented and new databases are under development for mission-critical materials (funded by HEDP and LDRD).

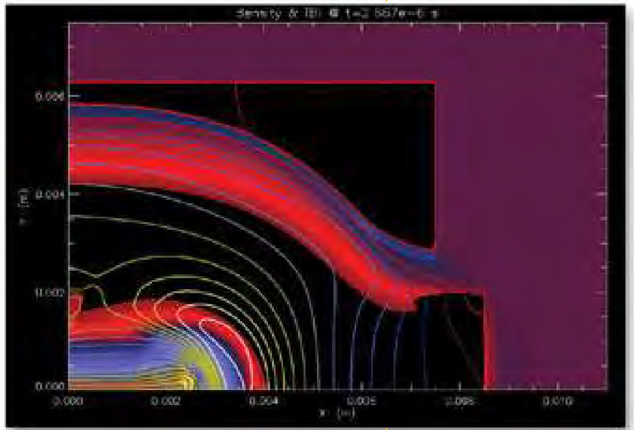
Contribution to the Stockpile Stewardship Program (SSP)

ALEGRA-HEDP is contributing to the SSP through simulations of the HEDP x-ray environments required for the Campaigns 4, 7, and 10 applications leading to increased understanding of the initiation, implosion and stagnation of the plasmas from these inherently 3-D wire array z-pinches. During FY03, ALEGRA-HEDP was successful in modeling the transition of single, micron-sized wires from cold solid to coronal plasma surrounding heated cores, and the results were compared with experimental data from Cornell University. The results from these simulations were used to guide 2- and 3-D simulations of wire array ablation (see figure). In particular, 3-D simulations have provided physical insight into experimentally observed non-uniform mass ablation along the length of the wires. ALEGRA-HEDP simulations support the hypothesis that the non-uniform mass ablation is a result of the "sausage" (m=0) instability, which leads to variations in the strength of the local magnetic field within the global field of the wire array. These simulations have resulted in the generation of new theory and understanding associated with wire array ablation, and these results have been presented at the American Physical Society's Division of Plasma Physics, the International Conference on Inertial Fusion Sciences & Applications, the International Conference on the Numerical Simulation of Plasmas. Various articles have also been submitted to Physics of Plasmas.

ALEGRA-HEDP is also contributing to the SSP through the design, fielding and analysis of experiments in support of the C-2 dynamic materials program on the Z machine. A predictive capability has been developed for modeling the launching of flyer plates using magnetic forces. The Isentropic Compression Experiment (ICE) technique is used to



perform EOS measurements of materials shocked by flyer plates launched at speeds up to 28 km/s. ALEGRA-HEDP has played a key role in guiding the C-2 program.

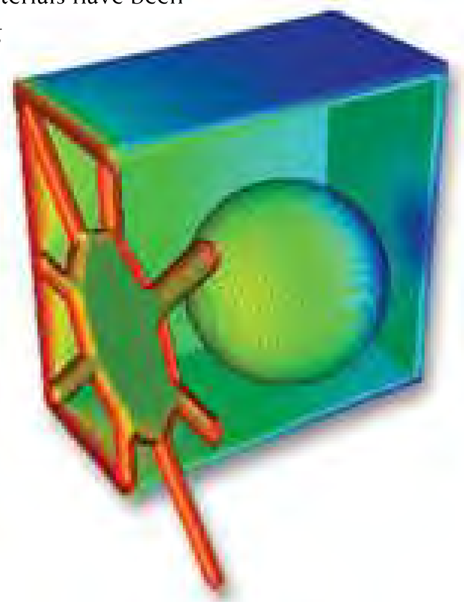


After an initial period of algorithm and database development, ALEGRA-HEDP was validated against existing Z data and has subsequently been used to design the necessary configurations to meet a variety of program requirements. Specifically, ALEGRA-HEDP was instrumental in designing the configuration that enabled the C-2 team to successfully reach the 28 km/s flyer plate velocity that was an FY03 Lockheed Martin Corporate Milestone (see figure above).

Benefits to ASC and to Sandia

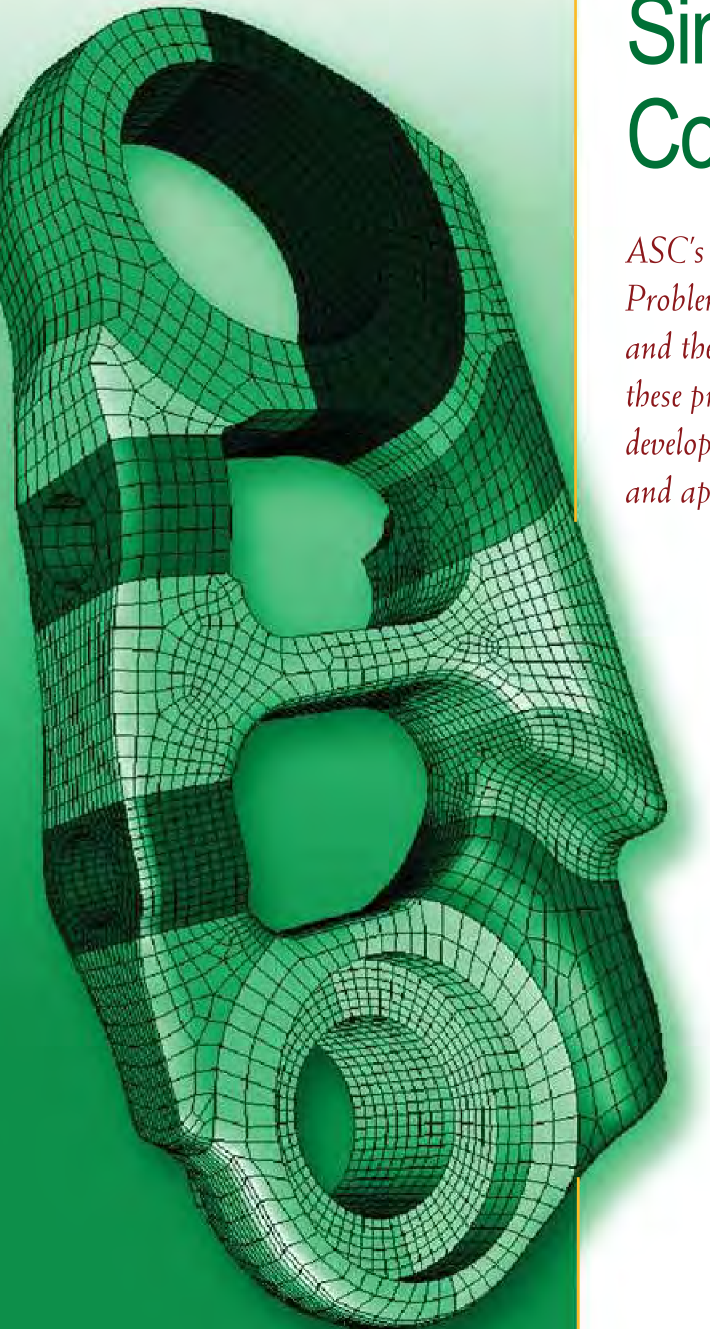
Since radiation plays such a key role on the Z machine, accurate radiation transport is necessary for success in the numerical modeling effort. During FY03, collaboration between Sandia and Lawrence Livermore resulted in the exchange and implementation of the Kull implicit Monte Carlo (IMC) package into ALEGRA-HEDP. Investigations are currently under way to compare IMC results (see figure at right) with those obtained using the flux limited diffusion approximation, comparing accuracy versus computational cost. To date, we have tested the scaling of the IMC package with up to 100 million particles and 4 million nodes on 250 processors.

The development and support of ALEGRA-HEDP have impacted multiple departments at Sandia. In order to obtain a solution to the magnetic field, a state-of-the-art algebraic multi-level iterative solver geared toward the magnetic induction equation was created (Depts. 9214, Computational Math/Algorithms and 9231, Computational Physics R&D). Significant emphasis has been placed on the scalability of this algorithm in order to obtain efficient solutions on ~1000 processors on ASC Red and Cplant™. Significant enhancements to material models were also required in order for simulations to match experimental data. Quantum molecular dynamics simulations (Depts. 1674, HEDP Theory/ICF Target Design & 9235, Computational Materials and Molecular Biology) are currently being used to modify conductivity models, EOS, and opacity models. Various materials have been upgraded including copper, tungsten, and stainless steel.



Future Developments

The development and use of ALEGRA-HEDP in the Z experimental program is an excellent example of the NNSA's goal to enhance synergy between ASC code development and HEDP experimental programs. Future software development is planned to meet a proposed FY05 Verification & Validation (V&V) milestone involving simulation support for the Z machine refurbishment (ZR). The ALEGRA-HEDP group has also provided justification for the acquisition of ASC Red Storm due to the significant computational demands of the associated algorithms and the needs of the Z experimental program. Future algorithmic development and simulation provide requirements for the development of Petaflop computers to tackle simulations in support of inertial confinement fusion.



Simulation and Computer Science

ASC's Simulation and Computer Science (S&CS) component is composed of four elements: Problem Solving Environment (PSE), Distance Computing (DisCom), PathForward, and the Visual Interactive Environment for Weapons Simulation (VIEWS). Together these program elements provide solutions to weapons designers and engineers, application developers, and integrators of the computer platforms and other systems to develop, execute, and apply the simulations.

Providing Scalable I/O Infrastructure

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The Scalable I/O project works with vendors and researchers to provide reliable, high-performance input/output for all SSP simulations…

Illustrated on the right is the relationship of the file system (driven by the I/O libraries) to the other high-performance system components.

Description

The Scalable I/O (input/output) project provides scalable I/O infrastructure for ASC and Stockpile Stewardship Program (SSP) computations, such as coupled multi-physics simulations, and for shared use of resources, such as distance computing for 10–30 teraOPS systems. These may involve high-fidelity, full-system simulation capabilities. The project includes work with vendors and researchers to provide reliable, high-performance, easily used scalable I/O libraries and file systems that make optimum use of disk I/O rates of 25 gigabytes/s and beyond. The project's goal is also to educate users on how to ensure optimum I/O performance from their applications.

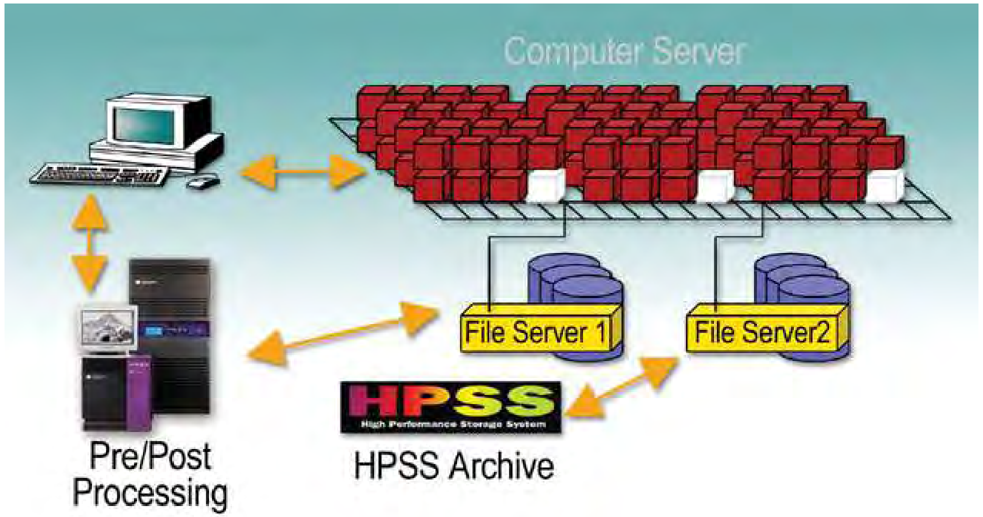
Technical Significance

The Scalable I/O libraries contribute to the integration of current and future compute platforms, visualization-rendering engines, and data management, pre- and post-processor servers. To support advanced data management capabilities, the project ensures that higher-level I/O libraries effectively use the lower level software and capabilities. In particular, the layers of the tri-lab high-level I/O model (e.g., SAF, HDF5, MPI-I/O, and industry and research file systems) must work well together on all ASC platforms. The project will continue end-to-end testing of these layers and help to analyze and improve the overall performance seen by the applications.

The Scalable I/O File Systems work provides immediate solutions for ASC and SSP applications, as well as a prototype data strategy to support future platform disk I/O rates of 25 gigabytes and beyond. The File Systems work provides a migration path to ASC Scalable Global Secure File System (SGSFS), a commercial file system that can be used on the largest tri-lab platforms and addresses performance needs.

In particular, the project will

- Work with vendors and researchers to promote, monitor, and guide development of new, more capable future I/O libraries and file systems,
- Provide parallel file system capability for cluster computing platforms,
- Work with researchers to improve the Parallel Virtual File System (PVFS) for Sandia's cluster computing platforms, and
- Investigate solutions for an ASC-wide, global parallel file system for SGSFS risk mitigation and to provide a viable replacement for distributed file systems (DFS).



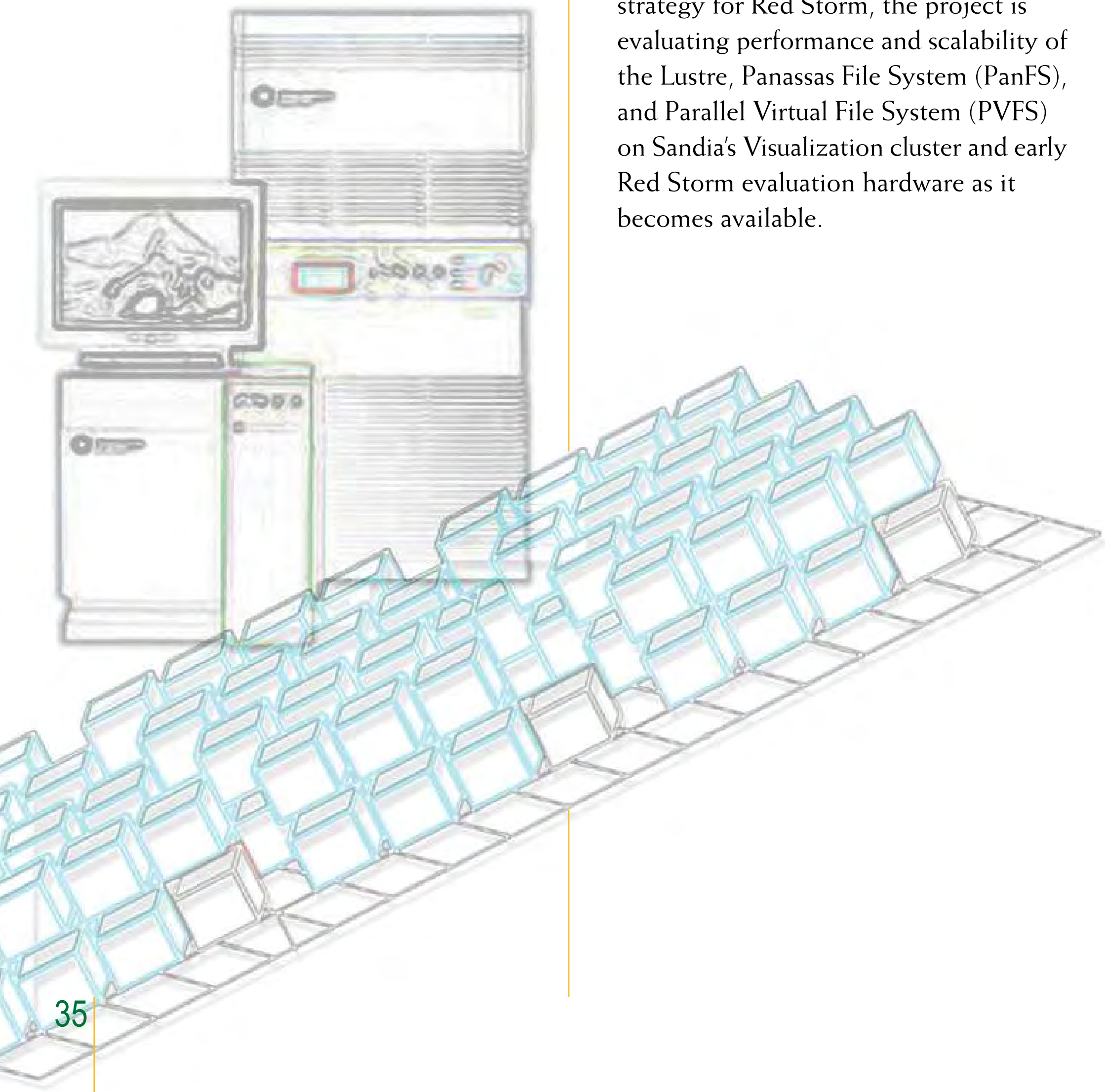
Contribution to the Stockpile Stewardship Program (SSP)

The Scalable I/O project works with vendors and researchers to provide reliable, high-performance input/output for all SSP simulations, data pre- and post-processing, visualization, and analysis on Sandia's current and future ASC and cluster computing platforms.

Input/output infrastructure used by SSP applications includes intermediate I/O libraries, such as MPI-I/O and parallel HDF5, and parallel file systems for current and future platforms.

Benefits to ASC and to Sandia

The Scalable I/O project works with vendors and researchers to provide reliable, high-performance input/output for all ASC simulations, data pre- and post-processing, visualization, and analysis on Sandia's current and future ASC and cluster computing platforms.



Red Storm parallel file system capability and performance, as well as the performance and scalability of intermediate I/O libraries such as MPI-I/O and parallel HDF5, depend on the Scalable I/O project. In turn, applications such as the SIERRA framework, through the sets and fields (SAF) project, and post-processing data management also depend on it.

The project has developed an application-level I/O library that provides a virtual file system capability for Red Storm compute nodes. As a risk-mitigation strategy for Red Storm, the project is evaluating performance and scalability of the Lustre, Panassas File System (PanFS), and Parallel Virtual File System (PVFS) on Sandia's Visualization cluster and early Red Storm evaluation hardware as it becomes available.

In particular, the project provides the following benefits to ASC and Sandia:

- Optimum performance and improved reliability of intermediate I/O libraries,
- Parallel file system capability for Sandia's current and future ASC and cluster computing platforms,
- Integration of external commercial servers for data storage, and
- User education and guidance to ensure optimum I/O performance from their applications.

Future Developments

A key element for accomplishing these goals is the continued development of SGSFS, a commercial file system that can be used on the largest tri-lab platforms and addresses our performance needs.

We will continue to promote, monitor, and guide development of new, more capable future file systems, including SGSFS. We will also mitigate SGSFS risk and provide a viable replacement for DFS, investigate solutions for an ASC-wide global file system, including possible new path-forward proposals.

We are also investigating I/O issues for data processing and performance for large data simulation and visualization issues that involve integrating the optimized I/O libraries with scalable data services, providing end-to-end I/O support for scalable data services, and delivering scalable architectures for I/O and data manipulation.

The project will work with researchers to analyze and improve the overall end-to-end I/O performance as seen by the applications. This work includes:

- Investigating distributed file systems to identify end-to-end I/O issues related to network design and/or operating system kernel implementations,
- Exploring optimizations for smaller data transfers in a scalable, portable way using MPI-I/O,
- Modifying NFS version 4 standard to provide Wide Area Network (WAN) enabled access to file servers, and
- Exploring scalable meta-data services, alternate data cache coherency mechanisms, and extensions to object-based disk (OBD) storage.

Creating a Distance Computing Environment for the ASC Program

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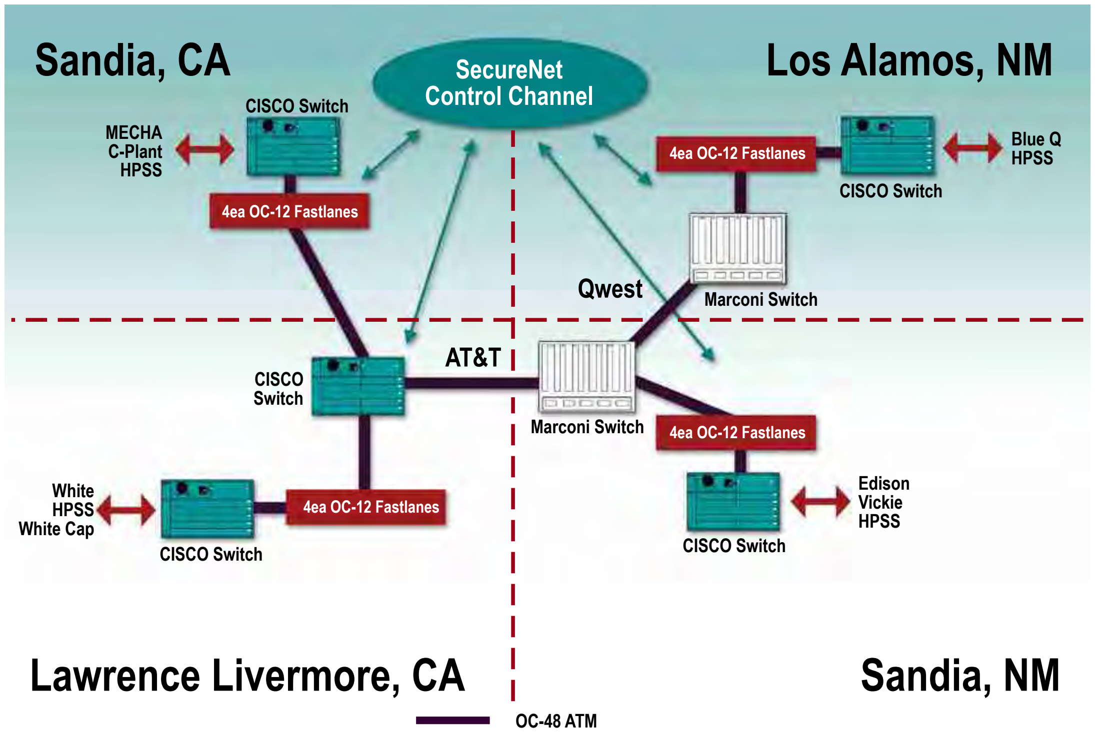
This work demonstrates how ASC was able to use the capability machines at remote locations as if they were local resources by creating a distance computing environment.

Description

Distance Computing (DisCom) is an important aspect of the ASC program. The primary goal of the DisCom Wide Area Network (WAN) is to ensure that ASC resources are shared among the labs, thereby better utilizing programmatic funds.

From an infrastructure viewpoint, the ASC effort has been focused on the supercomputers, visualization systems, and assorted support systems primarily located at the three weapons laboratories: Los Alamos, Lawrence Livermore, and Sandia. Part of the implementation strategy for these expensive hardware systems was to create an environment for efficiently sharing these expensive resources. Sandia network engineers led the tri-lab team effort to design the high-performance network that integrates the three laboratories in support of ASC's mission. Thus DisCom makes resource sharing possible and allows users to utilize remote ASC resources as if they were located locally. The performance of the DisCom WAN determines the practicality of such resource sharing. This resource has enabled code developers and analysts to use the best and most powerful machines in support of their stockpile stewardship work.

The DisCom WAN (illustrated below) is based on two 2.5 gigabit per second (OC-48) network links provided by AT&T and Qwest Communications. Various network technologies were used to create the network including Asynchronous Transfer Mode (ATM), Ethernet, and the ubiquitous TCP/IP protocol set. Given the initial ASC/DisCom performance goal of achieving a 100 megabyte per second transfer rate for large data files, the DisCom WAN engineering included support for multiple data streams in order to overcome performance limitations of existing network elements and of the network interface card implementations in ASC resources. The network element that limited performance was the NSA defined Type I encryptors. In fact, four 622 (OC-12) megabit per second Type I encryptors had to be installed in parallel at each site in order to achieve performance commensurate with the 2.5 gigabit per second network links. The network design utilized the existing SecureNet/ESNet to provide a secure and reliable control channel for file transfers while it reserved the expensive 2.5 gigabit per second DisCom WAN file transfers.



Network links of the Wide Area Network

Technical Significance

In conjunction with the creation of the parallel version of the File Transfer Protocol (FTP) application created for ASC compute resources, the DisCom WAN has provided users the capability to transfer large data files among laboratories at speeds up to 100 megabytes per second.This file-transfer capability allows distance computing by making it possible for a user to model a physical phenomenon on a remote ASC

The WAN is monitored continuously

resource, transfer the resulting output to a second remote ASC resource for post-processing, and finally store the visualization output on local storage. Such activity has become routine for ASC users.

Contribution to the Stockpile Stewardship Program (SSP)

The ASC distance computing environment made the next generation capability machine available to remote users to support ASC modeling and simulation activities for DSW and SSP work. This work includes W76 and W80 modeling and simulation activities.

Benefits to ASC and to Sandia

Through DisCom, ASC researchers have been able to use capability machines at remote locations as if they were local resources. Moreover, these capability machines have been used remotely for: code development, porting, and file transfers; all work related to Level 1 milestones associated with ASC's Applications and Simulation & Computer Science program elements; and W76 and W80 DSW activities.

Future Developments

While the initial implementation of the DisCom WAN utilized the best technology available, continued development means that new alternatives are becoming available. In particular, higher speed encryptors can be used to replace the four parallel encryptors, thereby reducing complexity. In the longer term, IP-based encryptors can be used to replace the current ATM encryptors, further simplifying the network design by reducing the number of technologies deployed. Modeling and simulation is being used and will continue to grow in helping to optimize WAN performance. In addition, operational procedures are continually evaluated to improve reliability and availability.

Improving ASC Customer Support Through the Synchronized Account Request Automated ProcEss (SARAPE)

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This work demonstrates how ASC can use everyday Web technologies to significantly improve processes to better support its customer.

Description

Previously, computer accounts at Sandia were issued by individuals accessing the WebCARS application on Sandia's internal restricted network. This network is not accessible to external customers of the laboratory or to customers who do not have account authorization. Therefore, requesting an account for these users was completed via hard copy and manual processing. This paper process was cumbersome and unreliable with account requests faxed among the users' origination site, the host computer site and eventually password administration.

To address the needs to improve the turn around time for getting an account, simplify the account request process, and improve the robustness of the process, we developed Sandia Account Request Automated ProcEss (SARAPE). SARAPE is an automated front-end process designed to reduce the necessity for manual intervention and to complement the current local manual account request process at each of the resource laboratories.

This Web-based application is an access point on Sandia's external open network that will allow any ASC/NWC/tri-lab customer to initiate an account request. The previous manual process is duplicated via code and electronic messages. The data are subsequently handled by a corporate database in the restricted network and protected as restricted.

The joint effort of two teams within Sandia's Division 9000, High Performance Computing and DisCom, gained consensus and successful inter-site collaboration to create an application for remote users to easily request accounts on high-performance computing systems at Sandia.

This application can be accessed at: https://sasr089.sandia.gov/cfdocs/prod/sarape/sarape.cfm

Technical Significance

SARAPE utilized existing technologies to provide a new solution to an old problem. The Cold Fusion application is used to collect data from external customers and then securely passes the information to a secured database on the internal restricted network, thus allowing external customers to make requests for ASC resources while protecting their private information. Access to this database by reviewers of the request is Kerberos authenticated, and upon approval, the information is securely entered into the existing workflow operations of WebCARS.

Contribution to the Stockpile Stewardship Program (SSP)

SARAPE directly supports the SSP by providing partners throughout the Complex access to obtain request for Sandia's weapon engineering applications in an automated and timely manner. SARAPE supports the SSP by improving the productivity of the analysts at the other sites by providing improved service in obtaining accounts on Sandia's ASC platforms. In addition, it will provide a trusted electronic record of all requests and approvals for these accounts.

Below: A screen shot of an account initiation request.

Benefits to ASC and to Sandia

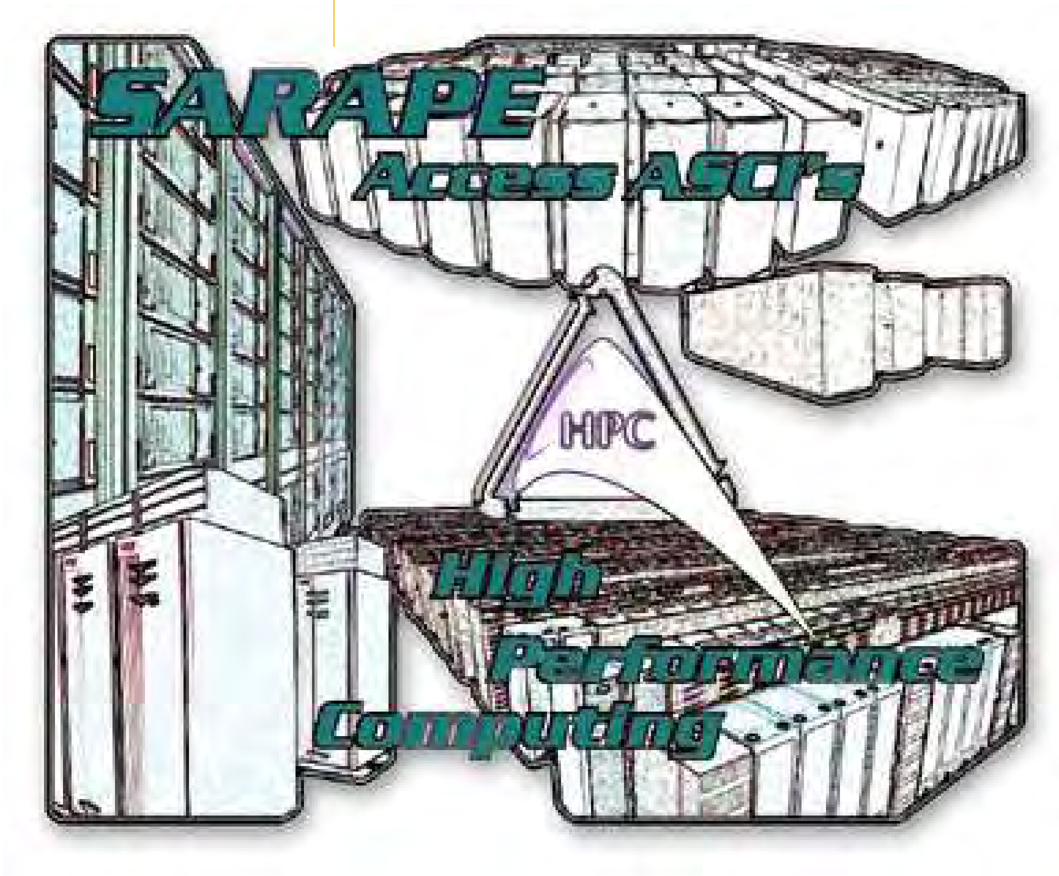
This work demonstrates how ASC can use everyday Web technologies to significantly improve processes to better support its customers. This application has been very well received by our customers with time to request accounts being shortened from months to days. This effort required the interaction and cooperation of many various departments and individuals within the Complex and we are elated to release it for use by all.

We serve as a central point for all ASC platform account and applications account requests. SARAPE reflects the expanded scope of the application. The project is scheduled to automate requests for resources within the confines of the three defense laboratories by the end of FY03.

The Sandia weapons engineering groups also saw an opportunity to put the SARAPE application to use by allowing requests from throughout the Complex for accounts to access weapons engineering applications—an opportunity that has been realized.

Future Developments

The near-term goal is to stand up a production capability that supports obtaining requests for ASC resources at Los Alamos and Lawrence Livermore and supports the weapons engineering application access for the DOE Complex. The longer-term goal of SARAPE is to include the ability to compile remote user account information among the resource sites so that we can ensure the timeliness of accounts.



Guiding Design-Through-Analysis Activities

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The DTA capability will permit more rapid turnaround of Sandia's simulations for the nuclear weapons stockpile.

Description

ASC's investment in advancing Sandia's computational capabilities and hardware resources has greatly reduced the time to perform a computational simulation. As a result, a greater percentage of the design-through-analysis (DTA) cycle is spent in problem set-up. Further exacerbating this problem, faster computations have made it possible to simulate larger and more complicated systems. To assist analysts in developing large, complex models, ASC has funded several problem set-up, post-processing, and visualization tools like Materials WISDM, SIMBA, CUBIT, GridServices, SimTracker, and Data Services. More complex problems (see figure below) have resulted in slower DTA cycle times and a greater vulnerability to error. This can be mitigated to some degree by coupling with the greater number of tools and improving the integration among them.

Technical Significance

The Design-Through-Analysis Roadmap Team (DART) was assembled to guide Sandia's DTA activities with the goal of achieving a 75% reduction in the DTA cycle time in the next three years. The team is composed of analysts, DTA tool developers, and managers with representatives from engineering sciences and weapons programs. DART was funded by both ASC and DSW.

DART is composed of several subcommittees to handle planning and technical details.

Metadata — This subcommittee identifies critical metadata lost among, and generated during, the DTA process and prototypes a simple communication mechanism between processes for metadata.

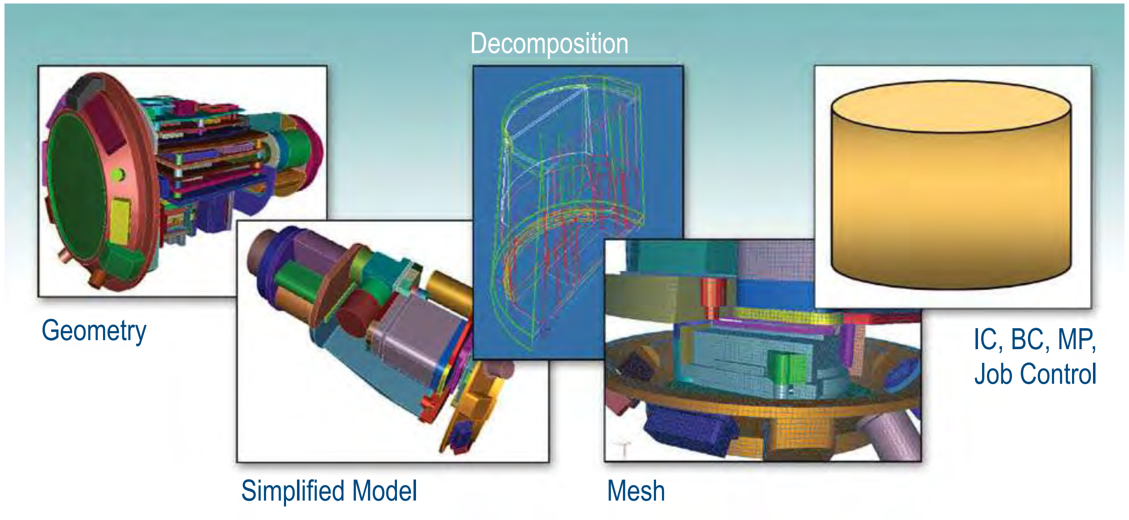
Communications — This subcommittee captures best practices and "tribal knowledge" used by experienced analysts in the DTA process and provides this information to all analysts, thereby institutionalizing these processes.

CAD Translation — This subcommittee improves cycle time by decreasing the complexity of, and creating consistency within, the CAD translation process.

SAF Format — This subcommittee keeps DART current with developments regarding the SAF mesh-data format, the interface to ASC Apps, and a sensible migration plan for DTA tools based on ExodusII.

Metrics — This subcommittee develops qualitative and quantitative measures for gauging performance of the DTA process, benchmarking the existing process to identify bottlenecks, providing input for prioritizing DART-supported activities, and evaluating the effects of DTA process changes, both qualitatively and quantitatively.

Post-Processing Action — This subcommittee surveys data mining and post-processing tools to identify needs that will improve the ability of analysts to interrogate large ASC-level simulations.

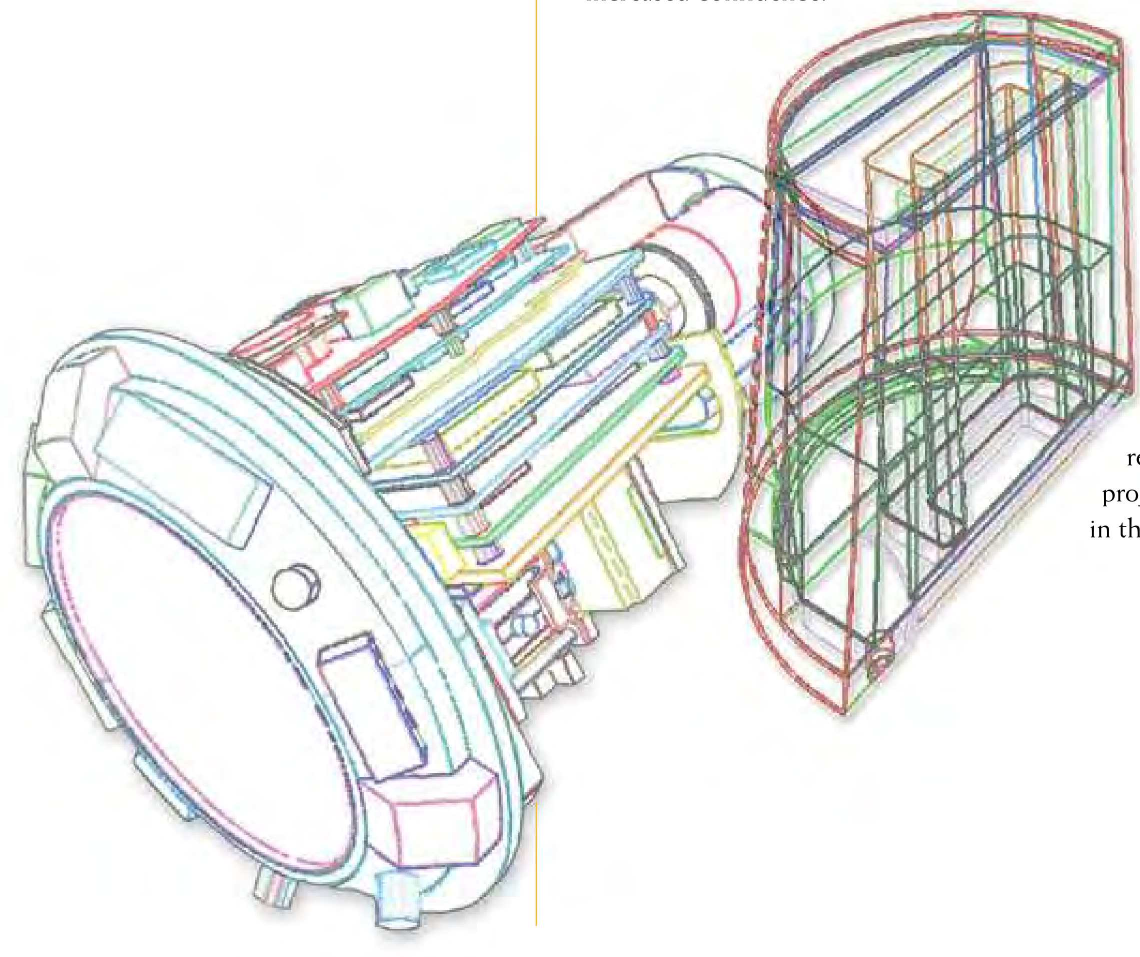


Five steps are needed to define geometries for single element mesh.

Analysis Process — This subcommittee integrates the engineering science's analysis process requirements into the DART process integration activities.

Contributions to Stockpile Stewardship (SSP)

The DTA capability will permit more rapid turnaround of Sandia's simulations for the nuclear weapons stockpile. In other words, simulations will be performed with greater geometric fidelity, increased physics and mechanics, and will generate increased confidence.



Benefits to ASC and to Sandia

A reduction in the DTA cycle time will provide Sandia weapons programs with a more responsive model-based engineering infrastructure that will allow it to better support the needs of a rapidly changing stockpile. With this increasing role of modeling and simulation in the design and qualification of weapon systems, the definition of a seamlessly integrated DTA process is critical for the successful integration of ASC-developed resources into weapons engineering activities. This capability is critical for Sandia's leadership role in engineering sciences.

Future Developments

Major objectives for FY04 are the completion of the DART Roadmap and Project Plan to outline the path to seamless integration of DTA tools. Toward this end, DART will identify gaps and overlaps in the DTA process, identify the need for new DTA tools, and enable the realignment of priorities of DTA projects to achieve the desired reduction in the DTA cycle time.

Managing Model-Based Material Properties for Modeling and Simulation Studies

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WISDM complements Sandia's broad library of constitutive models used in model-based design and certification of weapon systems.

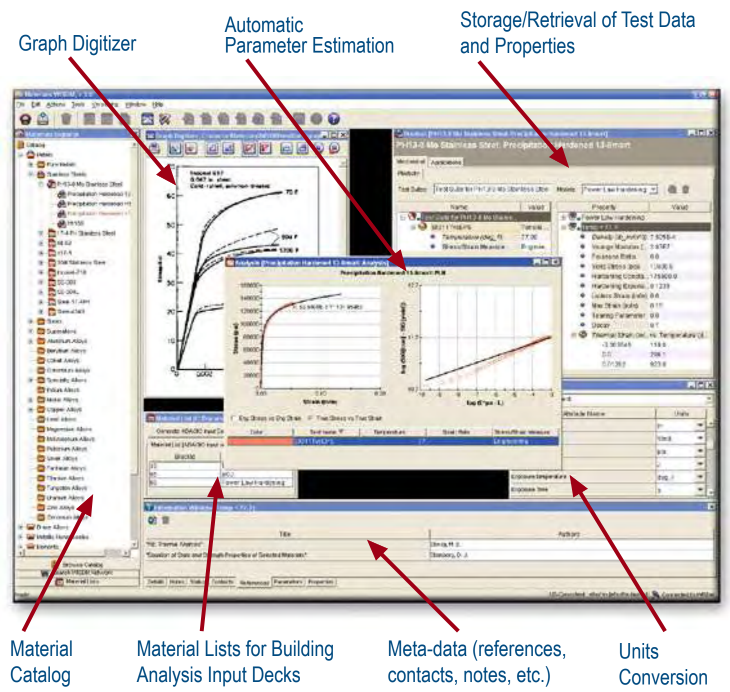
Description

Materials WISDM (Weapon Information System and Data Management), funded through the ASC Problem Solving Environment (PSE), is a materials information system to manage the entire lifecycle of materials-property generation.

Technical Significance

As the screen shot below illustrates, the Materials WISDM application supports storage and retrieval of materials test data and properties, graph digitization, units conversion, parameterization of properties from test data, and generation of analysis input decks. It also provides enterprise-level version control and change management of both raw test data and materials properties. Furthermore, the application is extensible to new material response modes and constitutive models as they are developed.

Materials WISDM has been deployed in the unclassified production computing environment at Sandia and is currently being deployed in the classified environment as well. As the first production Sandia application developed with the Java 2 Enterprise Environment (J2EE), this tool has driven the creation of robust, secure J2EE development and production deployment infrastructures on both the Sandia Restricted Network and the Sandia Classified Network.



Annotated screenshot of the Materials WISDM client, illustrating the application's functionality.

Contribution to the Stockpile Stewardship Program (SSP)

Many of these constitutive models have been developed to accommodate the specific needs of stockpile stewardship and therefore utilize materials properties not readily available from commercial materials data libraries. Preservation of these properties is essential, as their generation typically requires extensive testing and specialized codes operated by materials experts. Ultimately, these materials properties form the scientific basis for model fidelity and confidence in Sandia's modeling and simulation capabilities.

Benefits to ASC and to Sandia

WISDM complements Sandia's broad library of constitutive models used in model-based design and certification of weapon systems. Most importantly, it may reduce materials-property generation time, increase accessibility of materials property information, improve Sandia's ability to verify and validate simulation-based studies, provide long-term traceability of data, and promote the re-use of data in future weapon system activities. By providing greater accessibility to high-quality materials data, Materials WISDM plays a vital role in fast-response, simulation-based, high-consequence engineering studies—a primary focus of ASC.

Future Developments

In FY04, version 3.0 of the Materials WISDM application will be released. This version will include further enhancements to both the application architecture and its functionality, including support for additional constitutive models, links between materials and their weapons applications, and an advanced interface for integration with other ASC-developed applications.

Building and Managing Simulation Models

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In conjunction with assembling meshes and building complete simulation models and associated input files, SIMBA also manages models and organizes, stores, and archives them.

Description

Simulation Manager and Builder for Analysts (SIMBA) is an analyst's tool for building and managing simulation models currently in production use at Sandia. The principal goals of SIMBA are to:

1. Enable better understanding of the purpose, provenance, organization, properties, assumptions, and context of simulation models—leading to higher quality and analyst productivity.
2. Provide tools for managing multiple simulation models in context.
3. Track and archive the steps, decisions, and data sources used to build a simulation model—allowing annotation (electronic notebook) and reproducibility.
4. Reduce the time needed to create simulation models by providing a powerful model-building environment.

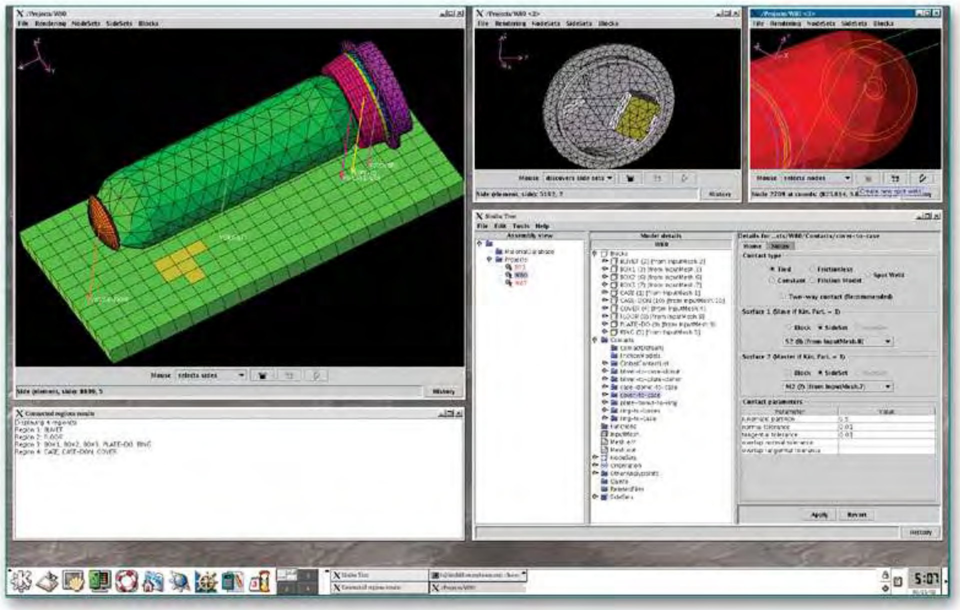
SIMBA is not a mesh generator; rather it uses meshes generated by Sandia and commercial tools. Analysts use SIMBA after some, but not all, of their component meshes are generated, work in SIMBA to build complete simulation models, and continue to use SIMBA while simulations are being run (see below). In conjunction with assembling meshes and building complete simulation models and associated input files, SIMBA also manages models and organizes, stores, and archives them.

Technical Significance

SIMBA's model management features have been influenced by the observation that analysts do not build single models in isolation; rather, they increasingly need to build and manage families of related models.

Building and managing families of related models is important for several reasons:

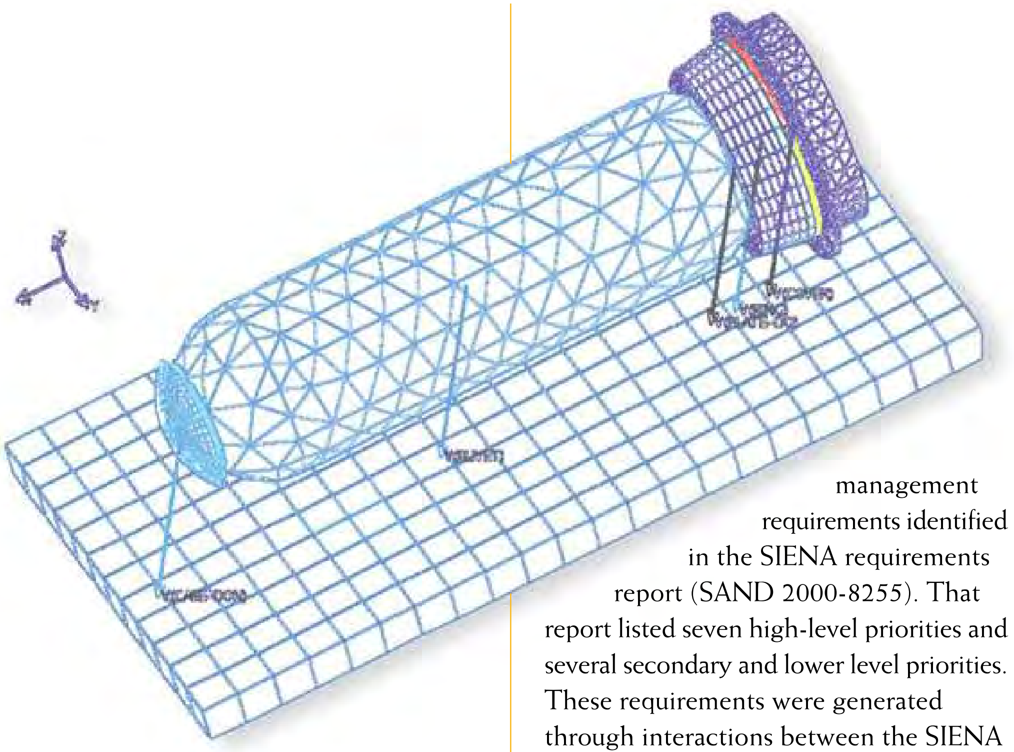
- During the design stage, an analyst may want to compare many alternate designs, perhaps varying geometry or material selection.
- High-fidelity finite element models can be built with several purposes in mind. For example, a weapon model may be constructed in such a way that it can be used for structural and thermal analyses, for crash followed by fire analysis, and for earth penetrator weapon case design. In order to support this reuse, the ability to use "plug and play" component meshes at varying levels of fidelity is valuable.
- Analysts often need to build and manage families of models because they make many runs to test individual code features and combinations of features to ensure that they are working correctly.
- As part of ASC's Verification & Validation program, weapon analysts need to construct models of validation experiments to specify the experiments and design the fixtures, and to compare simulations with the experimental results. It is extremely useful to be able to manage these analyses together and in context.



SIMBA's graphical workspace

Contribution to the Stockpile Stewardship Program (SSP)

SIMBA is in the development phase and is sponsored by the ASC Problem Solving Environment program. SIMBA development began about three years ago, spurred on by model-building and



management requirements identified in the SIENA requirements report (SAND 2000-8255). That report listed seven high-level priorities and several secondary and lower level priorities. These requirements were generated through interactions between the SIENA team and analysts. Four of the top-level requirements are directly related to model building and management; one is directly related to management of materials data, and one refers to archiving. SIMBA has substantially addressed the four top-level requirements relating to model building and model management and has partially addressed the more widespread issues of artifact representation and archiving. The WISDM project has substantially addressed the requirement related to management of materials data.

SIMBA is highly portable and is available for Solaris, IRIX, Linux, and Windows.

Benefits to ASC and to Sandia

Many analysts use SIMBA in day-to-day work and on special projects, including ASC milestone calculations. It is running on both classified and unclassified desktops, both in New Mexico and in California. SIMBA has allowed the W80-3 Abnormal Environment modeling team to rapidly import meshes developed by the NM-based Production Meshing team and to quickly assemble and use a system model. SIMBA has also been used to build models for the W87 and the B83.

Future Developments

More functionality is being added to support the generation of input decks and extend the simulation setup capabilities to other ASC codes, such as Calore for thermal analysis. This functionality will include an interface to extract materials property data from Materials WISDM. SIMBA will be enhanced to improve its ability to detect problems of mesh quality, block overlap, and contact data and provide mechanisms to correct the problems before job submission.

Organizing and Managing Results from Computer Simulations

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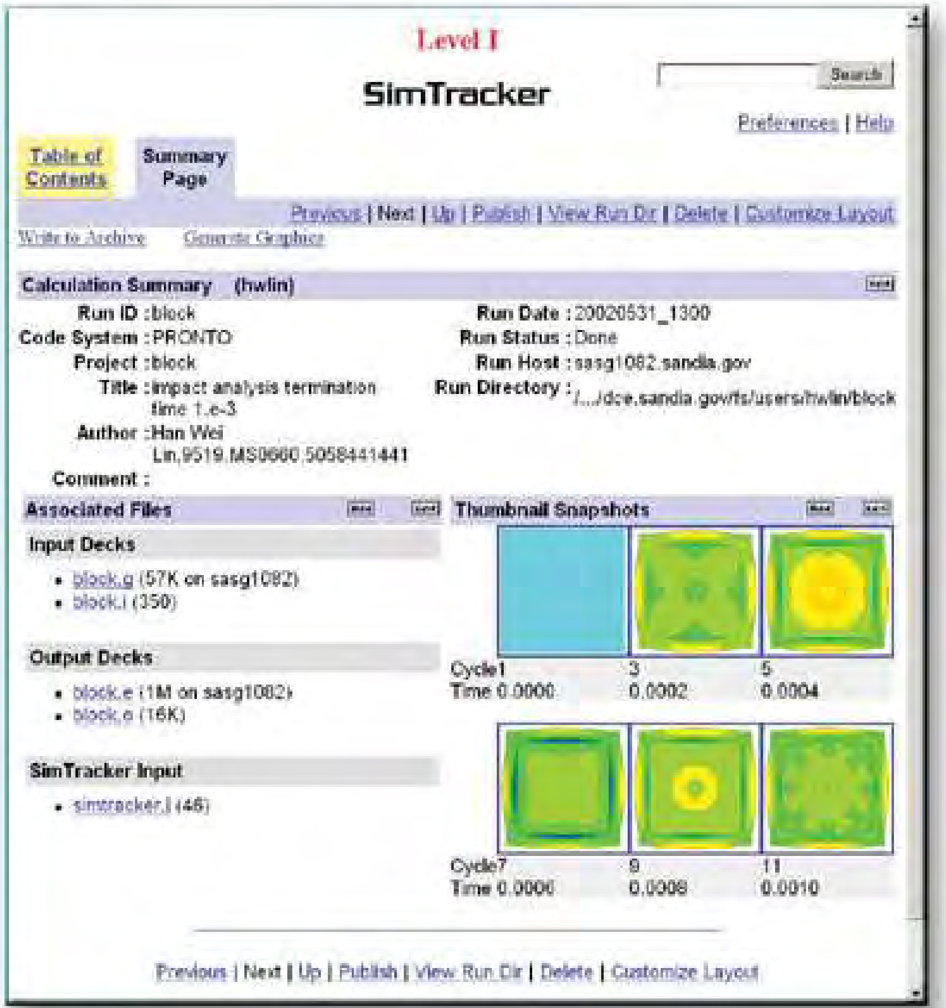
Large-scale computer simulations, in the ASC class, often take days or weeks to run and can produce massive amounts of output.

Description

Efficient exploration of results from supercomputer calculations requires filtering and summarizing the data. The SimTracker tool summarizes calculation results by automatically generating metadata (e.g., text and image snapshots) both during and after a calculation. The metadata are presented via dynamically generated Web pages.

Technical Significance

Thumbnail sketches with hypertext links to applications and data can be used to monitor the calculation as it runs, to review results, and to document the calculation for future reference. Large-scale computer simulations, in the ASC class, often take days or weeks to run and can produce massive amounts of output. A typical environment includes multiple hardware platforms, a large collection of eclectic software applications, data stored on many devices in many formats, and little standard documentation about the data. The exploration of simulation results is laborious, requiring knowledge of this complex environment and of many application programs. This is especially important when trying to review results of past experiments.



An example of a SimTracker calculation

Contribution to the Stockpile Stewardship Program (SSP)

Web-Based Solution

SimTracker offers a Web-based approach for exploring simulation results both during and after a calculation. The figure at left shows how this tool automatically generates metadata summaries that serve as a quick overview and index to the archived results of simulations. These summaries provide convenient access to the data sets and associated analysis tool. They include graphical thumbnail images, pointers to all relevant files for the simulation, and fields ranging from location and time of the calculation to comments and scalar physics values. The ability to access simulation databases and make runtime decisions are critical to efficient use of ASC computing resources.

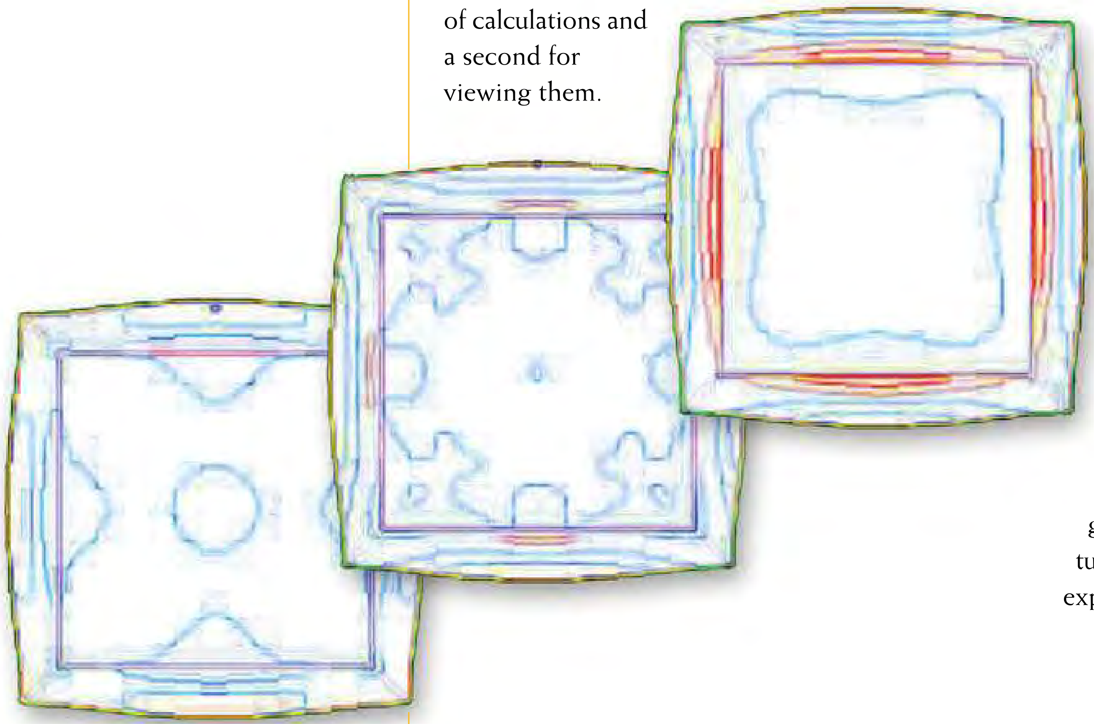
SimTracker is an extensible application easily adapted for use with different simulation codes, and it has been deployed at the three defense laboratories. It works with nine different physics and engineering simulation codes at Sandia, including the SIERRA framework, and 21 different codes in the tri-lab computing environment. This

Contact:

Web-based approach to monitoring and documenting simulations can be applied to other areas as well. Environments in which users run many simulations or generate large numbers of data files could benefit from SimTracker's high-level framework for conveniently viewing and organizing simulation results.

Benefits to ASC and to Sandia

Because SimTracker is "nonintrusive," its components are separate from the code system. End users and code developers are not required to make extensive changes to their current mode of operation to use the tool. SimTracker consists of two components: one for generating summaries of calculations and a second for viewing them.



The generation component creates calculation summaries from simulation output. This component runs data translation and conversion utilities, compresses data files, creates metadata that describe the calculation and where it is stored, runs postprocessors to create visualizations, and copies requested result data and metadata to archival storage.

Future Developments

The SimTracker team at Sandia is working with various analysis groups to support the improvements they need in the Design-Through-Analysis Process. This effort converts weapon-design information to a mathematical boundary value problem that can be solved with computational mechanics codes. This allows computational prototyping of various design options and, when done in a timely manner, can have tremendous impact in the final design. The improved organization and management of simulation metadata provided by SimTracker and other metadata tools will aid these groups in improving the turnaround time of such experiments.

Integrating Mathematical Software Components

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SIGMA is a systematic effort to increase the interoperability of these software components in order to improve their efficiency and ease of use. . . .

Description

The use of modeling and simulation in design and analysis raises many questions, the answers to which are necessary to ensure high-quality designs. Examples of such questions include: how sensitive is the simulation to model parameters? To what extent do simulation parameters contribute to model error? How does modeling help us design a reliable product given specified operating uncertainties? To perform the design exploration and analysis required to answer these questions, a range of uncertainty quantification, statistics, and optimization software tools is needed. While many such tools exist, they are often developed independently of each other. Any interactions between such tools are either manually reconciled or handled in the context of a framework like DAKOTA. In both cases, the various components are black boxes to each other.

SIGMA is a systematic effort to increase the interoperability of these software components in order to improve their efficiency and ease of use and to facilitate the introduction of new algorithms (resulting from research efforts) that rely on the interactions between statistics and optimization. In addition, we are working to ensure the portability, scalability, and robustness of the components by leveraging other Sandia codes to replace obsolete codes and by following improved software quality practices. The resulting interoperable components are deployed via DAKOTA and can also be used as a set of libraries residing on the same computer system.

Technical Significance

The primary challenges that the SIGMA packages address are those associated with the prohibitive computational expense of large-scale ASC simulation codes as well as the high cost of physical experiments. In particular, traditional techniques for determining optimal designs or for obtaining statistically meaningful data rely on the execution of a large number of simulations. Similarly, many physical experiments may be required. Given significant resource limitations, the expectation conducting the number of experiments called for by these techniques is unreasonable. These challenges are addressed by the development of quality software that implements both current techniques and the latest research techniques. New research is aimed at obtaining useful information while reducing the number of simulations and experiments needed. Interoperability between the different software packages, as mentioned above, is the key to the success of new algorithms because they depend on the interplay between statistics and optimization.

Contribution to the Stockpile Stewardship Program (SSP)

When coupled with analysis codes, SIGMA-developed software enhances the ability of weapons analysts to design, analyze and evaluate the quality of computational predictions. For example, we work directly with analysts who address questions about model uncertainty in the W80 and earth-penetrator (RNEP, PEN-X) programs. One problem of interest in the W80 program is predicting the response of the WES housing in abnormal mechanical scenarios (Figures 1 and 2). The ultimate goal is to build confidence in the computational predictions of models used for these scenarios, and a range of both physical and computational

Figure 1. W80 WES housing is modeled as a "can" with laser-welded lids to predict response of base metals, foams, welds, and component behavior to abnormal mechanical scenarios, such as handling drops.

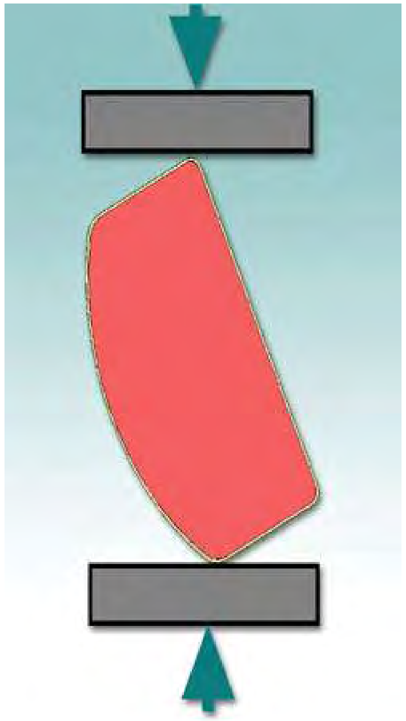

Figure 2. Design of Experiments is used to determine the total number of physical and computational "can crush" tests and combinations of parameters (such as can orientation, shown here) to determine the relative contribution of each parameter to weld response.

experiments is needed to accomplish that. We have worked closely with analysts in using design-of-experiments techniques to determine several test matrices for experiments to obtain response data with respect to various parameter combinations. Combined mathematical and analytical expertise was needed to ensure that main effects and importance rankings were computable within the prescribed resource limitations. Furthermore, tradeoffs were considered between different test matrices and to understand the relationships between the parameters in the physical domain and those in the computational domain. Work on statistical analysis of the data and on determining test matrices for computational experiments is ongoing. In addition, several areas in the capabilities provided by SIGMA have been targeted for improvement.

Benefits to ASC and to Sandia

As previously mentioned, SIGMA's software packages are deployed via the DAKOTA framework. As such, they are available on all ASC computing platforms as well as to analysts throughout the defense laboratories. Furthermore, with the DAKOTA integration into the SIERRA and NEVADA frameworks, these tools will become extremely easy to use in conjunction with many Sandia-developed ASC codes to solve a wide range of design, analysis, and validation problems. As a final note, the role of the software tools developed under the SIGMA project extends beyond the ASC program to all simulation-based science and engineering programs.

Future Developments

To continue to provide and improve support of the statistics, uncertainty quantification, and optimization needs of the SSP, several critical directions have been identified. The first is improved support for design of experiments. Making effective use of current technology requires statistical expertise beyond that of the average user. New software must assist the user by providing initial test matrices and information on how to modify and/or improve those matrices in a meaningful way. A second requirement is tools for statistical analysis of the data collected during experiments. Several such software tools exist, but they must be integrated into the software set that is provided to Sandia analysts. Third, to make the results of new and ongoing research efforts available to the analyst community, the development of new SIGMA software components (e.g., a Bayesian statistics package) is essential. Finally, inherent in the previously mentioned technical directions is the need for education of the users on the technology provided by these software tools. This will be accomplished via direct interactions between mathematicians and analysts as well as through tutorials on the fundamental concepts employed. The first tutorial was conducted in early October 2003, with follow-ups expected in the future.

By adhering to the goal of providing quality software deployment of state-of-the-art research in optimization and uncertainty quantification and addressing the critical needs outlined above, we expect to continue to add to the capabilities available in the SIGMA packages and deployed through DAKOTA. These capabilities will further the ability of mathematicians and analysts to provide more robust support to Sandia weapons programs with regard to design and analysis.

Establishing Security Infrastructure

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ASC users have one account to access all ASC systems, removing the need for multiple user names and passwords.

Description

The Problem Solving Environment Security project, provides the security infrastructure and resources for authentication, authorization, and file sharing across the ASC tri-lab systems and expanding to other Nuclear Weapons Complex (NWC) sites. The basis for the security infrastructure is DCE.

Technical Significance

DCE provides the Kerberos authentication services used throughout the NWC, including Los Alamos, Lawrence Livermore, Sandia (NM and CA), Kansas City Plant, Pantex, Y12, and Savannah River. DCE also provides the NWC registry for group information used for authorization decisions for the NWC community to access information at Sandia and Pantex.

Contribution to the Stockpile Stewardship Program (SSP)

The Security project has made a significant impact on a wide spectrum of activities that reflect the pervasive character of security requirements.

User Authentication across the NWC — User authentication is based on network login to existing DCE/Kerberos security systems established at each of the three laboratories and NWC partners. Users always log into their own DCE cell, and through cross-cell trust, this initial authentication is all that is necessary to access resources at other sites. This also places the responsibility for account and password management at the user's home site. ASC users have one account to access all ASC systems, removing the need for multiple user names and passwords. The formulation and establishment of the security criteria and inter-site agreements for enabling cross-cell trust over SecureNet was the responsibility of the Security Subproject.

NWC DCE Group Authorization — The Security project assisted in establishing the Complex's DCE groups. These groups are used within a number of applications such as Sandia's Web Fileshare and NWie Portal and Pantex's Data Mart and Interactive Electronic Procedures (IEP). Through the NWC groups, access can be granted to weapons information such as drawings, procedures, and stockpile surveillance data at Sandia and Pantex to engineers throughout the NWC.

Remote Access — Secure Shell with modification to support Kerberos authentication is used throughout the ASC sites to log into ASC systems. With Kerberos authentication, DCE cross-cell trust, and ticket forwarding, Secure Shell provides a single sign-on capability from desktops to ASC systems across all sites.

Benefits to ASC and to Sandia

The inherently secure technologies developed at Sandia benefit not only how internal business is conducted, but also affects the broader ASC communications by ensuring its security. Noteworthy areas include:

Software Support — The Security project provides the software packages, which allow applications to utilize the security infrastructure. Grid Services and Data Services utilize the MIT Kerberos and GSSAPI libraries, as well as the Generalized Security Framework (GSF) tool kit, within their applications.

Application and Web Service Support — Web Server authentication and authorization modules are provided by the Security project for widely available Web servers such as Apache and IPlanet. Recent work includes modules utilizing Kerberos tickets for authentication, eliminating the user name and password prompts for typical web authentication.

NWC Distributed File System (DFS) — DFS provides a global name space for a secure shared file system. DFS is used by ASC users to share files across sites. Because of the security features of DFS, it is used by Web servers and Web applications to provide need-to-know access controls for Web documents. The Security project is also looking at NFS V4 as the most likely replacement for DFS.

Future Developments

The PSE Security project is actively looking at a replacement to DCE and DFS. DCE's major vendor IBM has announced a service termination date for the product; therefore, this project is looking at transitioning the major areas listed above to other technologies based on Kerberos and LDAP. Sandia, in particular, is looking at the use of Microsoft's Active Directory as a replacement technology.

Extending Data Storage Capacity Through the HPSS

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The HPSS software marshals the resources of multiple computing and storage platforms to present the user a single, unified storage system.

Above: A StorageTek PowderHorn Tape Library. Each library has a capacity of more than 5000 tapes and can mount 450 tapes an hour. Each has a capacity of up to 2 petabytes. Sandia currently has six PowderHorn libraries in production.

Description

The High Performance Storage System (HPSS) is a hierarchical network-centric storage system to manage and store many petabytes (10^{15}) of data. The HPSS software marshals the resources of multiple computing and storage platforms to present the user a single, unified storage system. The HPSS software was produced through, and continues to be maintained and enhanced by, the cooperative efforts of Sandia, Lawrence Livermore, Los Alamos, Oak Ridge National Laboratory, and the IBM Corporation.

Technical Significance

Funded through the ASC Problem Solving Environment and the Integrated Computing Systems Projects, HPSS provides ASC users with storage capacity for the very large data sets generated by high-performance computing vital to the SSP and other ASC projects.

Version 4.5 of the software provided significant improvements with respect to the media types supported, media capacity, and performance. The primary means for data transfer is the Parallel FTP Client and Daemon. Other protocols have been added to this component to provide unprecedented performance across the Wide Area Network (WAN). These efforts have been leveraged to provide higher speed transfers between the ASC high-performance machines at each of the three laboratories. Transfers of large multi-gigabyte files have occurred at speeds up to 200 megabytes/second over the WAN (1200 mile) between Lawrence Livermore and Sandia. This has allowed Sandia's ASC Applications personnel to make use of the ASC White machine at Lawrence Livermore (and also the ASC Blue Mountain and Q machines at Los Alamos) while storing their data here at Sandia.

Version 5 of the software has been developed and will be generally available in the next quarter with deployment at the three defense laboratories in 2004. Highlights of this release will be additional performance, technology insertion, replacement of the aging metadata facilities, and an additional performance protocol for the Parallel FTP suite.

The StorageTek system, shown at left, is used extensively in Sandia's HPSS.

Contribution to the Stockpile Stewardship Program (SSP)

The extreme requirements presented to any computing infrastructure by the ASC and the Stockpile Stewardship Programs cannot be addressed by products designed for the commercial world. The HPSS project supports the large storage capacity and high speed data transfer needs of the computational scientists and engineers working on weapons simulation and modeling on weapon effects. Without the HPSS' capabilities, multi-gigabyte and terabyte data files representing significant computer usage and analyst effort would be lost or destroyed.

Benefits to ASC and to Sandia

Moving large datasets from site to site and from system to system using non-HPSS techniques can take weeks. The capabilities provided by HPSS throughout the three laboratories' computing infrastructure permit analysts to work on their data where and when they choose, mitigating constraints of transfer time or storage capacity. A common compatible hierarchical storage system used throughout the laboratories' computing environments simplifies customer training, leverages ASC development dollars, and improves problem solving by replicating production systems and increasing knowledge and experience with the product.

Future Developments

The Sandia HPSS implementation team is focusing on providing a tighter integration between HPSS and the ASC VIEWS project to provide customers with high-performance data transfer easily and reliably from the platforms on which they generate and view their data. This will also provide storage services for the ASC Red Storm platform expected to provide the computational resources for continued enhancements with respect to the SSP.

The HPSS services currently provide approximately 100 terabytes of storage to ASC computer users. This is expected to increase by the end of FY05 to nearly 16 petabytes.

Advancing Scalable Visualization

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By providing an environment that allows large-scale display and interaction with data, we aid understanding of spatial relationships and appreciation of their properties by physically moving through their environment.

Description

Visualization is an essential analytical tool for qualitatively and quantitatively understanding the volumes of data produced by the ASC program. Sandia has set new standards for high-performance graphics rendering and high-resolution display for scientific visualizations. A 2001 ASC Level 1 milestone for the Visual Interactive Environment for Weapons Simulations (VIEWS) program was to drive a large, tiled display containing at least 60 million pixels. The scalable software and hardware that drive these high-resolution displays continue to evolve.

Technical Significance

The tiled display is a Sandia-designed installation of 48 high-end Digital Projection, Inc., DLP™ technology light engines arrayed to form a 48-tile composite of rear-projected images. The composite image is 15,360 pixels wide by 4096 pixels high (62.9 million pixels) and is about 12 meters by 3 meters. From ten feet away, the pixel density is about as fine as the human eye can perceive. The primary image-rendering source is a nearby cluster of 64 HP (Compaq) SP750 personal computer workstations. A secondary image-rendering source is a cluster of 128 Dell Precision 430 personal computer workstations. Both clusters are outfitted with NVidia geForce3™ graphics adapters. The clusters use the Linux operating system and run a variety of commercial and research visualization application codes.

The rendering software, which drives the large tiled display, uses algorithmic approaches that provide excellent scalability with increases in data size. To "stress" test the rendering software, Sandia used a data set created at Lawrence Livermore. The data shown in the photograph are derived from Lawrence Livermore's 1999 Gordon Bell Award winning supercomputer simulation of compressible turbulence. A 470-million polygon iso-surface of a single timestep of the simulation was used as the source data. These data were used for their extreme size and because they are unclassified.

Advancement of scalable rendering and advanced display technologies complement other ASC/VIEWS research in data management, data exploration and development, and deployment of effective scientific visualization infrastructure for science and engineering.

Researcher interacting with the 60 M pixel display of a simulation of compressible turbulence that won the 1999 Gordon Bell Award for Lawrence Livermore

Contribution to the Stockpile Stewardship Program (SSP)

The VIEWS Corridor is a scalable data analysis and visualization environment that matches the scale of computational output from Sandia's (and from Lawrence Livermore's and Los Alamos') massively parallel processing supercomputing systems. The name VIEWS Corridor is a metaphor that encapsulates the goals of creating a wide path through which massive quantities of data can easily flow and through which scientists and engineers can collaboratively explore data.

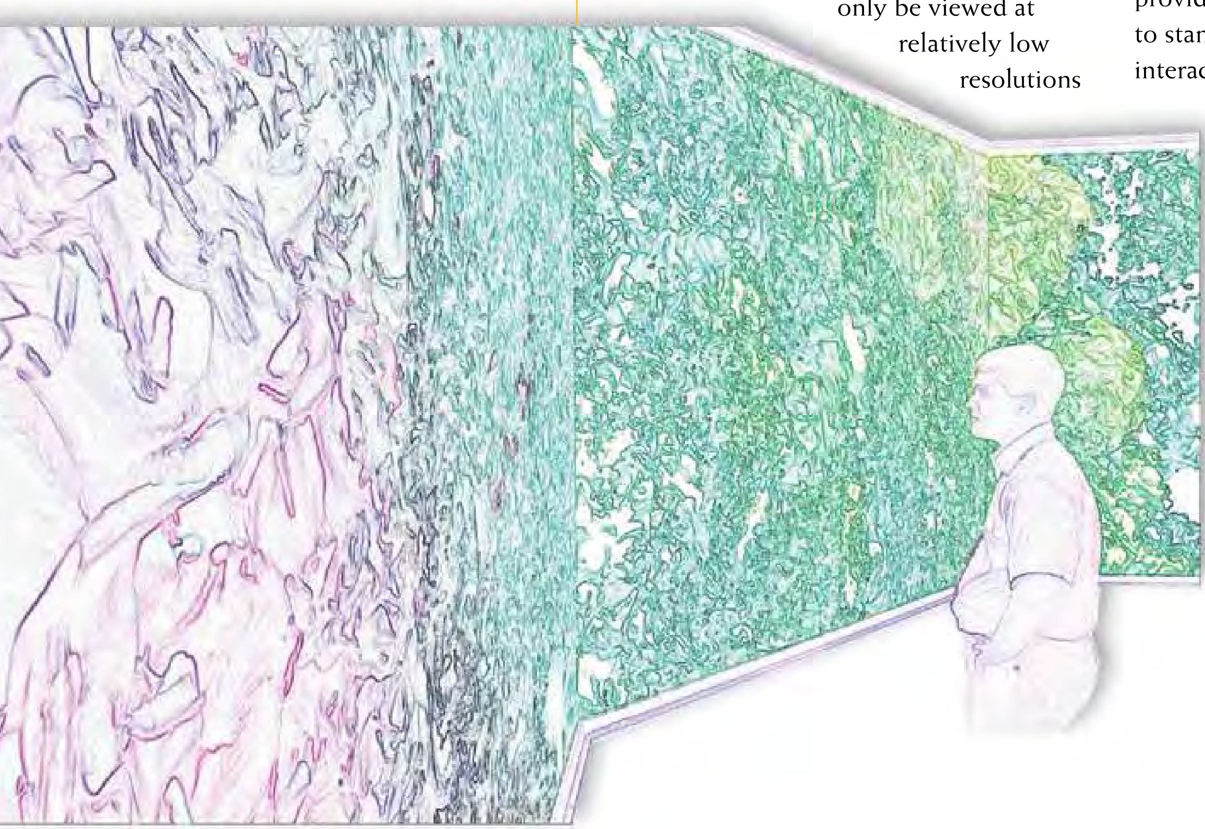
Massively parallel processing applies as many as thousands of processors to complex physics problems to create predictive models and simulate complex events such as impact, explosion, and fire. These models and simulations are powerful problem-solving tools for weapons engineering, homeland security, biotechnology, and weather.

Benefits to ASC and to Sandia

Before the VIEWS Corridor, the output of thousands of processors performing trillions of calculations per second could only be viewed at relatively low resolutions on a desktop computer monitor. Consequently, it was difficult to see critical details in the output and it was difficult for groups to collaborate and analyze the output.

The VIEWS Corridor concept allows us to look at large quantities of data according to former VIEWS tri-lab lead Philip Heermann – data that are " . . .getting truly huge. And what I mean by huge is that we're looking at data sets that are getting so large that a person can't even stand to look at them fully. We need to have ways that people can fully understand the information." Dino Pavlakos, Manager of Visualization and Data Analysis Department elaborates: "We would like to provide technology that allows end users to stand in front of a display like this and interact with the display and the data in a much more intuitive way."

By providing an environment that allows large-scale display and interaction with data, we aid understanding of spatial relationships and appreciation of their properties by physically moving through their environment. These new ways of interacting with data and displays are helping ASC engineers and scientists to learn more about the spatial relationships between the different parts of a data set.



Future Developments

Because these environments must be stable and powerful, innovations will continue to increase efficiency of pre- and post-processing Data Analysis and Visualization systems for the S&CS community in both Sandia Restricted Network and Sandia Classified Network environments and for both research and development and production use.

Further research and development, testing and evaluation, and production application of visualization technologies will continue with partners in the ASC/VIEWS program and with university and industry collaborators.

Speeding Up Mesh Generation Through CUBIT

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By addressing automation, efficiency, robustness, and capability of the tools in the geometry preparation and meshing steps, CUBIT will contribute significantly in reducing the time to take a design through the analysis process.

Description

CUBIT is a toolkit for robust generation of two- and three-dimensional finite element meshes (grids). Our main goal is to reduce the time to generate meshes, particularly large hex meshes of complicated, interlocking assemblies. VERDE and CGM are companion tools in the suite.

CUBIT is a solid-modeler based preprocessor that meshes volumes and surfaces for finite element analysis. Mesh generation algorithms include quadrilateral and triangular paving, 2D and 3d mapping, hex sweeping and multi-sweeping, tet meshing, and various special-purpose primitives. CUBIT contains many algorithms for controlling and automating much of the meshing process, such as automatic scheme selection, interval matching, sweep grouping, and sweep verification, and also includes state-of-the-art smoothing algorithms. One of CUBIT's strengths is its geometry module (CGM), for simplifying the underlying solid model into the model you wish to mesh, and includes a facet-based geometry kernel, as well as a strong virtual geometry capability.

Technical Significance

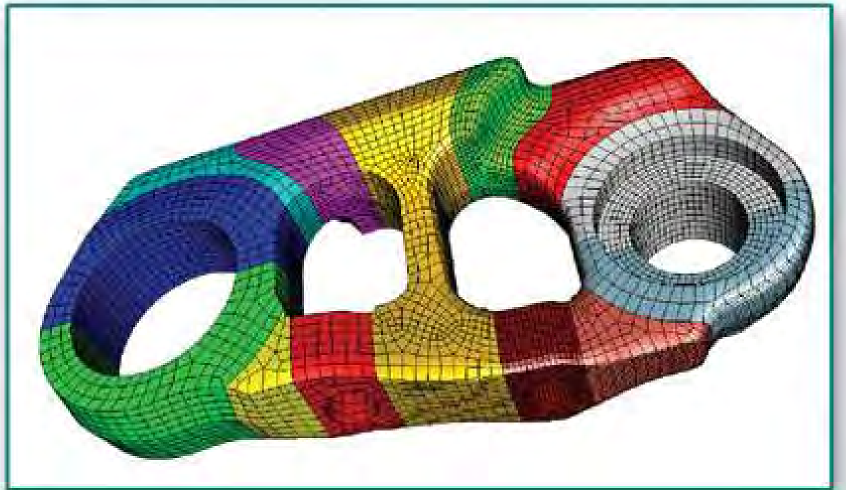
Recently, Sandia's Design-Through-Analysis (DTA) process has been identified for improvement. Several studies have shown that up to 80% of the DTA process is spent in geometry preparation and mesh generation steps. Therefore, the most significant impact to the DTA process could occur in the domain that CUBIT addresses. By addressing automation, efficiency, robustness, and capability of the tools in the geometry preparation and meshing steps, CUBIT will contribute significantly in reducing the time to take a design through the analysis process.

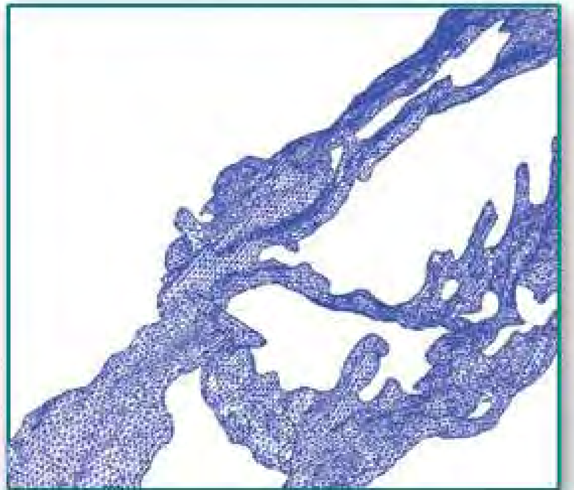
Contribution to the Stockpile Stewardship Program (SSP)

CUBIT has been used to generate meshes and/or clean up geometry on models for the B61, W76, W80, and W88 stockpile programs. The automation algorithms and scalability of the models that can be generated make it the only tool capable of processing some of the larger models needed for verification in the SSP.

Benefits to ASC and to Sandia

CUBIT has been used in areas other than weapons programs to obtain finite element meshes for a variety of simulations conducted by Sandia. The CUBIT development team maintains a strong presence in the mesh generation research community and hosts a conference and several symposia each year to promote the research in mesh generation. Because of the emphasis placed by Sandia and the

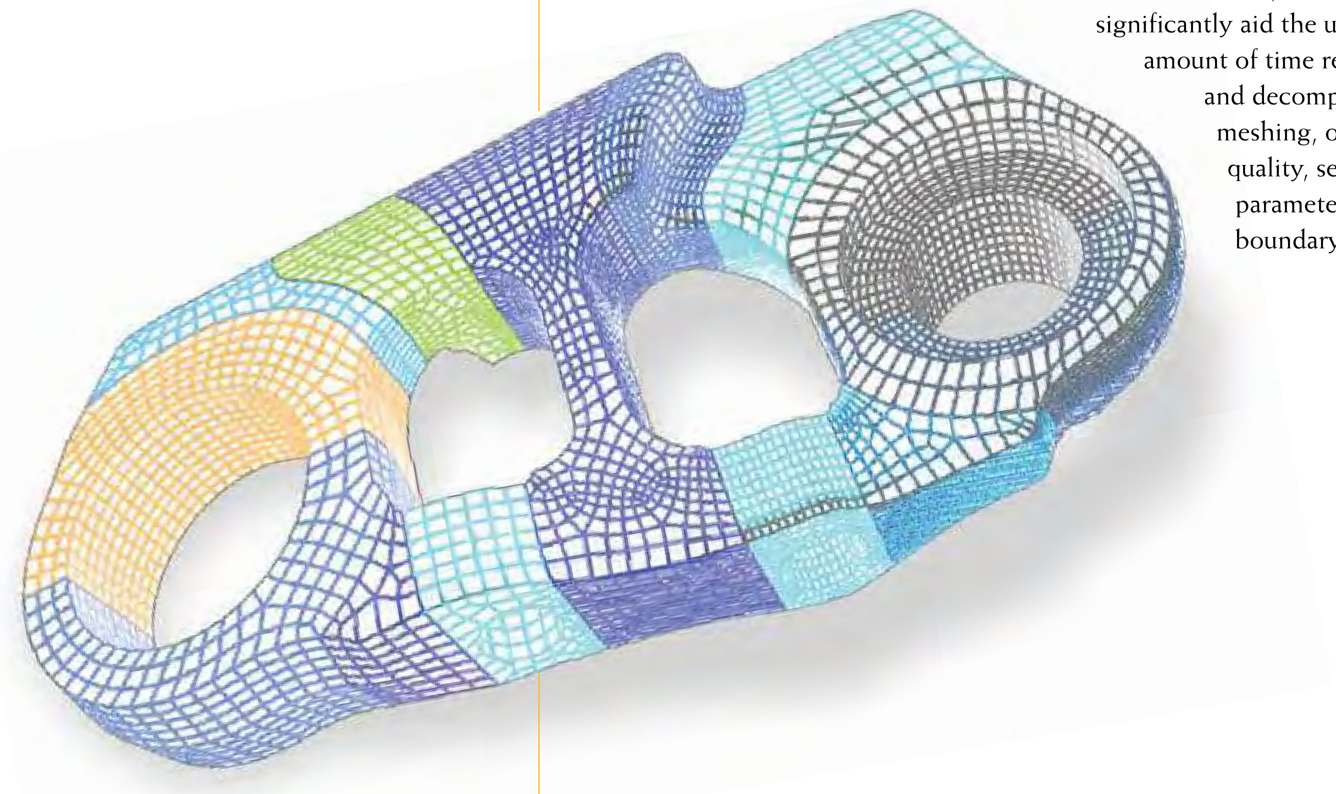




Two meshed examples generated using the CUBIT Mesh Generation Toolkit. The first example is a mechanical part showing the decomposition performed to generate meshable regions. The second model is part of a cell's endoplasmic reticulum. This model demonstrates CUBIT's facet-based geometry capabilities of complex models and the subsequent tetrahedral meshing of the model.

ASC program on high-performance computing, preparing the finite-element models efficiently has become a critical need for the program. By maintaining strong leadership in the mesh generation research and development community, Sandia and the ASC program are assured to have the latest and most efficient tools available to speed the step of preparing the finite-element model for engineering analysis.

Recent usage statistics show that CUBIT was used over 70,000 times by 173 different users in 2003. With each unique user averaging over 400 runs of CUBIT, we are having a significant impact on the engineering teams trying to generate models for analysis. In addition to these usage statistics, we estimate another 30% to 50% of our users are running CUBIT on the Windows platform that is not tracked by these statistics.

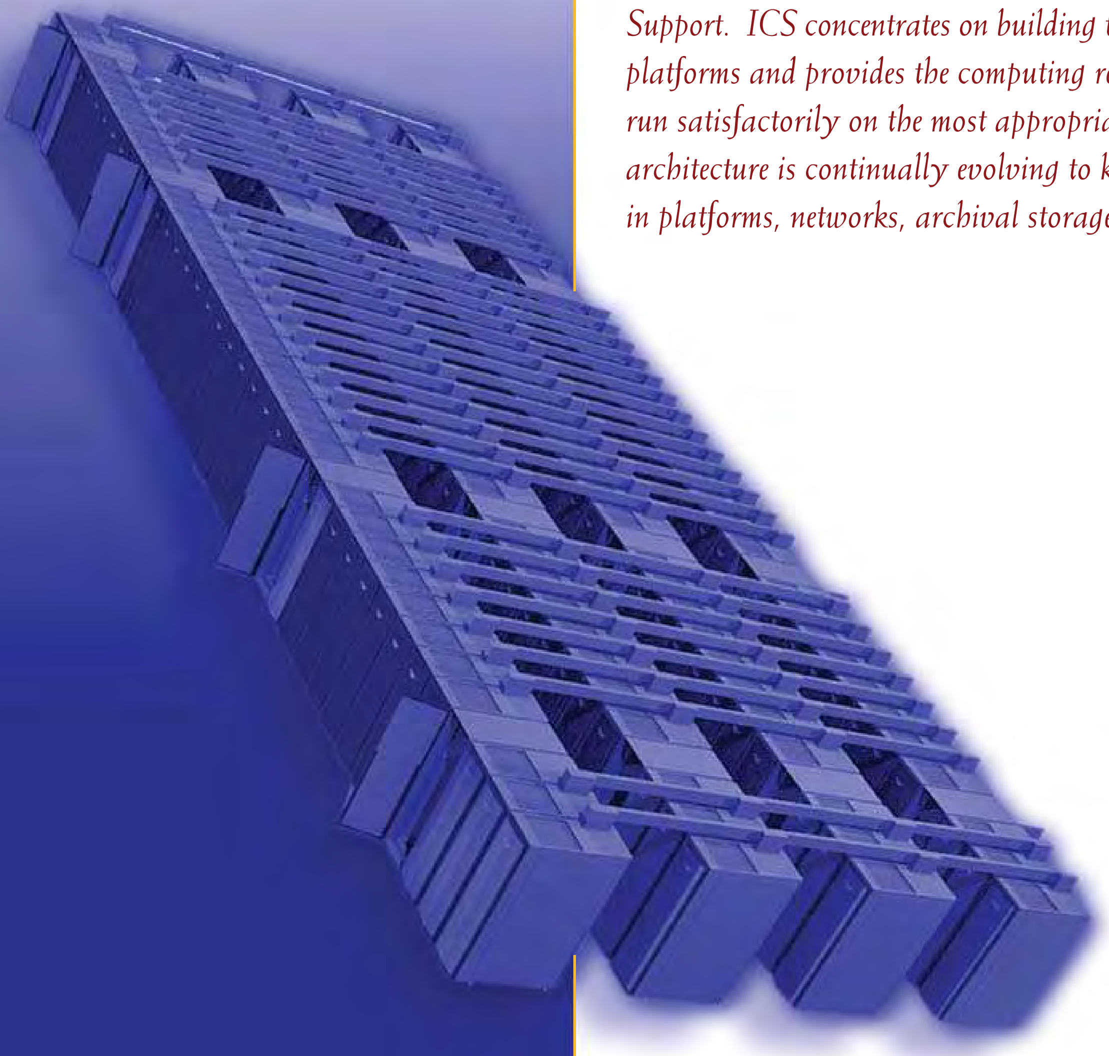


Future Developments

Near-term goals for the CUBIT team include adding the ability to generate large element meshes (>100M elements) on small memory machines (<2GB), adding a new graphical user interface to aid the new and intermittent users of CUBIT to come up to speed quickly with the meshing process, and automation, or "helper," tools to significantly aid the user and reduce the amount of time required to clean-up and decompose models for meshing, optimizing mesh quality, setting meshing parameters, and setting up boundary conditions.

Integrated Computing Systems

ASC's Integrated Computing Systems (ICS) component is composed of three elements: Physical Infrastructure and Platforms (PI&P), Computational Systems, and Simulation Support. ICS concentrates on building the infrastructure that supports the large computer platforms and provides the computing resources needed to ensure that applications run satisfactorily on the most appropriate machines, at any given time. The ICS architecture is continually evolving to keep pace with changes and replacements in platforms, networks, archival storage, and visualization facilities.



Operating and Maintaining ASC Platforms

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Sandia's production systems have supported "several national-security relevant calculations . . . as well as analysis of data and supporting simulations addressing the NASA Shuttle Columbia catastrophe."

Description

Production Systems involves the operation and maintenance of Sandia's ASC Platforms including the original ASC teraOPS platform, ASC Red, the Cplant™ systems in New Mexico and California. Commercial platforms are also maintained such as Origin 2000, Onyx 2 and Origin 3800 visualization servers, the HP ES45 SIERRA cluster (a mini-Q instantiation) and network storage devices represented by Network Appliance and BlueArc systems. These systems operate on the Sandia Restricted Network, the Sandia Open Network, and the Sandia Classified Network.

Technical Significance

ASC Red provides much-needed capacity to Sandia and University Alliance developers and analysts. ASC Red provides a stable, mature platform that can demonstrate scalability of codes up to several thousand nodes. In addition, the Parallel File System supports research and development of the SAF library for collective input/output of engineering science framework codes. The lightweight kernel operating system Cougar, supported by Sandia, is the prototype for the next-generation lightweight kernel to be used on Red Storm.

Contribution to the Stockpile Stewardship Program (SSP)

The capacity provided by ASC Red and Cplant™ permits selective high-priority runs for ASC milestones and DSW to be accomplished on ASC White and Q machines while supporting small- and medium-sized runs locally. In addition, several national-security relevant calculations have been supported as well as analysis of data and supporting simulations addressing the NASA Shuttle Columbia catastrophe. Cplant™ in particular has provided significant support to basic research efforts in materials science funded by ASC.

Benefits to ASC and to Sandia

When Sandia assumed full responsibility for support of ASC Red hardware and software, the situation demanded a cooperative effort between the computer science researchers in 9200 and the operations staff in 9300. This effort provided excellent training for the subsequent agreement with Cray, Inc., concerning the Lightweight Kernel support for Red Storm to be supplied by Sandia.

Future Developments

We will carry forward this operational experience and system support activity with Red Storm and regain world preeminence in scientific computing by demonstrating superior performance with the MPLINPACK code and attempt to surpass the Earth Simulator on the ToP 500 list of supercomputers. We will translate operational excellence and cluster management skills gained through construction and operation of the CPlant™ clusters into highly effective operation of commercial clusters for both New Mexico and California needs in general scientific computing and simulation.

Pioneering Platform and Operating System Designs:

Red Storm/Thor's Hammer Platform

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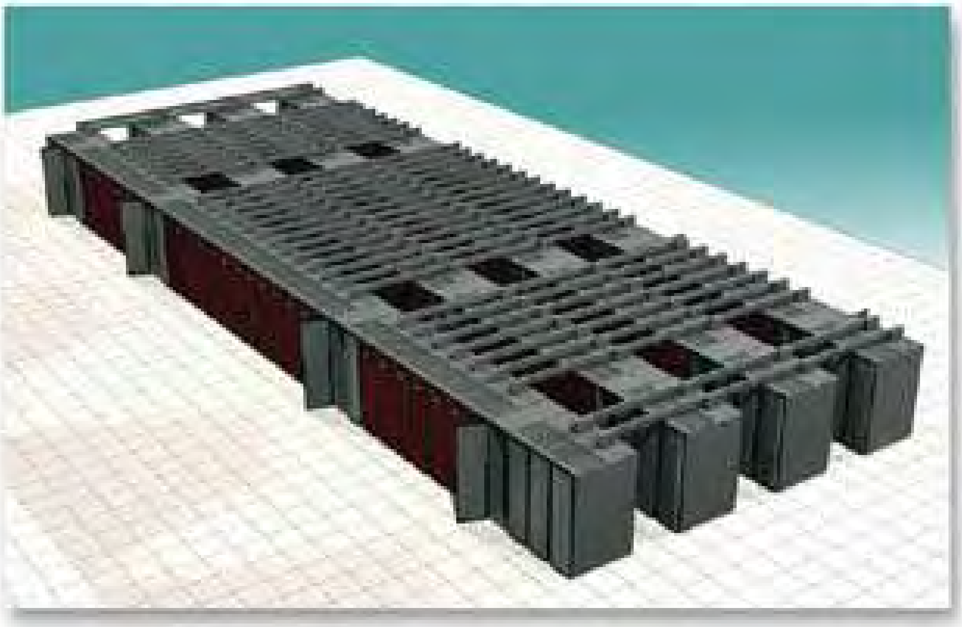
The nominal, theoretical peak performance of Thor's Hammer is rated at ~ 40 teraOPS. It consists of 10,368 processors in a central compute partition and 256 processors in each of two service and I/O partitions.

Description

In 2003 the Red Storm platform project extended ASCI Red, the first compute platform to achieve over one trillion operations per second – a teraOPS. Engineered and implemented in partnership with Cray, Inc., Red Storm is the modern architectural design for a new massively parallel MIMD (Multiple Instruction, Multiple Data) supercomputer using a new commodity processor – the 64 bit AMD Opteron™. Red Storm architecture scales from a single cabinet and relatively few processors to hundreds of cabinets and tens of thousands of processors. Opteron processor nodes are interconnected in a 3-D mesh high-speed network enabled by an Application Specific Integrated Circuit (ASIC), designed by Cray. The Red Storm operating system is a successor to the Intel UNIX & Cougar operating system employed on ASCI Red.

The first implementation of Red Storm is a machine called Thor's Hammer (Hammer is a reference to the "SledgeHammer" development code name of the AMD Opteron processor.) The nominal theoretical peak performance of Thor's Hammer is rated at ~ 40 teraOPS. It consists of 10,368 processors in a central compute partition and 256 processors in each of two service and I/O partitions. (A unique feature of both the ASCI Red and Thor's Hammer platforms is their ability to segment into two distinct machines with complete physical separation. This allows one segment to reside in a classified partition and the other to operate in an unclassified partition, and is typically done on a regular rotation in order to make large computational resource available for both classified and unclassified workload.)

Another key feature of the Red Storm Thor's Hammer implementation is its relatively low power consumption and air-cooled mechanical design engineered into a small footprint. Each compute cabinet consumes about 15 kW for total Thor's Hammer power consumption of less than 2 MW. The footprint of the total system is less than 3000 ft². (By comparison, the Earth Simulator ~ 40 teraOPS machine, currently listed as the fastest in the world, consumes on the order of 100 MW in a footprint of about 25000 ft².)



Rendering of Thor's Hammer showing the following features: compute partitions in red, service I/O partitions in grey, overhead cable trays, and separation points shown by open doors.

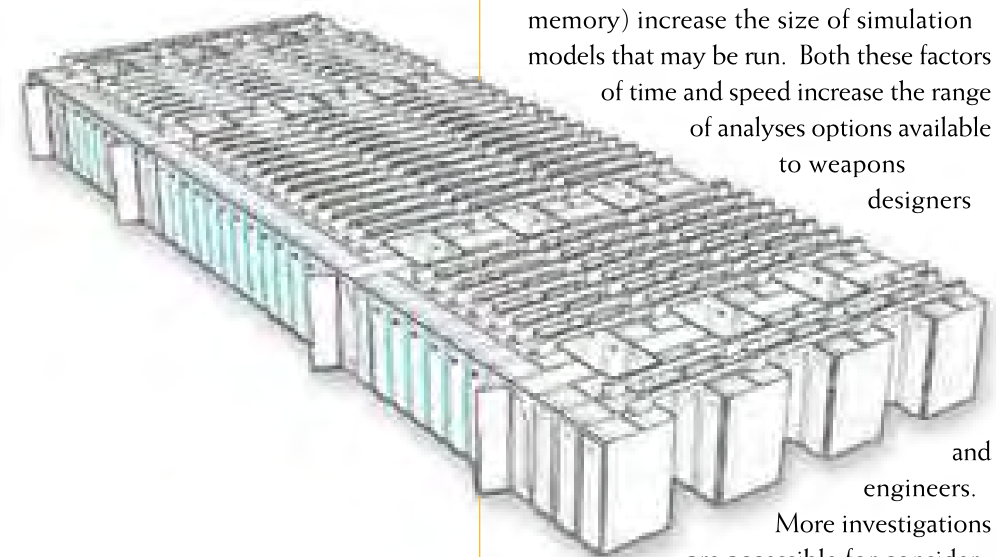
Technical Significance

Red Storm hardware architecture features a highly scalable combination of 1) a custom ASIC-enabled high-speed-network for processor-to-processor communication in a 3D-mesh topology, and 2) a commodity processor (AMD Opteron) with its own integrated DDR DRAM memory controller. The result is a much more balanced and tightly coupled MPP design that exhibits high inter-processor and memory bandwidths with low latencies.

Red Storm operating system architecture (SUSE Linux / SNL-Cray Catamount LWK) addresses scalability of applications and operating systems services. Moreover, Red Storm systems architecture supports an extremely high-performance scalable parallel file system and a very high performance network bandwidth to support intensive local and off-machine data transport. Along with selective direct engagement with sub-system, providers to tune performance (e.g., compiler and debugging and performance assessment tool vendors), these balanced combinations of commodity strengths and custom development ensure that Red Storm is a design that leverages applications and O/S performance at scale better than other conventional O/S and architecture constructs.

Contribution to the Stockpile Stewardship Program (SSP)

Increases in computational speed and efficiency decrease the time it takes to run any given application computation. Increases in machine size (particularly number of nodes and available application memory) increase the size of simulation models that may be run. Both these factors of time and speed increase the range of analyses options available to weapons designers



and engineers. More investigations are accessible for consider-ation and greater fidelity and resolution may be applied to problems that can benefit from more model detail. Addi-tional physics (more calculations per time step) may also be included in some analyses.

Faster computation also allows analysts to run computations for longer ranges of time steps to investigate phenomena over longer simulated time spans.

All of these factors contribute to increased scientific understanding of complex phenomena in our problem sets and help increase confidence in the stockpile.

Benefits to ASC and to Sandia

Along with the direct scientific and engineering contributions to stockpile stewardship, the investment in state-of-the-art computation is an investment in people and in reputation. Challenging leading-edge computational science attracts the talents of the very best computer scientists and engineers. Additionally, it enhances the reputation of Sandia both within the DOE Complex and in the external technical and political circles. It helps ASC and Sandia compete for personnel and technical resources and improves our ability to succeed in our missions. Projects like Red Storm bring the very best to ASC and to Sandia.

Future Developments

Platform acquisitions are both strategic and dynamic decisions. They require carefully planned requirements-driven specification development as they are competed for procurement. Yet, they also require agile, technology-driven oppor-tunities to foster and reward innovation that may enhance application performance for NNSA/ASC missions. A variety of future developments are anticipated:

- Follow-on increases in scale are contemplated to double or triple the size of Thor's Hammer via direct addition of more system nodes to the 3-D mesh. The current machine could easily reach above 100 teraOPS for a relative fraction of original cost.
- Hybrid architectures are also contemplated, such as Processor-in-Memory methods to improve processor-memory data bandwidth, and selectively incorporating vector-processing techniques to improve application efficiencies.
- Interconnect technology evolution may provide opportunity to increase inter-processor messaging bandwidth and decrease latency.
- Enhancements to service and I/O sub-systems, such as modernization of the adapter bus, are also under consideration to improve machine pre- and post- processing capabilities for data services and visualization.

All of these possibilities are likely contributors to increase computing capability to, and beyond, a petaOPS (1000 teraOPS), and along with off-machine infrastructure improvements, application improvements, and algorithms improvements, promise to continue the growth and importance of ASC .

Supporting ASC with State-of-the-Art Facilities:

DISL – The Distributed Information Systems Laboratory

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DISL provides a facility for research, development, prototyping, and production usage of leading-edge, high-performance computer and communications technologies required to make distributed computing and collaborative engineering a reality.

Description

The Distributed Information Systems Laboratory (DISL) is a line item (~$38M) project construction of an ~71,500 ft^2 office and computer laboratory building to house ~180 staff and visiting researchers. DISL is in the Sandia/CA Technical Area.

The DISL building is a two-story structure consisting of offices for computer science and weapons engineering staff and laboratories supporting research and development in several computer-science disciplines. DISL straddles a limited area boundary with about two-thirds of the building in the limited area and capable of classified operations and about one-third open to unclassified collaboration and interaction with visiting researchers.

In addition to offices, DISL has:

1. Computer labs – a High-Performance Computing lab, a Network/Partnerships lab, a Collaboration lab, a Visualization lab, a Network Security and Cyber Security lab, and a Technology Deployment lab;
2. Visualization Design Center – a large first-floor facility with state-of-the-art information displays and communications capabilities and with high-performance, large-format immersive displays;
3. Large and small conference rooms;
4. Central communications distribution rooms that are the core of the advanced network switching and optical fiber and copper infrastructure, supporting as much as 10-Gb bandwidth to every desktop or computing function in the facility;
5. A senior management suite.

DISL provides a facility for research, development, prototyping, and production usage of leading-edge, high-performance computer and communications technologies required to make distributed computing and collaborative engineering a reality. The focus is on enabling the distributed computing environment for Complex-wide integration and engineering collaboration. These technologies are crucial to achieving the virtual enterprise of the future, which is distributed but totally interconnected, where every piece knows what every other piece is doing, and where designers, analysts, and experimenters can interact with each other as if they were in the same room. Moreover, DISL uses as well as develops this leading-edge technology. DISL is a prototype demonstrating a science and engineering workplace of the 21st century.


An aerial view of DISL.

Technical Significance

DISL brings together elements of Sandia's network security and communications, distributed computing and collaborative engineering, and visualization communities to enhance collaboration and improve effectiveness needed for science-based stockpile stewardship (SBSS) across the Complex.

The primary tenants of DISL are from Weapons Design, Technology Deployment, Enterprise Modeling, Visualization R&D, Cyber Security R&D, Network/Cluster Computing R&D, and Computer Sciences R&D organizations. Workgroups in DISL from these groups are the Distance Computing and Enterprise Collaboration backbone of ASC's modeling and simulation.

Contribution to the Stockpile Stewardship Program (SSP)

DISL is the Sandia/CA center of activities supporting the ASC program (as JCEL – the Joint Computational Engineering Laboratory, is the Sandia/NM center) and is a key contributor to ASC's success. DISL's mission is to develop and employ advanced secure communications and distributed information tools supporting SBSS. Capability developed within DISL will ultimately support a more effective and efficient and distributed Complex-wide enterprise.

Benefits to ASC and to Sandia

The process of attracting the brightest technical talent to the nuclear weapons complex and retaining them is immeasurably enhanced by offering world-class facilities and technical capabilities. DISL, JCEL, and the Microsystems & Engineering Sciences Applications (MESA), the three newest of Sandia's major facilities, recognize the need to compete for talent and provide staff with the best working environments and resources available. Facilities such as DISL can be critical recruiting differentiators, and building DISL with the appearance and the functionality of a world-class R&D workplace of the 21st century is an important long-term benefit to ASC and Sandia.

Future Developments

The location of DISL in the center of the California site is a step toward more effective collocation of secure communications and distributed information technologies and capabilities essential to ASC and SBSS. These are essential missions for the Sandia/CA laboratory and are an important base for future growth. The California site will continue to be the center of this technology research and development for the Complex and the nation. Information systems science and cyber security and communications science contribute greatly to Complex-wide collaborations. They merge with ASC-enabled modeling and simulation into a uniquely functional and attractive center of world-class research, development, and applications supporting SBSS.

Supporting ASC with State-of-the-Art Facilities:

JCEL – The Joint Computational Engineering Laboratory

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The primary mission of JCEL is to ensure the rapid development and application of high-performance computing, modeling, analysis, design, and simulation, which is a foundation of the SBSS vision as it is supported by the ASC program.

Description

The Joint Computational Engineering Laboratory (JCEL) is a line item (~$31M) project construction of ~65,000 ft² office and computer laboratory building to house ~175 staff. JCEL is sited in the SW corner of Sandia/NM's Technical Area I close to the Central Computing and Communications Facility, the SuperComputing Annex (and site of Thor's Hammer/Red Storm, Sandia's newest largest computing platform), and to the MESA (Microsystems Engineering Sciences Applications) complex currently under construction.

The JCEL building is a three-story structure consisting primarily of office/staff pods, each built to TSRD specification for secure, common need-to-know workgroups. Each workgroup pod supports approximately 20 people, including management, administrative support, and conferencing space. In addition to the office pods, there are the following:

1. Computer labs – an unclassified lab area and a classified lab area supporting the state-of-the-art ASC computing infrastructure.
2. Visualization labs – a large first floor "visualization corridor" facility with a large-format, very-high-resolution tiled display (~20 ft × 10 ft × 30 million pixel) and a smaller second floor work room with a custom visualization display table and user workstations.
3. Large and small conference rooms with multiple advanced displays.
4. Area outside the need-to-know boundaries for visiting researchers.
5. Central communications distribution rooms that are the core of the advanced network switching and optical fiber and copper infrastructure, supporting up to 10-Gb bandwidth to every desktop or computing function in the facility.
6. A senior management suite.

The primary mission of JCEL is to ensure the rapid development and application of high-performance computing, modeling, analysis, design, and simulation, which is a foundation of the SBSS vision as it is supported by the ASC program. JCEL is a prototype and demonstration of a science and engineering workplace of the 21st century.

Technical Significance

JCEL brings together elements of Sandia's design, computational simulation, and analysis communities to enhance collaboration and improve effectiveness needed for SBSS. JCEL will be occupied by the Stockpile Resource Center (2900); the Computation, Computers, Information and Mathematics Center (9200); and the Engineering Sciences Center (9100). Center 2900 is largely responsible for supporting War Reserve engineering design and CAD/CAM model development, Center 9200 is largely responsible for algorithms and computational tools development, and Center 9100 is largely responsible for simulation codes development, simulation models, and analysis. Workgroups in JCEL from these centers are the Design-Through-Analysis backbone of ASC's modeling and simulation vision for nuclear weapons science-based model-based engineering.

Contribution to the Stockpile Stewardship Program (SSP)

JCEL is Sandia/NM's center of activities supporting the ASC program (as DISL is the Sandia/CA center) and is a key contributor to ASC's success. JCEL's mission is to develop and employ advanced SBSS tools. In JCEL, design alternatives will be developed and explored using iterative simulations of virtual prototypes. Surety, reliability, and performance assessments will be model-based and incorporate fundamental understanding of critical component response to the full range and all credible combinations of environmental inputs defined for weapon systems in Normal, Abnormal, and Hostile environments. Tools developed within JCEL will ultimately support manufacturing efforts elsewhere within Sandia and the NWC by enabling product design alternatives to be modeled, analyzed, evaluated, and modified as necessary by engineers—all through the use of simulation.

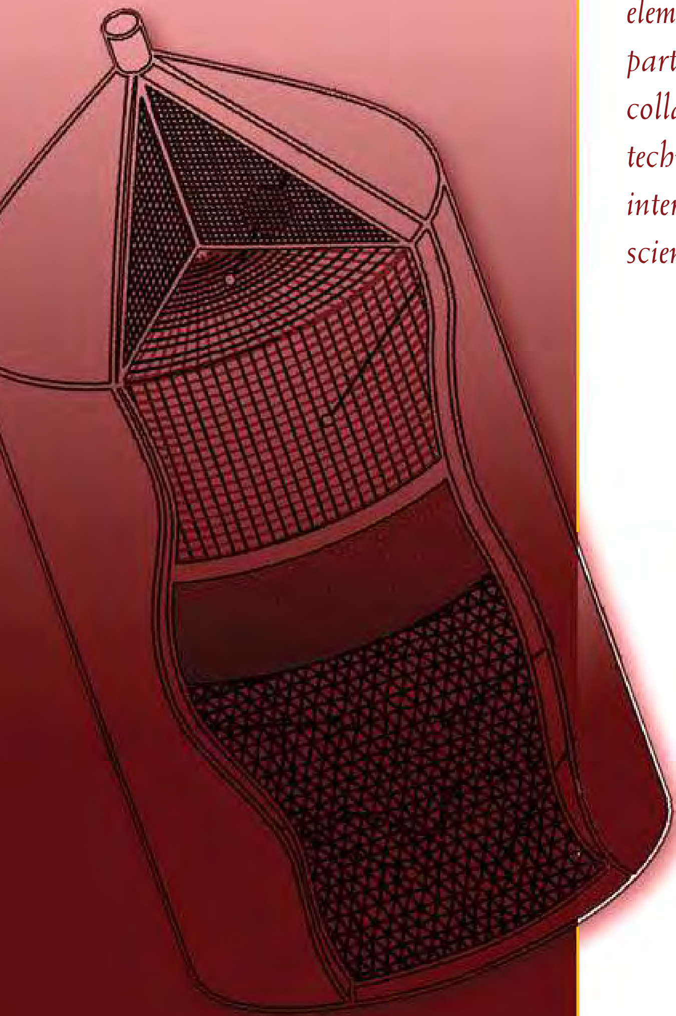
Benefits to ASC and to Sandia

As with DISL the process of attracting the brightest technical talent to the nuclear weapons complex is immeasurably enhanced by offering top facilities and world-class technical capabilities. JCEL, DISL, and MESA, the three newest of Sandia's major facilities, all recognize the need to compete for talent and provide staff with the best working environments and resources available. Facilities such as JCEL can be critical recruiting differentiators, and building JCEL with the appearance and the functionality of a world-class R&D workplace of the 21st century is an important long-term benefit to ASC and Sandia.

Future Developments

The location of JCEL in Sandia/NM Tech Area I near the established Central Computing Facility, the newly completed SuperComputing Annex, and emerging MESA facilities (particularly the MESA Weapons Integration Facility sited directly east of JCEL) is a step toward more effective co-location of critical computation, engineering design, and modeling and simulation capabilities. Together, these facilities with their intensive communications infrastructure and their large electrical and mechanical loads form a synergistic "Computing District" as defined within Sandia's Comprehensive Site Plan. General site improvements will build this part of the Sandia Technical Area I into a uniquely functional and attractive center of world-class research, development, and application of computational and engineering science for SBSS.

University Partnerships



ASC's University Partnerships (UP) component at Sandia is composed of two elements: Academic Strategic Alliance Program (ASAP) and Institutes. Sandia is a participant in ASAP, which is run as a tri-lab program. The crux of ASAP is to collaborate with academia in the areas of science-based modeling and simulation technologies. Computer science institutes are focal points for laboratory-university interactions and serve as vehicles for fostering increased basic and applied scientific research at the laboratories.

Partnering with Universities

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Research conducted through this partnership is contributing to the knowledge base required to demonstrate the powerful capabilities of modeling and simulation across a broad spectrum of science and engineering applications, using massively parallel computers.

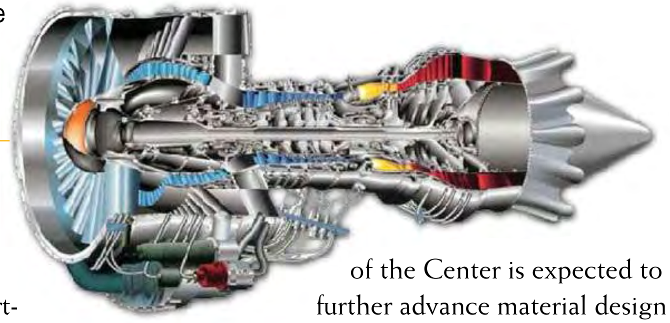
Description

Academic Strategic Alliance Program (ASAP), through partnerships with five universities, pursues advances in the development of computational science, computer systems, mathematical modeling, and numerical mathematics important to ASC. The participating universities are developing new computational frameworks as they make advances in several scientific areas, such as material sciences, fluid dynamics, turbulence, solid mechanics, and radiation physics. The ultimate goal is to integrate large computer models from these various disciplines into single, comprehensive models to solve critical scientific and engineering problems.

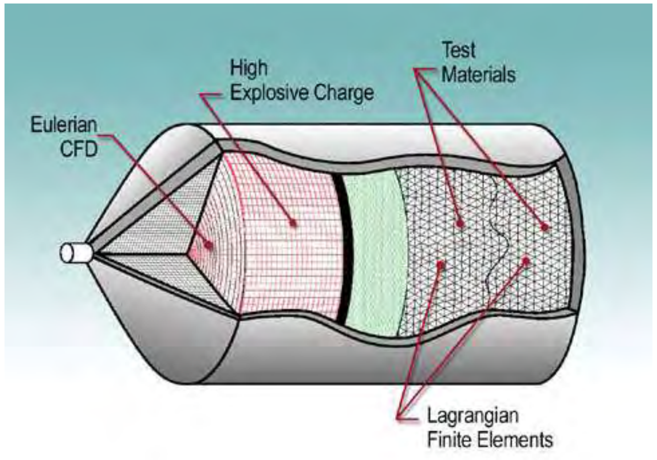
Technical Significance

Five university-based Centers of Excellence were chosen competitively from among almost 50 proposals to undertake computer-based simulations of similar magnitude and multi-disciplinary complexity to those required of the Defense Program laboratories . Thus, multiple disciplines and departments are engaged at each of the centers, working with the three laboratories' sponsoring teams consisting of experts in areas of computational mathematics and computer science, as well as the science and engineering disciplines relevant to the simulation at each center.

A description of the five centers' technical focus follows.



Integrated turbulence simulation: a detailed simulation of a jet engine—Stanford University.



Dynamic response of materials—Caltech.

• California Institute of Technology (Caltech), Center for Simulating the Dynamic Response of Materials –The Center is developing simulation codes for its virtual shock physics test facility (VTF). The VTF allows researchers to introduce strong shock and detonation waves that collide with targets, to compute the subsequent dynamic response of the target materials, and to validate these computations against experimental data. Understanding the dynamic response of materials is a key technical issue for ASC, since this response is at the heart of essentially all processes governing the performance, safety, and reliability of the nuclear stockpile. The work of the Center is expected to further advance material design and have applications in other areas such as geophysics related to oil exploration, earthquake prediction, and weather analysis and forecasting.

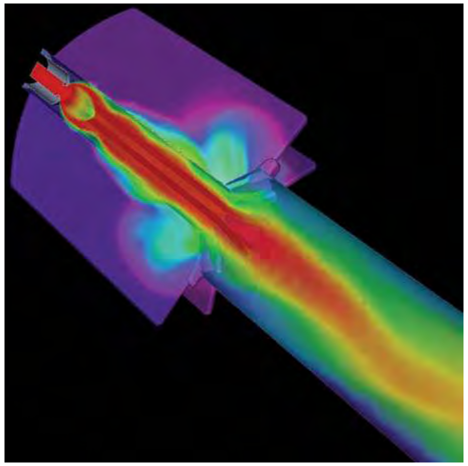
• Stanford University, Center for Integrated Turbulence Simulation – This Center's research focuses on the simulation of compressor, combustor, and turbine components of aircraft turbine engines. The resulting integrated simulations examine, for example, rotating stall in the compressor, aero-elastic blade vibrations, combustor instabilities, and heat transfer from the hot combustion products to the first blade rows of the turbine. Code development work at the Center involves producing massively parallel codes for high-fidelity flow and combustion simulation. Improvements in turbulence and transport modeling, and combustion and compressible flow computations, will help Stanford establish a new design paradigm that will shorten the design cycle, reduce testing expense, and improve reliability of turbine engines. Other key components of the program are research on numerical methods, compilers, operating systems, and computer architectures, driven by (and supporting) the massively parallel turbulence simulations.

Studying the stars: what happens when stars die? where are complex atoms produced? how big is the universe? how old is the universe?— University of Chicago

• University of Chicago, Center for Astrophysical Thermonuclear Flashes – At the University of Chicago's Center, scientists study the physics of thermonuclear explosions of extremely compact and dense stars. Such explosions occur when matter from a companion star falls onto the surface of the compact star, where it is crushed and heated by gravity. The Center is developing simulations and analyses of these thermonuclear flashes. The goal of the Center is to provide an understanding of the physics of nuclear ignition, detonation, and turbulent mixing of complex multi-component fluids and other materials. The proposed integrated calculation will be the highest resolution calculation ever done for the initiation of a nova outburst.

• University of Illinois, Urbana/Champaign, Center for Simulation of Advanced Rockets – The Center is using the National Aeronautics and Space Administration Space Shuttle as the simulation vehicle for the detailed, whole-system simulation of solid propellant rockets. Solid propellant rockets provide the immense thrust required to launch large payloads into space. Although the individual component technologies are reasonably well understood, lacking has been high-resolution, fully three-dimensional, integrated modeling and simulation of their complex interactions and the resulting potential instabilities and failures. The design of solid-propellant rockets is a sophisticated problem requiring expertise in diverse disciplines, including ignition and combustion, solid mechanics, fluid dynamics, shock physics and quantum chemistry, the aging and damage of components, and the analysis of various potential failure modes.

• University of Utah, Center for the Simulation of Accidental Fires & Explosions – The Center's focus is to provide state-of-the-art, science-based tools for the numerical simulation of accidental fires and explosions, especially within the context of handling and storing highly flammable materials. These simulations will also help to better evaluate the risks and safety issues associated with fires and explosions in the aerospace, chemical, and petroleum industries. The ultimate goal of the Center is to simulate fires involving a diverse range of accident scenarios. These problems require knowledge of fundamental gas- and condensed-phase chemistry, structural mechanics, turbulent flows, convective and radiative heat transfer, and mass transfer. These simulation computations must be time-accurate and contain full-physics simulation of accidental fires.



Simulation of Advanced Rockets — University of Illinois

Simulation of accidental fires & explosions — University of Utah.

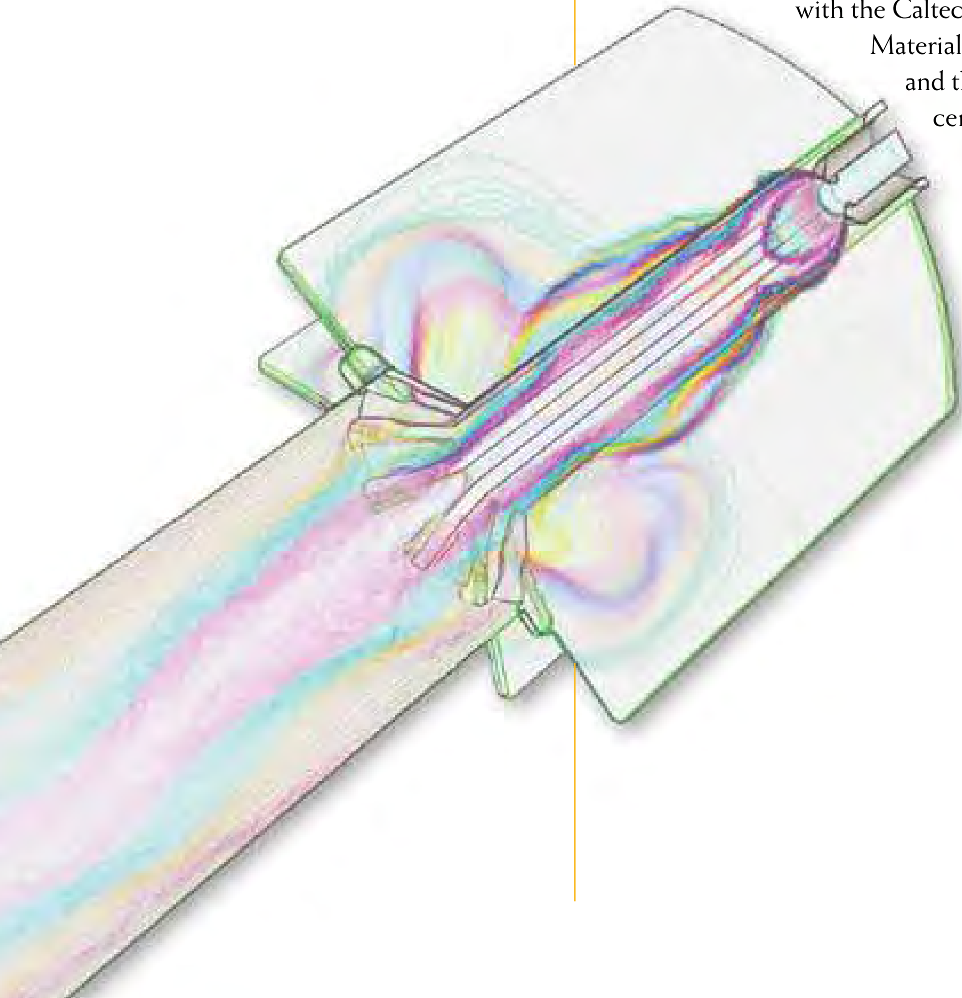
Contribution to the Stockpile Stewardship Program (SSP)

ASAP was formed to involve the U.S. academic community in advancing science-based modeling and simulation technologies. Research conducted through this partnership is contributing to the knowledge base required to demonstrate the powerful capabilities of modeling and simulation across a broad spectrum of science and engineering applications, using massively parallel computers. The computing problems tackled by ASAP do not involve nuclear weapons research, but the methodologies and tools developed for their solutions are having a positive impact on stockpile stewardship, as well as other national scientific, economic, and social needs.

Benefits to ASC and to Sandia

The three Defense Program laboratories have an unprecedented opportunity to collaborate with the Centers in areas of common interest. Through shared experiences using massively parallel computers and through workshops, site visits, and staff exchanges, both entities form strong interactive bonds that are mutually beneficial. The universities are also establishing new computational sciences curriculums, providing a pipeline of students for ASC tri-lab staffing needs.

Sandia has exchanged staff with the Caltech center in the area of molecular dynamics and jointly sponsored workshops with the Caltech center on Materials Modeling and the Stanford center on turbulent combustion. Sandia has hired 10 students/staff from ASAP centers. In the last year, Caltech, University of Chicago, University of Illinois, and University of Utah made site visits to Sandia/NM and Sandia/CA. In each of these visits, the universities brought 20–40 faculty, staff, and students to Sandia; presented overview technical talks; held detailed technical discussions with Sandia staff; and presented poster papers. These activities have resulted in successive collaborations.



Future Developments

ASAP was initially planned as a five-year program. In 2002, the program was extended for another five years to 2007. External reviews have regarded ASAP as an extremely successful program. All five centers are progressing to accomplish their goals. The future of the program after 2007 is being discussed and will be reported when a decision is reached.

Establishing Research Centers:

The Computer Science Research Institute

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The CSRI "…provides both a physical and technical focal point for identifying problems, for conducting research and for developing and strengthening interactions between the university and laboratory researchers."

Description

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. During each of the past several years, the CSRI has hosted over 200 short-term visitors and over 60 long-term visitors including summer faculty, sabbaticals and student internships. These participants represented over 100 institutions. Participants are encouraged to develop long-term collaborative relationships with laboratory scientists and researchers.

The CSRI has facilities in Albuquerque, New Mexico and Livermore, California. These facilities include office space for over 75 staff and collaborators, conference rooms, collaborative work areas and extensive computing facilities. These facilities include the Intel Teraflops computer, Cplant™, (a scalable cluster-based computer) an SGI Origin 2000, a Compaq SIERRA cluster, and other computers available for research.

Technical Significance

The CSRI sponsors studies in computer science, computational science and mathematics that impact large-scale modeling and simulation. One of the key technical issues is that of scaling; the CSRI is interested in developing algorithms and software that scale both as the size and complexity of the problems increase and as the number of processors increase to the thousands or tens of thousands. The CSRI is also interested in computer platforms, including hardware and system software that scale to thousands of processors.

Some of the technical areas of interest include:

Computer Science

- Scalable cluster computers and heterogeneous computers.
- Data-intensive computing.
- Environments for scalable computing.
- Parallel I/O.
- Advanced Algorithms.

Mathematics and Algorithms.

- Scalable solvers.
- Optimization.
- Adaptivity and mesh refinement.
- Algorithms for solution of differential and integral equations.
- Graph-based, discrete and combinatorial algorithms.
- Uncertainty estimation and verification and validation.

Enabling Technologies

- Mesh generation.

Top row: Curt Ober, Sandia; Simon Tavener, Colorado State University; Donald Estep, Colorado State University; Jim Teresco, Williams College; Max Gunzburger, Florida State University; Joe Flaherty, Rensselaer Polytechnic Institute; Martin Berggren, Sandia; Bill Hart, Sandia; John Shadid, Sandia; Roscoe Bartlett, Sandia

Bottom row: Karen Devine, Pavel Bochev, Rich Lehoucq, and David Ropp, all Sandia

Benefits to ASC and to Sandia

The CSRI complements existing laboratory research programs and ASC university alliances. It provides both a physical and technical focal point for identifying problems, for conducting research and for developing and strengthening interactions between the university and laboratory researchers.

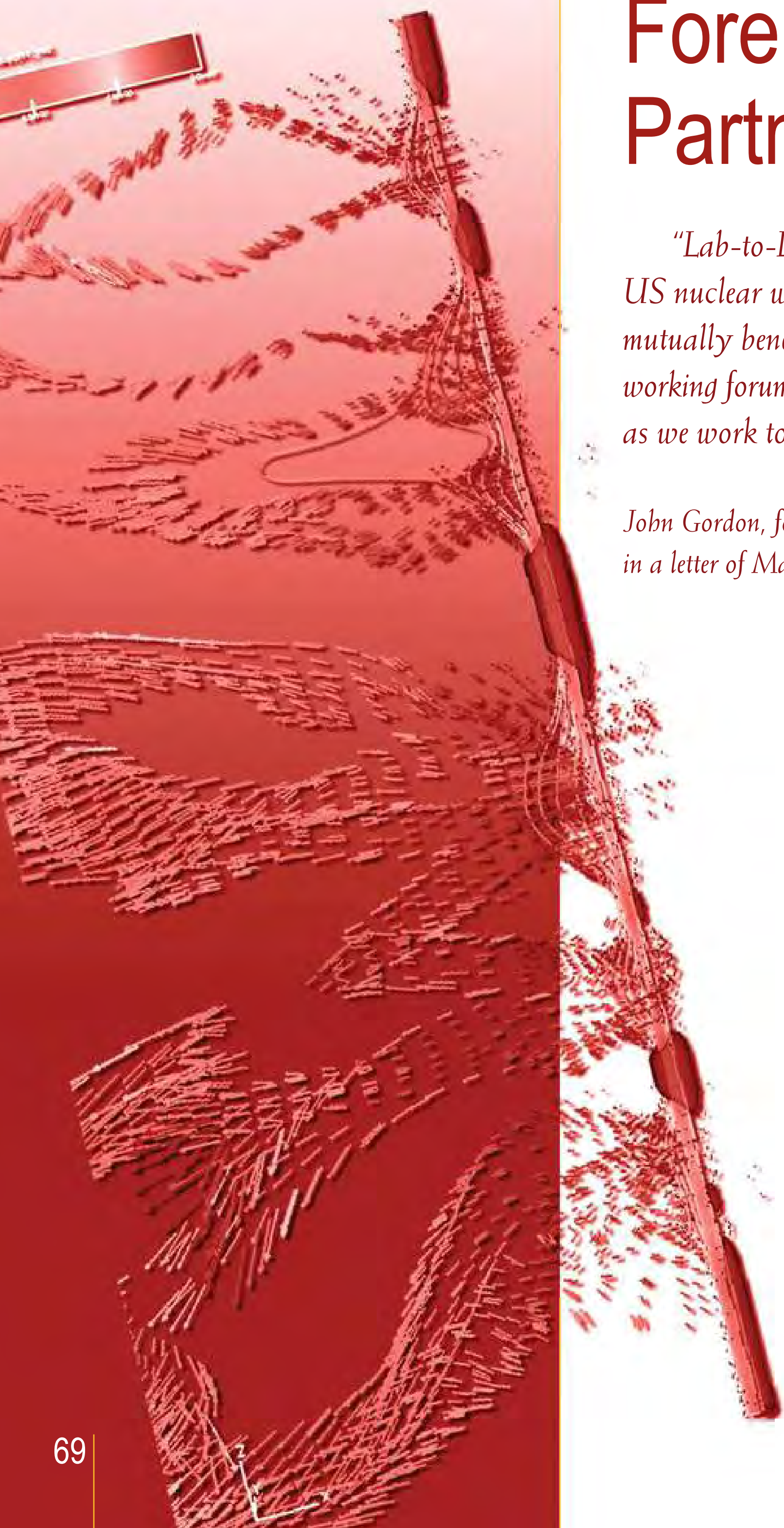
University and industry researchers participate in the CSRI through collaborative research projects, short-term visits, extended visits, summer positions, sabbaticals, and workshops. The CSRI also supports both graduate and undergraduate student programs. These include post-doctoral positions, summer jobs and graduate fellowships. The CSRI encourages students to choose careers in computer science, computational science, and mathematics that support directly the challenges of national security.

The CSRI presents many opportunities for collaborations between university researchers and laboratory scientists in the areas of computer science, computational science and mathematics:

- Faculty sabbaticals lasting from a semester to a year,
- Summer faculty positions,
- Graduate fellowships through the NPSC and HPCS (Krell Institute) programs,
- Summer student positions,
- Technical visits of lengths from one week to three months,
- Post-doctoral positions lasting up to two years,
- Conference sponsorships,
- A CSRI colloquium series,
- Visits by laboratory staff to universities.

Future Developments

The nature of science institutes is to continue to nurture collaborative efforts among the laboratories and universities with the ultimate goal of enhancing existing, and developing newer, capabilities in modeling and simulations.



Foreign Partnerships

"Lab-to-Lab interactions between the Russian nuclear weapons initiatives and the US nuclear weapons laboratories that began some ten years ago have proven to be mutually beneficial. Continuing technical and scientific collaboration also provides a working forum that will materially contribute to the new US/Russian strategic relationship as we work to address areas of mutual interest and concern."

John Gordon, former Administrator, National Nuclear Security Administration
in a letter of May 14, 2002.

Collaborating With the Russian Federal Nuclear Institutes

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Out of these collaborations we hope to uncover extensions to our research and development activities, and perhaps insights into alternative approaches to difficult problems.

Description

In the summer of 2002, John Gordon, Administrator of NNSA, and L. D. Ryabev, First Deputy Minister of Ministry for Atomic Energy of the Russian Federation (Minatom), agreed to renewed lab-to-lab interactions between the U.S. nuclear weapons R&D laboratories and the Russian Federal Nuclear Institutes. The new collaborations would focus on Science and Technology (S&T), principally in the areas of materials science, computational methods, and experiments and technologies in pulsed power. The U.S. participants are Sandia, Los Alamos, and Lawrence Livermore, and the Russian participants are VNIEEF at Sarov, VNIETF at Chelyabinsk, and VNIIA in Moscow. At Sandia, a portion of our commitment to these collaborations is supported by the ASC Program. During 2003 the ASC Program placed contracts with the Federal Institutes in computational algorithms for Z-pinch applications, and we held substantive discussions in the areas of molecular dynamics (Figure 1), sub-grid scale mechanics, and computer architectures – discussions that will hopefully lead to additional contracts in 2004.

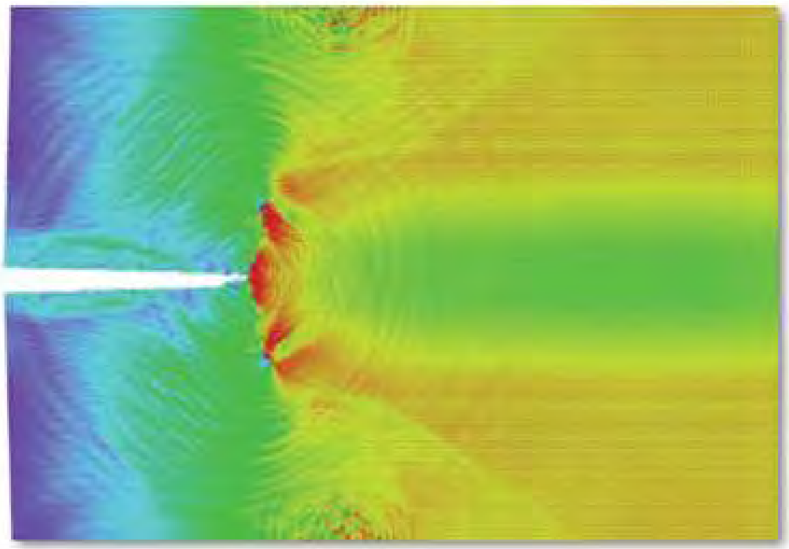


Figure 1. Steady-state, dynamic crack propagation using molecular dynamics.

Technical Significance

The technical significance of these collaborations is based on the opportunities offered to Sandia's engineers and scientists to access unique analytical, simulation and experimental methods at the Russian Federal Nuclear Institutes. Out of these collaborations we hope to uncover extensions to our research and development activities, and perhaps insights into alternative approaches to difficult problems. Moreover, the Russian Institutes offer low-cost and high-quality technical staff and experimental facilities.

Contribution to the Stockpile Stewardship Program (SSP)

The current Administrator of NNSA, Dr. Ev Beckner, continues NNSA's support of these lab-to-lab collaborations, and he believes there is the potential of significant technical benefit to the US laboratories' staff by focusing on science and technology projects. Projects already placed, *"Development of Hybrid PIC Code for Simulating PW Laser Interactions with Dense Matter,"* and *"Numerical Simulation of Wire Array Implosions,"*

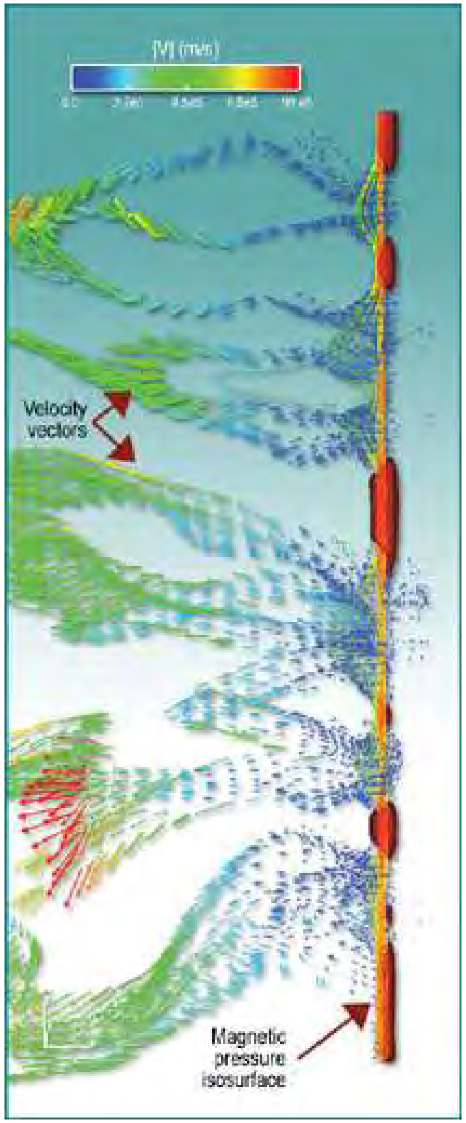


Figure 2. Velocity vectors with current density stream lines, plus isosurface of maximum in magnetic pressure.

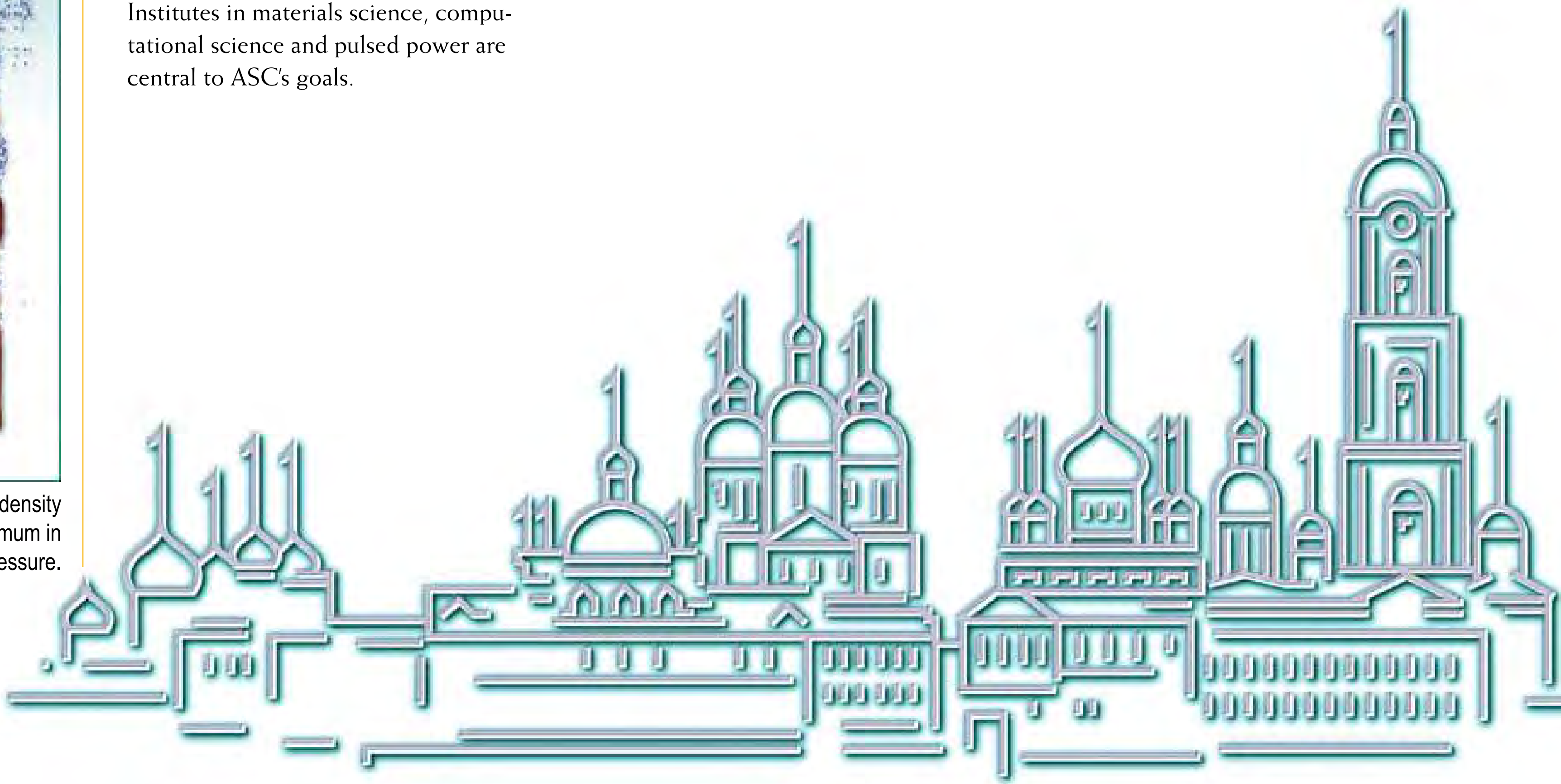
are central to simulation of Z-pinch physics (Figure 2) in proposed upgrades to Sandia's pulsed power facilities.

Benefits to ASC and to Sandia

These collaborations encourage interactions among Sandia's engineers and scientists working on leading- edge research and development for the ASC program. The goal of ASC is to deliver physics-based simulation capabilities, and central to this goal is an understanding of the underpinning physics, including experimental discovery, theoretical models, and numerical algorithms. Our S&T collaborations with the Russian Federal Institutes in materials science, computational science and pulsed power are central to ASC's goals.

Future Developments

Collaborations with the Russian Federal Nuclear Institutes and the ASC Program are off to an excellent start, with the signing of four contracts in 2003. We expect additional contracts in materials science (Figure 2) and computational sciences to be negotiated and started in 2004. With the possible introduction of government-to-government agreements covering these collaborations, we may in the future be able to work with Russian Institutes outside of Minatom.



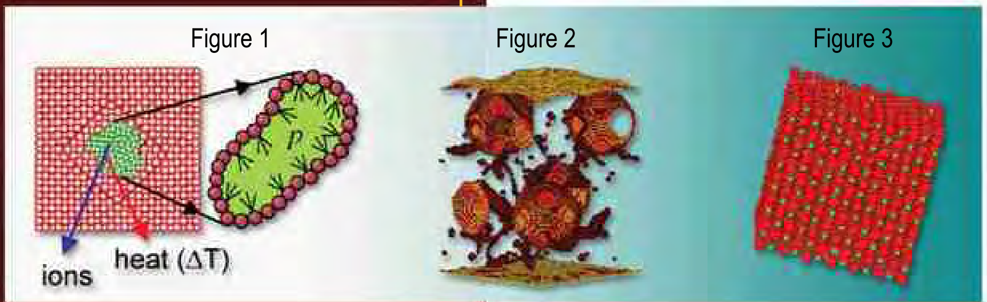


Figure 1. Atomistic model of Helium bubble – A bubble of helium atoms (green) is placed within a metallic lattice (red) to study the material defects created during bubble growth. Over time, additional helium atoms are created within the bubble to simulate aging processes. It was determined that the nearly spherical growth of the bubbles is also accomplished with a force-field of expanding range that acts on metal atoms adjacent to the bubble surface. Doing-so relieves the computational requirements for simulating bubble growth.

Figure 2. Helium bubble growth near a free surface – Growth of multiple Helium bubbles is simulated within a metallic lattice in which the Helium bubbles are placed in proximity to a free surface. The bubbles themselves are modeled using force-fields with time-varying ranges. The growing bubbles produce crystalline defects including vacancies, dislocation threads, and stacking fault tetrahedra. The dislocation threads are observed to not only interconnect the bubbles, but also create paths to the free surface.

Figure 3. Model of Metal-Hydride – It is in aging metal-tritides that Helium bubbles develop and grow. As such, an inter-atomic potential is being developed to accurately model the physical and mechanical properties of hydrogen atoms (green) positioned interstitially within a metallic lattice (red). This potential should reproduce such features as metal-hydride lattice parameter, miscibility gap as a function of hydrogen content, and occupancy of the lowest energy interstitial site at thermodynamic equilibrium.