2014 HPC ANNUAL REPORT

SANDIA MISSION COMPUTING

Sandia National Laboratories

SNLSimMagic©

AUGMENTED REALITY APP

Scanning this code with an iPhone or iPad will provide access to SNLSimMagic; an augmented reality iOS application that can be downloaded to the device. Readers with the application can use their mobile devices to scan images in this document that show the AR icon, and an associated movie clip will be played on their device. SNLSimMagic was developed at Sandia National Laboratories.

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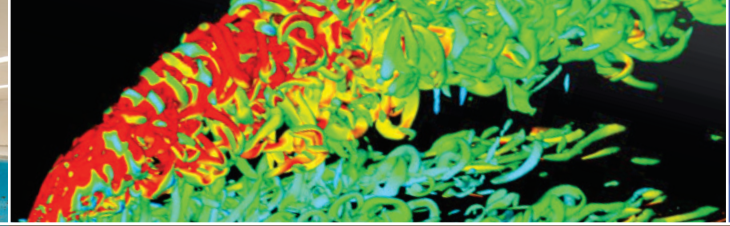
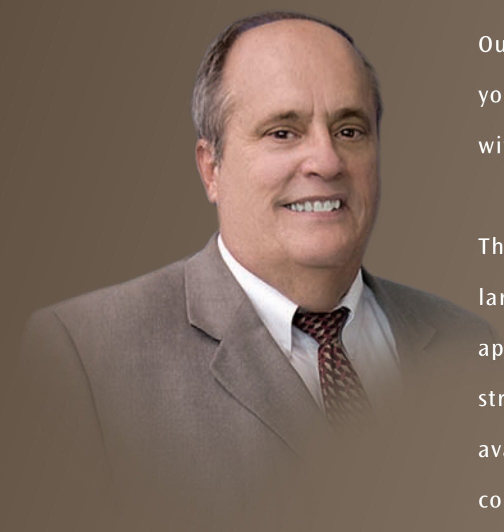



SUSTAINING MISSION EXCELLENCE

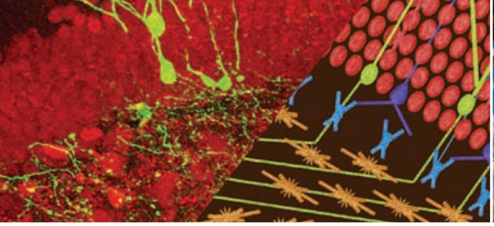


Our commitment is to support you through delivery of an IT environment that provides mission value by transforming the way you use, protect, and access information. We approach this through technical innovation, risk management, and relationships with our workforce, Laboratories leadership, and policy makers nationwide.

This second edition of our HPC Annual Report continues our commitment to communicate the details and impact of Sandia's large-scale computing resources that support the programs associated with our diverse mission areas. A key tenet to our approach is to work with our mission partners to understand and anticipate their requirements and formulate an investment strategy that is aligned with those Laboratories priorities. In doing this, our investments include not only expanding the resources available for scientific computing and modeling and simulation, but also acquiring large-scale systems for data analytics, cloud computing, and Emulytics. We are also investigating new computer architectures in our advanced systems test bed to guide future platform designs and prepare for changes in our code development models.

Our initial investments in large-scale institutional platforms that are optimized for Informatics and Emulytics work are serving a diverse customer base. We anticipate continued growth and expansion of these resources in the coming years as the use of these analytic techniques expands across our mission space. If your program could benefit from an investment in innovative systems, please work through your Program Management Unit's Mission Computing Council representatives to engage our teams.

Mike Vahle
Chief Information Office & IT Services



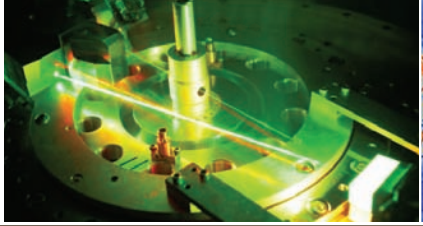
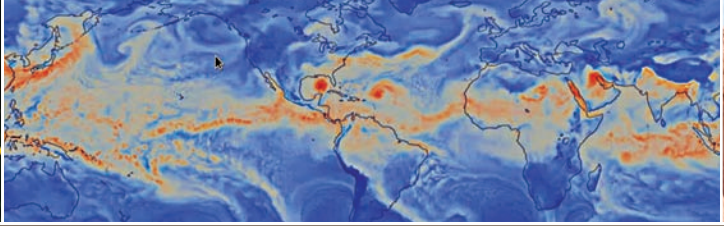

SUPPORTING YOU THROUGH DELIVERING SERVICES AND INFRASTRUCTURE

Center 9300 supplies computer and network services throughout Sandia, on multiple networks supporting diverse needs, from the Corporate Computing Help Desk, to critical services on the Sandia Classified Network, and enterprise-level services for the majority of our customers who use the Sandia Restricted Network. Recent customer growth has seen us expand offerings into the Sandia Open Network, the SiprNet for interactions with the Department of Defense, the upper level limited area network, and expanded interlaboratory communications and services. All of this effort is designed to improve your effectiveness in as many aspects of your work as we can support.

Recent expansion of mobile device support and providing the ability to use personal electronic devices inside Technical Areas are examples of our commitment to improve and expand your ability to obtain essential services on demand in more and more locations seamlessly. The research and development required for these new services leverages our cyber security knowledge, our networking and telecommunications services, and our Mission Computing Services for desktops and department resources. Scientific Computing systems, and the new Informatics and cloud services systems exist within this environment and also benefit from the knowledge and expertise of all the service groups within 9300. This synergy lowers costs and improves our ability to serve your needs, reacting with agility, as they change.

We deliver fundamental capabilities to the Laboratories. Let us know how we can partner with you to ensure your success. Whether it is colocation of computing resources in our central computing facilities, or helping expand your business with targeted investments or personnel, we stand ready to help.

John Zepper
Director, Computing & Network Services


SUSTAINING MISSION EXCELLENCE

It is very exciting to see the rapid progress being made in expanding our large-scale computing and computational simulation capabilities through the Sandia Institutional Computing Program. This program is a manifestation of a commitment by Sandia leadership to the continuous advancement and long-term sustainment of these capabilities for the benefit of all Sandia national security mission areas. We believe these capabilities are an important enabler of our national security missions, and a vital contributor to engineering excellence. We are particularly excited about the scientific, engineering, and technological advances that will be realized as we leverage the new capabilities being provided by our large-scale computing platforms. Tremendous advances have been made in high performance computing and computational simulation over the past twenty years, and further advances will be realized over the next twenty years, likely at an accelerating rate. These advances will create new opportunities for discovery and invention, which will open the door for continued innovation in our contributions to U.S. national and economic security. It is important to our mission, to our role as a Federally Funded Research and Development Center, and to our identity as a national laboratory that we remain on the cutting edge of computing and computational science and engineering, and that we continue exploiting these capabilities to the fullest extent possible in carrying out our national security missions. Evidence of mission impact from ongoing Sandia Institutional Computing Program investments is shown by the examples in this document. We hope these examples stimulate ideas and motivate your use of these new institutional computing resources. We encourage you to explore the possibilities for impactful use of large-scale computing in your programs and projects, and to take full advantage of the new computing architectures and platforms that will continue being provided by the Sandia Institutional Computing Program.

Stephen Rottler
Vice President, Energy & Climate Programs

DEFENSE SYSTEMS & ASSESSMENTS

We deliver advanced science and technology solutions to deter, detect, track, defeat, and defend against threats to our national security. We analyze the vulnerabilities of our adversaries and develop innovative systems, sensors, and technologies for the defense and national security community.

The Defense Systems and Assessments (DS&A) program management unit (PMU) exists to foster invention, innovation, maturation, and demonstration of technologies to enable future force capabilities. In addition to developing these capabilities across multiple domains (air, land, maritime, space, and cyber) we exploit these innovations and transition technology-enabled capabilities to the current force through our cooperative agreements with industrial partners. Implicit in this statement is the understanding that as a Federally Funded Research and Development Center, Sandia's ethos is that science and technology should serve the needs of the warfighter and provide our national security community with new and improved capabilities to perform their missions against current and future threats. National security threats remain many and varied, including those related to nuclear non-proliferation, cyber security, nuclear command and control, missile defense, reducing the vulnerability and increasing the resiliency of trusted systems, and preventing technological surprise. The DS&A PMU works strategically across these and many other threat areas with all levels of government to solve the nation's highest priority national security issues.

National security threats remain many and varied, including those related to nuclear non-proliferation, cyber security, command and control, and preventing technological surprise.

Anthony Thornton
Deputy for Technology & Programs

MULTIMILLION-ATOM TIGHT-BINDING SIMULATIONS
TO INVESTIGATE THE PHYSICS OF DONOR ATOMS IN THE CONTEXT OF QUANTUM COMPUTING

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PROCESSING HOURS

2,447,795

Quantum computing promises to disruptively change information processing using the laws of quantum physics. A team of researchers at Sandia National Laboratories used Red Sky to investigate the physics of donor atoms in silicon for use as qubits for quantum computing, as part of a project led by Malcolm Carroll. A qubit is the quantum mechanical analog of a computing bit. A classical bit can take the values 0 (off) or 1 (on), but a qubit can take these values, as well as any value in between. The researchers investigated the magnitude of energy barriers for transferring electrons between donor centers and electrostatically-defined quantum dots at the silicon oxide interface, using the NEMO3D tight-binding code from Purdue University.

Understanding energy barriers helps the research team design structures robust to noise and decoherence effects, and understand experimental results for preliminary qubit attempts. This work will continue in the future, in particular analyzing experimental results anticipated to come from collaborators at Sandia's Center for Integrated Nanotechnology. Red Sky was key to completing this work, because it required a scan of many different problem parameters (e.g., the distance of a P atom from the Si/SiO2 interface), and each parameter required a parallel calculation; Red Sky allowed the researchers to do this parameter scan in a reasonable amount of time. This work was completed with help from Rajib Rahman and Gerhard Klimeck at Purdue University.

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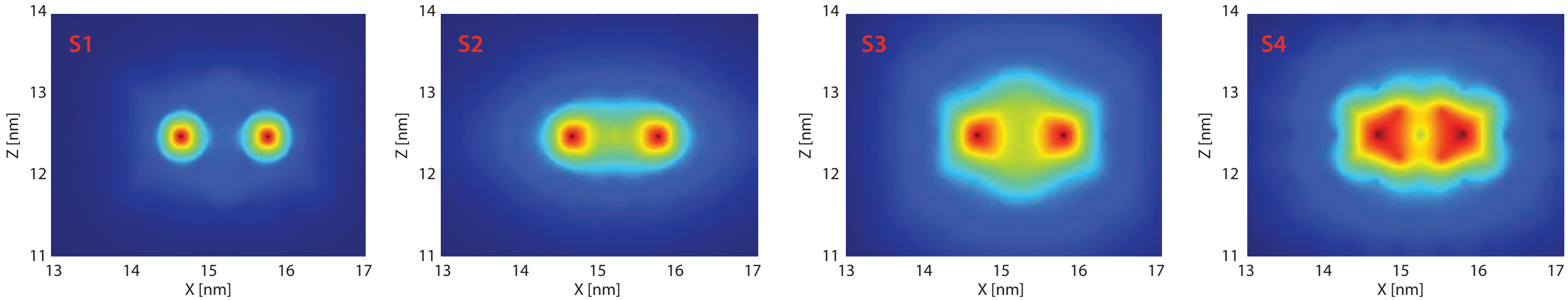

Atomistic tight-binding simulation of the four lowest electronic states of a P2+ donor molecule in Si (shown as 2D cuts).

MODELING THE CHELYABINSK AIRBURST: DEATH OF AN ASTEROID

In 2013, an asteroid pierced the earth's atmosphere and began a fiery descent toward the surface. Moving in excess of 19 km/s, it crossed over the glaciated plains of the Kurganskaya and Chelyabinskaya oblasts, trailing a pair of smoky-looking, iridescent plumes, repeatedly shedding debris while moving in excess of Mach 60 before being abruptly decelerated and destroyed in a final half-megaton detonation a little more than 15 seconds later. The asteroid passed approximately 40 km south of the Chelyabinsk city center, blasting residents with a shock wave from the explosion above several villages and the countryside, and hammering them with repeated sonic booms from trailing fragments. The proximity of the explosion to a population center led to many injuries and widespread blast damage, and also yielded a plethora of serendipitous data in the form of video footage from security and dashboard cameras. Combined with seismic, infrasound, and satellite records, data from this airburst was collected and provided a multi-faceted means to determine the projectile size and entry parameters, and to develop a self-consistent model of the airburst. This once-in-a-lifetime occurrence enabled a Sandia National Laboratories researcher to test out his theories and simulations on actual data.

Computational models are used to gain insight about the phenomena associated with airbursts caused by the hypervelocity entry, ablation, breakup, and explosion of asteroids and comets in planetary atmospheres. Among the resulting discoveries is the recognition that airbursts caused by downwardly-directed collisions do more damage at the surface than a nuclear explosion of the same yield and are therefore more dangerous than previously thought. Simulations run on Sandia's high performance computers using the multi-dimensional, multi-material shock-physics code, CTH, and applying adaptive mesh refinement to resolve phenomena across spatial scales over many orders of magnitude, led to the discovery of unexpected phenomena emerging from the highly-directed geometry of these events. These phenomena include ballistic plumes that rise to low-earth orbital altitudes before collapsing, ring vortices that descend to the surface and add to the list of damage mechanisms, and the splitting of shallow entry wakes into linear vortices that become visible as twin condensation trails. As scientific understanding has improved, these models are ready to be focused on systematic, high-fidelity, multi-scale, multi-physics-based quantitative risk assessments to objectively inform policy decisions associated with planetary defense.

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572,292

ELECTRONICS SURVIVABILITY

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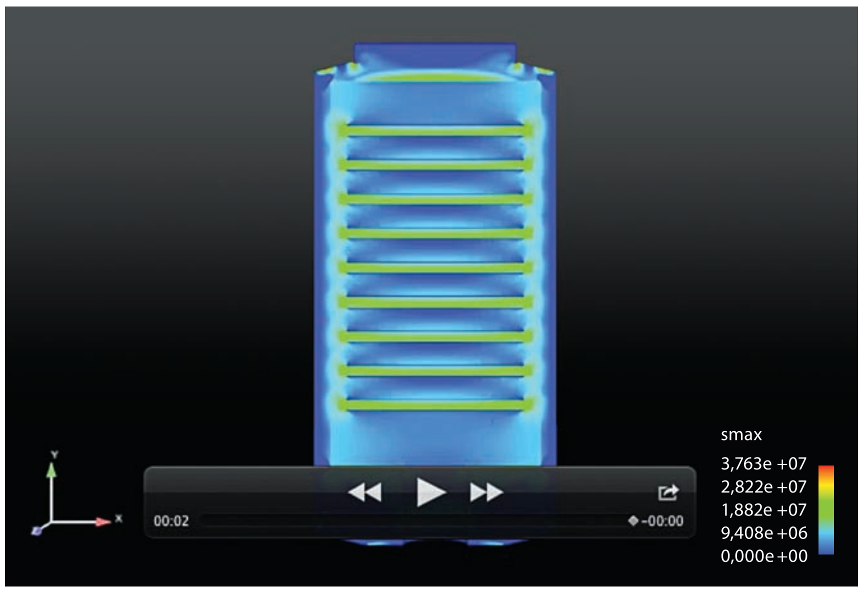
94,962

Surface mount technology, a method of placing components directly on printed circuit boards (PCBs) is quite common in the modern electronics industry. In some instances, PCBs may be encapsulated in foam or epoxy to improve survivability against hostile environments. In addition, PCBs may be encapsulated within a metal housing, prior to insertion or preloading into a final assembly. When designing PCBs to survive operational environments, it is important to understand the stresses and strains generated during manufacturing and thermal cycling in addition to dynamic loading.

While all high-G electronics are not subjected to harsh thermal environments, it is important to note that almost all packaged electronic weapon systems will be required to pass some level of thermal requirements. The large disparity in the coefficients of thermal expansion of polymers, ceramic components, metal solders, and PCBs can generate significant stress during thermal cycling. In many cases, thermal environments alone can result in stresses in excess of the material strength; cracking of encapsulants or ceramic components, underfill debonding, and solder fatigue are just a few of the potential failure mechanisms.

Many encapsulated designs have been successful; however, the mechanism behind the success may not be well understood. While dynamic stresses from vibration and impact are important, understanding the residual manufacturing stress is a critical first step for determining margins. For this effort, common packaging materials were characterized and nonlinear constitutive models were populated to perform computational simulations. Coupled physics, quasistatic thermal stress, preload, and dynamic impact simulations were utilized to investigate the advantages and disadvantages of various encapsulations, coating, and underfill choices. By leveraging SNL HPC capabilities, hundreds of permutations of packaging scenarios were quickly modeled, with the intent of developing generic packaging guidelines for encapsulating electronics subjected to harsh thermal and mechanical environments.

So far, the packaging strategies developed from this research have been successfully implemented in several Sandia NNSA components as well as in Air Force applications. The research findings are being published in a series of packaging design guide SAND Reports.



Packaged electronic device subjected to dynamic impact while under residual stress from encapsulation and preload.

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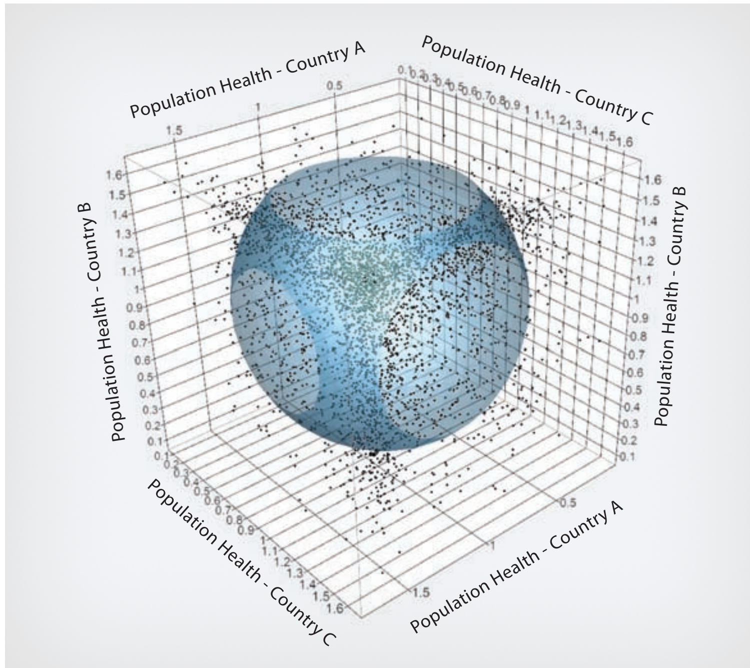
COMPLEXITY SCIENCE-BASED FRAMEWORK FOR GLOBAL JOINT OPERATIONS ANALYSIS TO SUPPORT FORCE PROJECTION

The national defense enterprise constitutes a complex adaptive system-of-systems, (CASoS) which coordinates the acquisition, planning, development, and deployment of national assets to accomplish effective global force projection. The military is undergoing a significant transformation as it modernizes for the information age and adapts to include an emerging asymmetric threat beyond traditional cold war era adversaries. The Office of the Secretary of Defense (OSD) must coordinate countless factors, over a short period of time, including civilian leadership objectives, budget limitations, and adaptive adversaries to determine the optimal trade-offs of resources and capabilities to accomplish national security missions. Understanding the dynamics of international economic relations aids in OSD-level decision making.



Distribution of household health in interacting national economies of three countries.

Researchers at Sandia developed an enterprise-modeling framework to simulate economies with different sectoral production coefficients. These economies interact through international markets for several resources, such as oil and manufactured goods. Differences among economies cause production to shift around the system over time. External disruptions to production or trade can also be introduced into the model, to simulate their propagation across the system.

Global economic models are typically built to study relatively small perturbations to existing systems, and so rely on a great deal of specific information about current conditions. This work is focused on finding general categories of system behavior, and understanding what features account for differences in behavior. Understanding the possible size and pace of shifts in economic activity, and the conditions that tend to increase or moderate those changes, can help decision-makers anticipate the conditions or locations where economic tensions might foster conflict.

This framework and constituent modeling objects advances the science of large-scale modeling and simulation, uncertainty quantification, and large scale optimization techniques. This work seeks to understand the tradeoff in capability investment across lethality, surveillance, reconnaissance, and intelligence (both space and terrestrial based), and cost as DoD invests in a prompt global strike mission capability.

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PROCESSING HOURS

5,363



ENERGY & CLIMATE

Seeking to create a secure energy future that is also sustainable by using high-performance computing and other capabilities to drive the development and deployment of energy resources.

The vision of the Energy & Climate (EC) Program Management Unit (PMU) is to enhance the nation's security and prosperity through sustainable, transformative approaches to our most challenging energy, climate, and infrastructure problems. EC goals and objectives seek to both leverage and enhance key competencies associated with Sandia's nuclear weapons mission to amplify our contributions to broader national security in energy generation and distribution and response to climate change. EC work furthers Sandia engineering excellence with an emphasis on connecting deep science to engineering solutions. EC PMU research programs work to:

- Ensure that the nation's energy infrastructure is resilient and effectively integrates renewable resources.
- Create the science, engineering, and system-level foundations for a safe, secure and robust nuclear energy future.
- Reduce dependence on petroleum-based fuels and develop sustainable alternative fuels and increased efficiency of vehicle technologies.
- Understand and prepare the nation for the national security implications of climate change.
- Provide a differentiating science understanding that supports the PMU and Sandia's mission technologies now and into the future.

EC management chose these objectives to help the nation meet national security missions identified by the Department of Energy to reduce our dependence on foreign oil, increase use of low-carbon stationary power generation, increase resilience of critical energy infrastructure, understand risks and enable mitigation of climate-change impacts, and strengthen the nation's science and technology base in energy generation and infrastructure and in effectively responding to climate change.

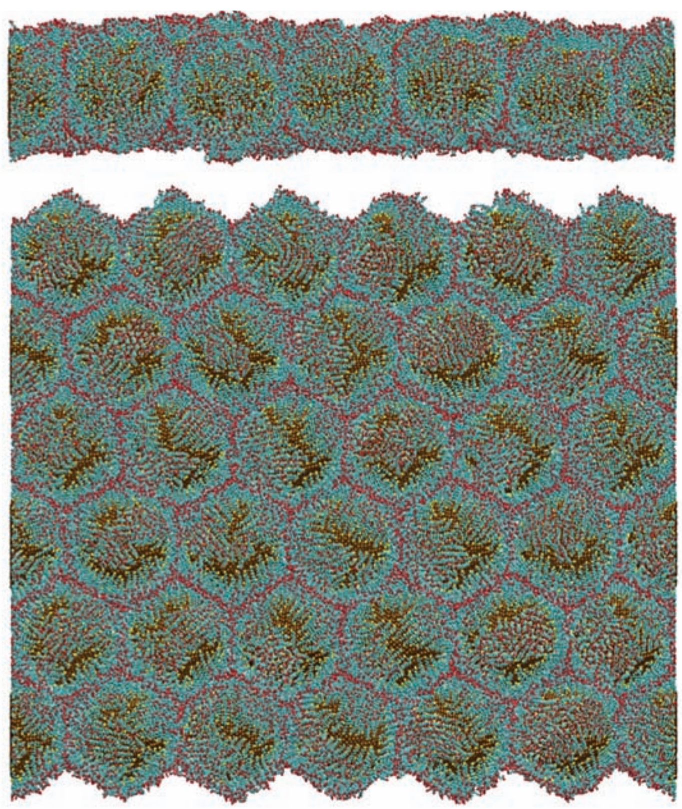
EC seeks to create a secure energy future that is also sustainable by using high-performance computing (HPC) and other capabilities to drive the development and deployment of energy resources that are safer; cleaner; more economical, reliable, and efficient; and less dependent on scarce natural resources. A sustainable future requires understanding and ensuring that the Earth's climate system supports the nation's energy systems while simultaneously mitigating the impact these energy systems have on the Earth. EC seeks to create this energy future—informed by a science-based understanding of the complex interdependencies between energy and climate.

Marcey Hoover
Chief Operating Officer for Energy & Climate Programs

UNIQUE HIGH STRENGTH, MOLECULARLY THIN NANOPARTICLE MEMBRANES

Thin membrane films composed of a single layer of inorganic nanocrystal cores encoded with organic ligands are currently of great interest for a range of applications from nanosieves to electric, magnetic, or photonic devices and sensors. While these membranes have been found experimentally to be flexible yet surprisingly strong under indentation, the underlying microscopic origin of their large tensile strength remains unresolved.

Sandia researchers used large-scale molecular dynamics simulations to probe the fundamental mechanisms underlying the unique mechanical strength of these two-dimensional membranes. Recent multi-million atom simulations of alkanethiol-coated gold nanoparticle membranes were carried out to simultaneously measure nanoscale interactions while directly comparing membrane properties to experiment. To replicate experimental conditions, researchers first formed the nanoparticle membranes at a water-vapor interface, and then removed the water to form free-standing membranes. Simulated membranes capture the experimental morphology and structural properties, which provides insight into their underlying mechanisms.



Free-standing alkanethiol gold nanoparticle membranes with COOH terminal groups viewed from the side (*top*) and above (*bottom*). The video shows how different membranes fail under strain.

Mechanical tests of the resulting membranes showed that interactions between end-groups on the encoded ligands play a dominant role in determining membrane strength and stiffness. The ligand end-group also affects how these membranes fail under tension as shown in the augmented video accompanying this article. Simulations provide unprecedented molecular detail that cannot be obtained experimentally, and the resulting insights can be used to design nanoparticle membranes with more finely tailored mechanical properties.

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PROCESSING HOURS

31,917,851

CRYOGENIC AND FIRE DAMAGE ANALYSIS ON LIQUEFIED NATURAL GAS SHIPS

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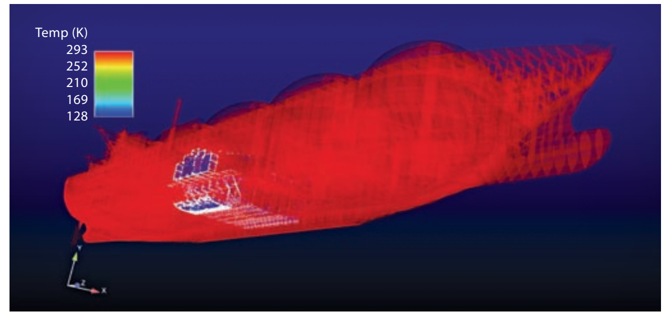
PROCESSING HOURS

416,078

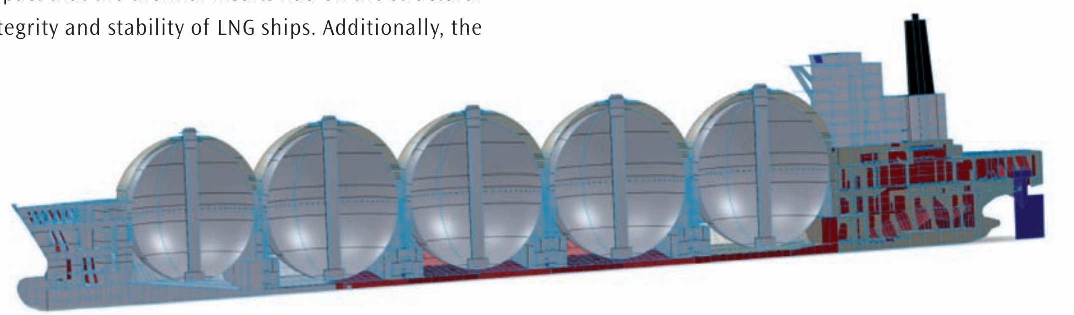
Liquefied Natural Gas (LNG) is transported around the globe in ships the size of modern aircraft carriers, carrying as much as 75 million gallons of LNG or the equivalent of over 6 billion cubic feet of natural gas. LNG is transported in multiple cargo tanks at cryogenic temperatures of about -250 °F. Because of their double hull design, these LNG ships have an exemplary safety record, but a large cargo tank breach could spill significant volumes of LNG. Sandia National Laboratories assembled a diverse, multi-disciplinary team of fire science, cryogenic damage, hazardous cargo transportation, and structural testing and modeling experts from across the Laboratories to support the U.S. Coast Guard and the Department of Energy in addressing potential ship damage and stability concerns from a large LNG spill. This group of experts developed analysis and modeling tools to estimate the damage to ship structure caused by internal flow of the cryogenic liquid and the effect of high temperatures ensuing from an external LNG spill fire. Analysis results were then used to assess the impact that the thermal insults had on the structural integrity and stability of LNG ships. Additionally, the analysis helped identify likely ship and spill behavior and related public safety concerns and hazards.



Sandia's team developed a series of novel approaches to testing, damage modeling, and structural analysis required for this project. These approaches were unique in their complexity, scale, and required integration. This effort included the development and execution of small and large-scale thermal and mechanical (including thermo-mechanical) tests of LNG ship materials and representative structures.

The need for detailed structural models to analyze the long-duration ship damage and stability behavior required several innovations in the use of high performance computing, damage modeling, and analysis approaches. These efforts have demonstrated to industry and federal agencies the depth and breadth of Sandia's modeling and testing capabilities and analysis expertise that can be applied to address complex engineering and safety problems.

This work was conducted in FY09-FY12.



(*Above left*) Modeling was conducted to determine the effects of fire on LNG ships. (*Above right*) Cryogenic damage to a ship from a large internal spill. (*Left*) Cross-sectional view of a LNG carrier.

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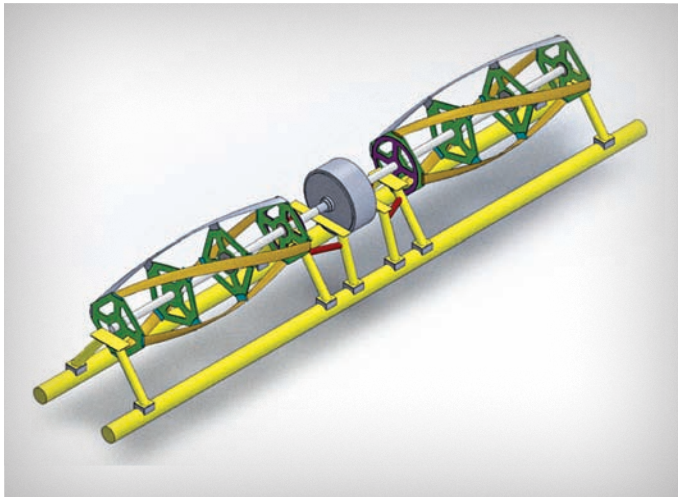
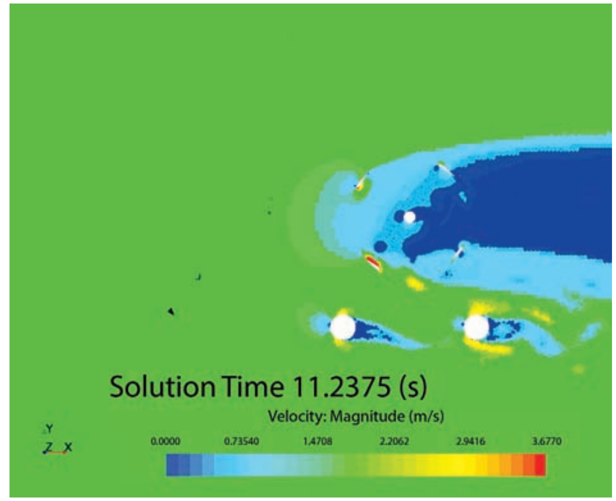
HIGH FIDELITY EVALUATION OF TIDAL TURBINE PERFORMANCE FOR INDUSTRY PARTNER





(*Above left*) Isometric view of RivGen TGU.

(*Above right*) Evolution of velocity magnitude at mid-section of turbine rotor showing vortex shedding from foils, shaft and base of support frame.

High performance computing at Sandia National Laboratories is playing a key role in the U.S. Department of Energy's Wind and Water Power Technology Office mission of advancing the commercialization of tidal energy converters; by improving their power performance and reducing their levelized cost of energy below the local "hurdle" price at which they can compete with other regional generation sources without subsidies. This was recently highlighted in a collaborative project between Sandia National Laboratories' water power technologies group and the U.S. tidal turbine developer, the Ocean Renewable Power Company (ORPC).

The Sandia-ORPC team applied high fidelity modeling to evaluate the performance of the RivGen® prototype turbine generation unit, a cross-flow turbine, which exhibits more complex flow physics than the more common axial-flow turbine. The 3D unsteady Reynolds-averaged Navier-Stokes (URANS) models used to predict power performance were first validated using a unique set of field measurements collected by ORPC in Cobscook Bay in 2014.

Numerical experiments, simulated on Glory, were then conducted to investigate and quantify parasitic drag effects on turbine performance and how these effects could be mitigated to improve performance. The results of this investigation provided a clear path for modifications to be made in the next design iteration of the RivGen turbine.

This study demonstrated the value of high fidelity modeling, and Sandia National Laboratories' HPC resources, when resolving the complex 3D flow effects on performance that are sometimes encountered with complex turbine architectures.

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PROCESSING HOURS

962,437

STATISTICAL MECHANICS WITH DENSITY FUNCTIONAL THEORY ACCURACY

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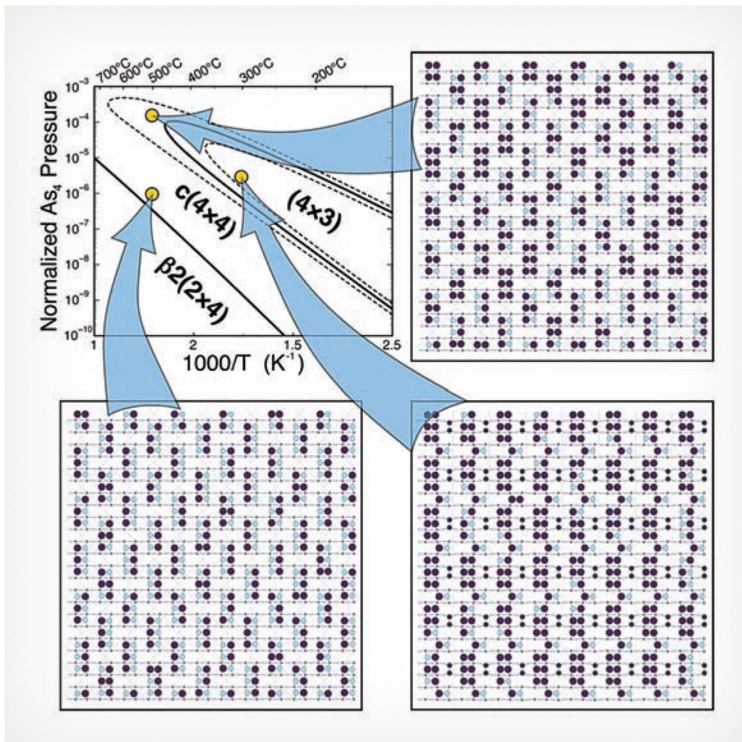
PROCESSING HOURS

1,202,420

Density Functional Theory (DFT) calculations allow the accurate determination of ground state and transition state energies but require thousands of processing hours for each structure. Monte-Carlo (MC) calculations allow the determination of finite-temperature thermodynamic and kinetic properties of disordered systems but require energy evaluations for millions or billions of structures. In a Center for Integrated Nanotechnologies (CINT) project, we have collaborated with users at several universities to combine these seemingly incompatible methods to obtain statistical properties with DFT accuracy. The "glue" that we use to bind DFT and MC together is the Cluster Expansion (CE) formalism. In the CE approach, the system of interest is mapped onto a generalized Ising-like model.



Calculated GaAs surface reconstruction phase diagram (*upper left*) as a function of inverse temperature and normalized partial pressure. Circles indicate the thermodynamic parameters corresponding to the instantaneous MC snapshots shown in the other three panels.

For example, a variable in a CE might represent the occupation of a site in an alloy, the formation of a dimer on a surface, or the presence of a vacancy at an interface. These variables parameterize the possible configurations of the system. Once the CE is fit to a training set of DFT energies that sample these configurations, it allows very rapid evaluation of the energy for an arbitrary configuration, while maintaining the accuracy of the underlying DFT calculations. These energy evaluations can then be used to drive statistical or kinetic MC calculations to obtain finite-temperature properties. As part of CINT projects and three Laboratory Directed Research and Development projects arising from this CINT work, our DFT/CE/MC approach has been or is being applied to obtain bulk, surface, interface, and point defect properties in III-V semiconductors and their alloys.

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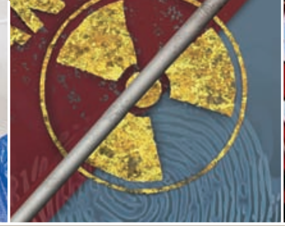


INTERNATIONAL, HOMELAND & NUCLEAR SECURITY

The International, Homeland, and Nuclear Security (IHNS) Program Management Unit (PMU) is responsible for integrating a large number of Sandia's programs in areas ranging from global nuclear security to homeland protection. The PMU missions are broad, and they draw on personnel and expertise from across Sandia.

The PMU brings together programs and capabilities for enhancing the security of dangerous materials, fighting terrorism, and supporting national emergency and incident response. Major program areas include safeguarding nuclear weapons and nuclear materials, protecting critical U.S. government assets and installations, facilitating nonproliferation and arms control activities, securing cyber and physical infrastructures, and reducing the risk of terrorist threats. Sandia's technical capabilities support PMU research and technology development in risk and threat analysis, monitoring, and detection, diagnosis and identification, decontamination and recovery, situational awareness, and vulnerability assessment. The PMU develops technologies for monitoring and verifying arms control agreements, detecting proliferation activities, and securing nuclear sites and materials.

IHNS supports a number of federal agencies, including the National Nuclear Security Administration; the Departments of Defense, Homeland Security, State, Health and Human Services, Treasury, and the Federal Aviation Administration.

IHNS projects use Sandia's HPC resources for predictive modeling and simulation of interdependent systems, modeling dynamic threats, forecasting adaptive behavior, enabling decision support, and processing large cyber data streams. The following pages highlight some of the PMU's current set of advanced computing projects.

Gary Laughlin
Technical Deputy for International, Homeland, and Nuclear Security

IHNS projects use Sandia's HPC resources for predictive modeling and simulation of interdependent systems, modeling dynamic threats, forecasting adaptive behavior, enabling decision support, and processing large cyber data streams.


MOLECULAR MODELING OF PROTEIN TRANSLOCATION THROUGH NANO-FLUIDIC PORES

TEAM MEMBERS

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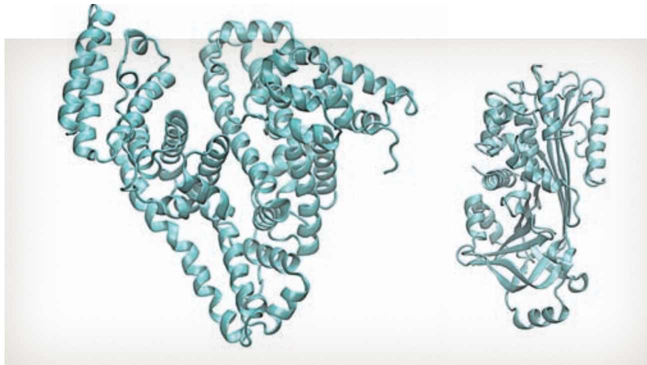
PROCESSING HOURS

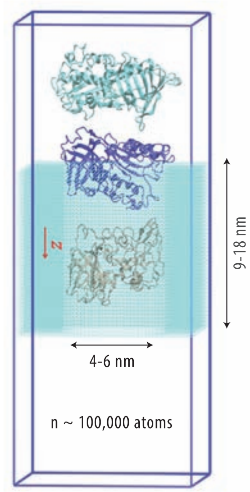
3,484,621

Experimentalists in the Center for Biological and Material Sciences at Sandia developed a novel technique to separate proteins from a mixture. The technique uses external voltage in a microfluidic device coupled with membranes that contain nanometer-sized pores with uniform diameter. Dr. Anson Hatch and his co-workers discovered a physical regime where tuning the applied voltages to force proteins into narrow synthetic pores permits highly selective entry and fractionation of proteins. The new technique is far more efficient than traditional size-exclusion methods for protein separation, which require multiple membranes with different pore sizes.



Molecular simulations can help us understand the macroscopic phenomena of voltage-driven protein separation at atomistic length-scales. A theoretical group, led by Dr. Susan Rempe, performs molecular dynamics simulations to determine which properties control the free energy barriers to protein entry into nanopores. Properties that can be controlled experimentally are the most interesting, including nanopore chemistry and diameter, applied voltage, and protein size. Sandia's high-performance computing clusters, like Red Mesa, are critical for these computationally challenging simulations.

Recent simulations reveal that proteins unfold to enter size-limited pores narrower than the protein's radius of gyration. Free energy barriers increase for larger proteins and smaller pores, which supports experimental observations of protein translocation. Applied voltages usually lower those free energy barriers. The simulations also reveal that one of the proteins responsible for anthrax toxicity, anthrax lethal factor, behaves differently from common proteins in blood serum. Current work is focused on understanding the basis for the unusual translocation behavior of anthrax proteins. The experimental team can use that information to fine-tune membrane design and external voltage to capture protein toxins. More importantly, theory and experiment together may reveal how those toxins cross cellular membranes through narrow, size-limited pores, which may lead to new ways of disrupting protein translocation and preventing infection.



(*Far left*) Structure of common proteins in blood serum: ovalbumin (*left*) and bovine serum albumin (*right*). These proteins encounter different free energy barriers when entering the membrane due mainly to size differences. Molecular simulations shed light on how the proteins change structurally (e.g., unfold) during entry. Because of differences in their charge states, these proteins also respond differently to the applied external voltages.

(*Above right*) Snapshots from molecular simulations showing different conformations of a protein during translocation across a nanometer-sized pore in a model membrane. These simulations use advanced sampling techniques to measure the free energy barriers to protein entry. Free energy calculations are computationally expensive, and hence require high performance clusters like Red Mesa.

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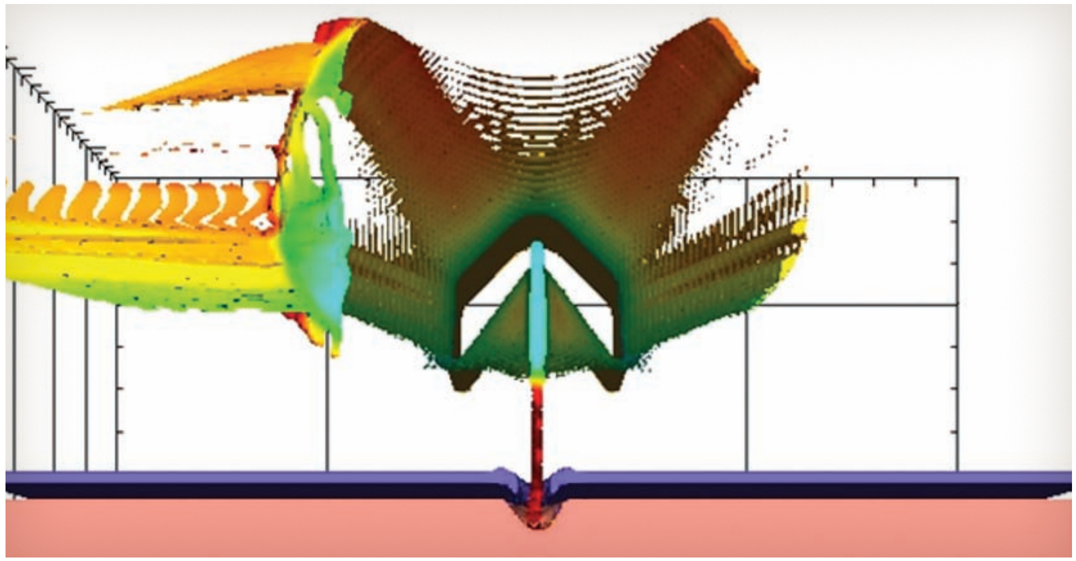
EVALUATION OF NUCLEAR POWER PLANT SECURITY DOORS

Sandia is evaluating nuclear power plant door designs for resistance to explosive attacks. These doors protect both man- and vehicle-sized entrance portals at many power plants. Twenty-seven different door designs were studied by both modeling and testing. HPC modeling results were used to plan two separate explosive test series and to improve door designs. The manufacturers will use the results obtained using Advanced Simulation & Computing codes run on Sandia HPC platforms, Sandia's test results, and any future results they may obtain with commercial codes, to improve explosive resistance of their products. Improving the security features of these doors prevents potential attackers from sabotaging these nuclear facilities and endangering surrounding populations.



CTH calculation of an explosively formed jet striking a security door.

HPC modeling results provided the door manufacturers with insight regarding the performance of specific components of their products and the effectiveness of various design changes, including specific material choices. Some of these data were not revealed by testing alone, but became apparent when numerical simulations were completed. The door manufacturers have found the modeling results extremely helpful and have greatly improved the blast resistance certainty in their designs. Future collaboration is likely to continue with this customer on similar projects. In addition, some of the door manufacturers have adopted numerical modeling to help understand the effects of explosive threats on their products. The manufacturers should then be able to provide government and civilian customers with improved security doors by early adoption of modeling in their design processes.

Explosive test on a door panel conducted at Sandia National Laboratories

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PROCESSING HOURS

103,886

BIO-COMPATIBLE DEGRADATION OF SMALL MOLECULES

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PROCESSING HOURS

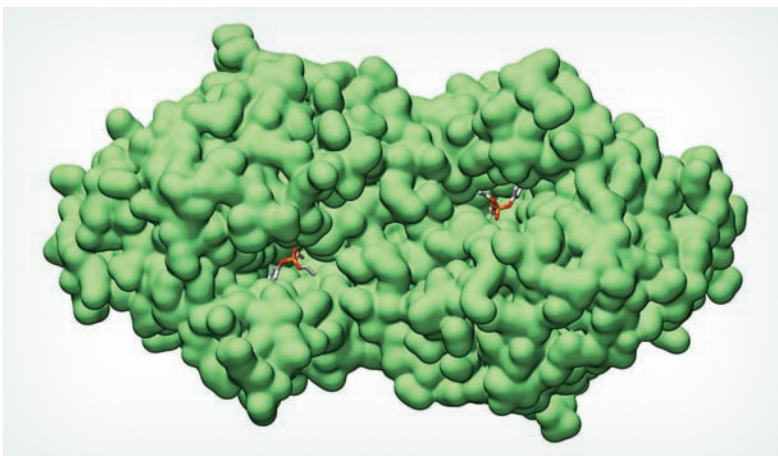
1,665,641

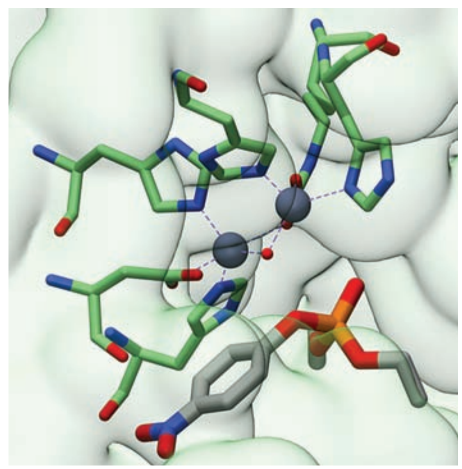
The efficient degradation of small molecules through bio-compatible methods has many important applications including decontamination of toxic sites and medical treatments. Biological enzymes are the perfect tool for this task due to their natural chemical selectivity and often very high catalytic rates. However, additional features must be engineered into these enzymes in order to make them effective tools.

In a joint effort with experimentalists at Sandia and collaborators at the University of North Carolina, the University of Maryland, and the MD Anderson Cancer Center, Sandia theorists are using a variety of computational tools to enhance the activity of enzymes for different applications. Through a combination of classical and quantum mechanical molecular simulations, they are able to explore properties such as thermal stability, chemical specificity, and reaction energetics. One of the enzymes currently being studied is an organophosphorous hydrolase (OPH), which is capable of degrading a variety of chemicals such as toxic nerve agents. OPH has great potential as a tool for rapid decontamination of sites exposed to nerve agents without leaving other toxic residues, yet its thermal and chemical stability must be improved before it can be used in the field.

Although exploring short time- (pico to nano seconds) and length- (few nanometers) scales, the molecular simulations used for these studies are computationally very expensive and require large HPC resources such as Red Sky. The ability to run many different types of simulations simultaneously is critical, and Red Sky provides the resources needed for this.

(*Below Right*) Surface representation of the dimeric organophosphate hydrolase enzyme with ligand bound in the active sites. The ligand shown is paraoxon, a commonly used analog in the study of the degradation of nerve agents.





(*Left*) Close-up of the active site of OPH with the paraoxon ligand. The active site is composed of two zinc ions, which are stabilized and activated by nearby histidine and electronegative amino acids. Improving the thermal stability of this enzyme requires the stabilization of these metal ions as the temperature increases.

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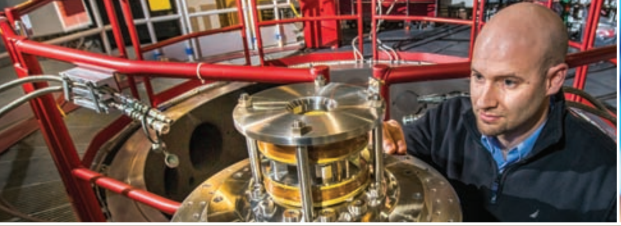


LABORATORY DIRECTED RESEARCH & DEVELOPMENT PROGRAM

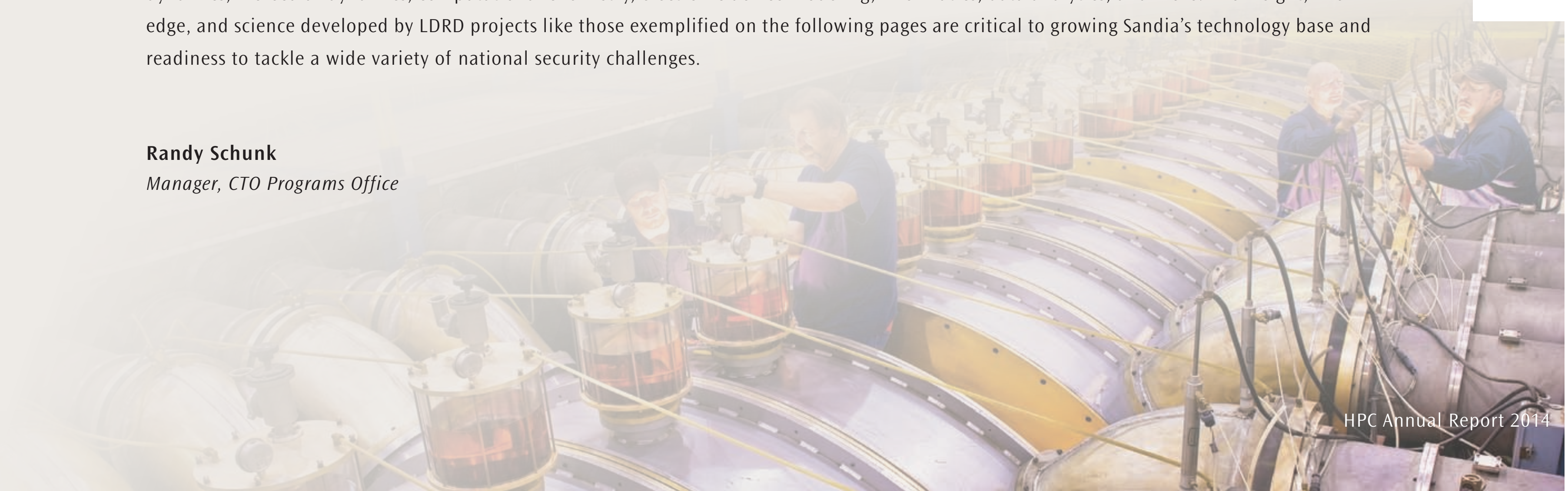
As Sandia's sole source of discretionary research and development funds, the Laboratory Directed Research and Development (LDRD) Program functions as a catalyst for the genesis of innovative science and applied advancements in engineering and technology that serve the Department of Energy and other national security missions. In fiscal year 2014, following a competitive review process, the LDRD Program Office awarded approximately 410 new and continuing projects (totaling $155 million) to Sandia's scientists and engineers.

LDRD proposals outlining R&D distinct from existing programs are reviewed and selected for funding by Investment Area (IA) team members in the following mission relevant IAs: Materials Science, Computing and Information Sciences, Engineering Sciences, Radiation Effects and High Energy Density Science, Nanodevices and Microsystems, Bioscience, Geoscience, Defense Systems & Assessment, Energy, Climate, and Infrastructure Security, International, Homeland and Nuclear Security, Nuclear Weapons, Grand Challenges, and Research Challenges. Significant investments in cyber security are managed throughout the program and are distributed across these investment areas according to mission need. Strategic Partnerships support the professional development of graduate students and new staff at Sandia through LDRD projects classified as Campus Executive, Early Career R&D, or Truman Fellowships.

Research activities throughout the LDRD program are high-risk but driven by anticipated mission needs. High performance computing capabilities and computational science expertise are key elements of risk mitigation in the program and are critical to the program's and Sandia's success. Throughout the program, HPC algorithms and expertise are being developed and deployed to a variety of scientifically challenging problems. Over a million processor hours are utilized on any given week by LDRD projects on problems ranging from computational solid mechanics, fluid dynamics, molecular dynamics, computational chemistry, electronic device modeling, informatics, data analytics, and more. The insight, knowledge, and science developed by LDRD projects like those exemplified on the following pages are critical to growing Sandia's technology base and readiness to tackle a wide variety of national security challenges.

Randy Schunk
Manager, CTO Programs Office

High performance computing capabilities and computational science expertise are key elements of risk mitigation in the program and are critical to the program's and Sandia's success.



HETEROGENEOUS NUCLEATION OF METHANE HYDRATES

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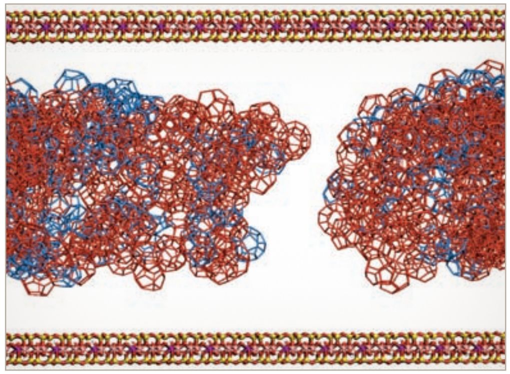
PROCESSING HOURS

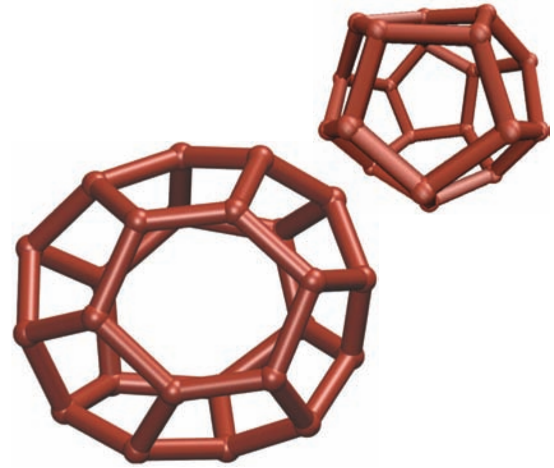
9,371,748

Understanding the nucleation and thermodynamic stability of natural methane hydrates will lead to more effective methods for extracting subsurface methane from hydrate deposits that occur in the Arctic permafrost and in shallow seafloors. Improved control of methane hydrate formation is critically important in the extraction of oil—for example, flow assurance in oil pipelines, the prevention of environmental disasters (and potentially the loss of human life), such as the 2010 oil blowout in the Gulf of Mexico. Ultimately, understanding how and where methane hydrates form is important to the future energy security of the United States.

Methane hydrates are crystalline materials formed when ice-like water cages trap methane molecules, which are the primary component of natural gas. At low temperatures (near 0 °C), moderate pressures, and appropriate chemical conditions, methane hydrates form in clay-rich sediments. Current estimates of methane hydrate deposits are in the trillions of cubic meters. To put that in perspective, the United States uses approximately 600 billion cubic meters of natural gas per year. In addition to representing a significant global resource for natural gas, the unwanted formation of methane hydrates is of environmental, safety, and economic concern. For example, the formation of methane hydrates hindered the containment efforts in the 2010 Macondo oil spill in the Gulf of Mexico. Further, strategies for preventing the formation of pipe-clogging methane hydrate plugs to maintain the flow of crude oil within pipelines are necessary for economic viability of hydrocarbon resources and for maintaining safe operating conditions.



Understanding the fundamental physical chemistry of methane hydrate nucleation may offer enhanced insights into controlling their formation. Specifically, molecular dynamic simulations can provide access to the time and spatial scales necessary to probe nucleation mechanisms. While the majority of molecular dynamics investigations to date have focused on simple nucleation processes (methane-water only), Sandia is using its substantial computing resources to study heterogeneous nucleation to investigate the influence of a mineral surface (methane-water-mineral). The Geosciences Research Foundation at Sandia is sponsoring this study as part of the Laboratory Directed Research and Development program.



Heterogeneous nucleation and thermodynamic stability of methane hydrates is critical to the energy security of the United States. Cutting-edge simulation methods using Sandia's supercomputers are required to address this challenge. Strategic experiments will both validate and inform the simulations. Outcome of this project is a comprehensive molecular-and macroscopic understanding of heterogeneous hydrates that supports Geosciences energy mission.

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MOLECULAR MECHANISM FOR ENTRY OF DENGUE VIRUS INTO HOST CELLS

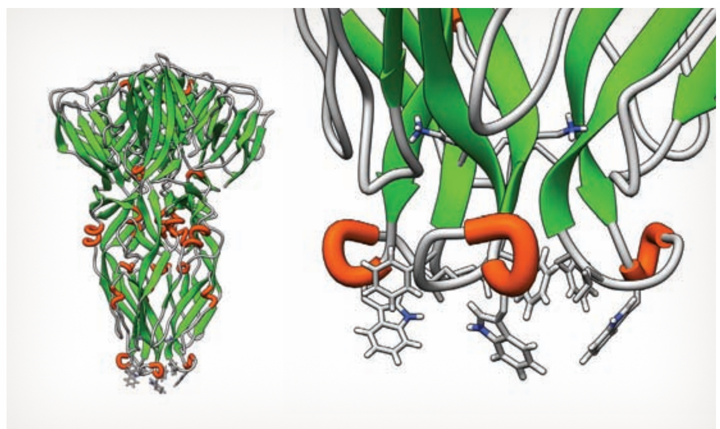
Sandia theorists, in collaboration with experimentalists, are undertaking computational bioscience research to understand how viruses infect cells. Their findings may help determine how to block viral infections and prevent pandemics. The virus under study is Dengue virus (DENV). DENV is endemic to tropical regions and infects some 50 to 100 million individuals, accounting for 500,000 hospitalizations annually, according to the World Health Organization.

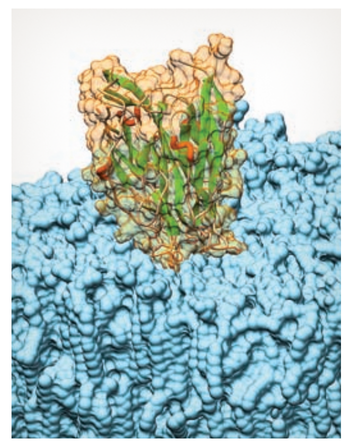
DENV is enveloped in a lipid membrane, which is in turn covered by a large number of symmetrically arranged E proteins. As cells try to destroy the virus through endocytosis, the low endosomal pH triggers a conformational change in the E proteins resulting in attachment to the inner membrane of the endosome. The E proteins ultimately fuse the DENV viral membrane with the endosome, which allows release of the viral genome into the cell cytoplasm. Sandia researchers are using molecular dynamics simulations run on Red Sky to understand how E protein catalyzes the fusion of the viral membrane to the endosome. The main goals of the computational and experimental work are to determine how different types of lipids modulate the behavior of the E protein, and how specific amino acids near the tip of the protein allow anchoring to the membrane. The combined simulation and experimental studies also suggest that the fusion loop may play a role beyond simply anchoring the E protein to the host membrane, such as facilitating lipid mixing between the two membranes by disturbing the host membrane structure.

While the experimentalists are able to study the virus at the macroscopic scale, the simulations provide detailed and valuable information at the atomic scale. These details allow researchers to understand the molecular features responsible for viral infectivity, which may be invaluable in the development of vaccines and therapeutics to block infection.

(*Below left*) Structure of the DENV E protein in the trimer form. (Right) Close-up of the E trimer "tip" highlighting some of the amino-acids in the fusion-loop region, which are critical for viral infectivity. The molecular mechanism of action of the fusion loop remains unknown.

(*Below right*) Snapshot of a molecular dynamics simulation showing a model lipid membrane (light blue) and a truncated version of the DENV E protein (transparent orange surface). These types of simulations are being used to understand the molecular features that allow the anchoring of the protein to the membrane, as well as fusing of the two lipid membranes.





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PROCESSING HOURS

5,263,249

EXPLORING NEW FRONTIERS IN KINETIC PHYSICS IN INERTIAL CONFINEMENT FUSION

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Harry S. Truman Fellow

Patrick Knapp

Stephanie Hansen

PROCESSING HOURS

2,368,598

Nuclear fusion is the bringing together of two light atomic nuclei; converting a small amount of mass to enormous amounts of energy. Fusion research is a critical component of the NNSA's Stockpile Stewardship Program, and it also holds the promise of one day providing the world with virtually limitless clean energy. At Sandia, the world-class Z Accelerator is being used to investigate Magnetized Liner Inertial Fusion (MagLIF), a cutting-edge approach to achieving fusion in the laboratory. MagLIF experiments begin with a solid beryllium can (liner) filled with deuterium fuel. The fuel is magnetized and preheated by a powerful laser before the liner implodes under the tremendous magnetic pressure of the Z Accelerator, compressing the fuel to thermonuclear conditions.

Experiments are modeled on HPC platforms using advanced physics simulations, which capture much of the physics governing the implosion. The goal of this Laboratory Directed Research and Development project is to understand some of the physical approximations made in the codes and develop computational tools and models to open up an expanded phenomenological space for investigation. The work focuses on plasma kinetics; that is, the behavior of individual energetic, electrically charged particles within the fuel, which often behave differently from the bulk fuel.

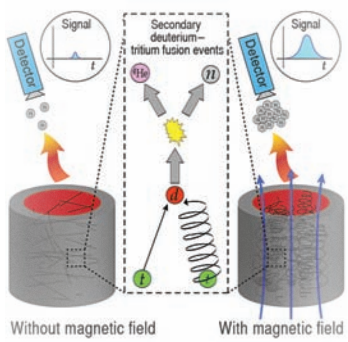
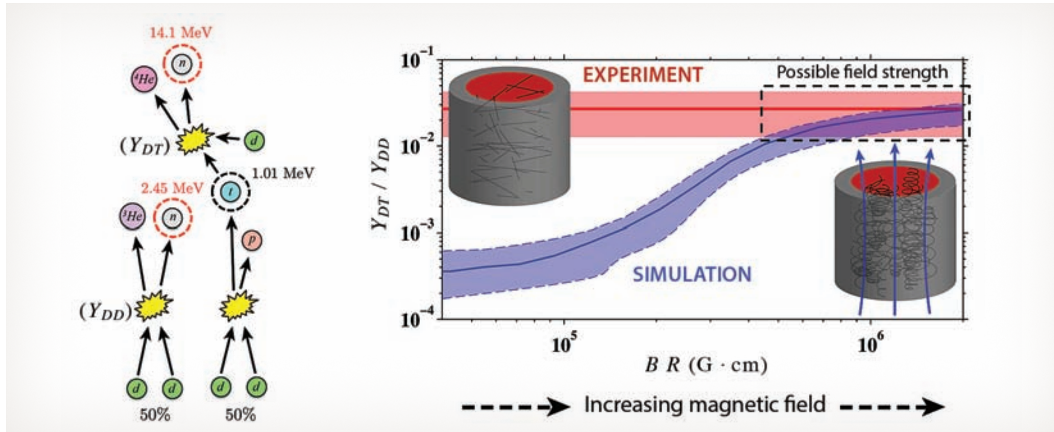


Illustration of the impact of extreme magnetic fields on a critical process in MagLIF fusion plasma.

This work has demonstrated that the magnetic field trapped in the fuel, which is vital to MagLIF's success, carries additional benefits. The field confines the most energetic fuel particles and fusion byproducts, enhancing the fusion reactivity and leading to nuclear signatures that provide our first glimpse of the extreme magnetic field strengths generated by the implosion.



(*Above left*) Fusion reaction pathways for pure deuterium fuel, with "primary" deuterium deuterium (DD) neutrons and "secondary" deuterium tritium (DT) neutrons (*red circles*), the latter produced by high-energy tritium nuclei (*black circle*) arising from one branch of the DD fusion reaction. (*Above right*) Comparison of measured and simulated ratio of DT to DD neutron yields vs. magnetic field strength, with cartoons showing typical triton trajectories through the fuel in the un-magnetized and magnetized limits.

Truman Fellows are expected to solve a major scientific or engineering problem in their thesis work or provide a new approach to a major problem.

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MODELING PRIMARY ATOMIZATION OF LIQUID FUELS
USING A MULTIPHASE DIRECT NUMERICAL SIMULATION/LARGE EDDY SIMULATION APPROACH

In the quest for high-efficiency, low-emissions, combustion devices, predicting the effect of liquid fuel injection in a high-pressure reacting environment is crucial. Developing a precise scientific understanding of the physical processes governing liquid fuel injection in a combustion chamber–and translating this knowledge to a validated predictive model–is a major objective at the Combustion Research Facility in Sandia, Livermore.

As part of a Laboratory Directed Research and Development (LDRD) project, a state-of-the-art multiphase simulation capability, developed by Professor Mark Sussman at Florida State University in Tallahassee, is being specialized at Sandia for high-pressure engine applications.

With sufficient computational power, the multiphase code can track fuel injection on a time scale of nanoseconds, capturing the fragmenting liquid interface with micrometer resolution. This capability is unique because it does not require any pre-existing knowledge of the spray characteristics. Spray simulations have been validated against experimental measurements in a number of configurations.

Even with access to Sandia's vast computational capabilities, the simulation of a realistic injector device at the level of accuracy displayed in the figure is limited to a small volume around the injector and requires several weeks of computer time, on a machine such as Red Sky, to collect sufficient spray statistics.

Snapshot of the fuel surface transitioning from internal to external flow in a Diesel injector (a 20x scaled-up model used for laboratory measurements). The jet disintegration is taking place outside of the injector (injector's walls are removed from the view for clarity–the smooth cylindrical surface on the top left side of the figure corresponds to fuel flow inside the injector's orifice). The insert on the top right side shows the typically convoluted shape of a liquid fragment from the jet before it is broken up into smaller droplets.

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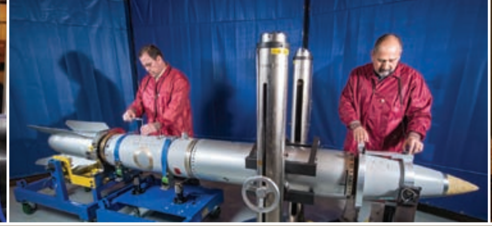
4,226,924


NUCLEAR WEAPONS

Computational simulation capabilities have been successfully leveraged across all of Sandia's mission areas, and have had significant impact with U.S. industries and universities.

Computational simulation, enabled by high performance computing, plays a critical role in the stewardship of the nation's nuclear deterrent, underpinning the technical basis and scientific understanding of the present stockpile, resolution of anomalies, and sustaining the stockpile into the future. Sandia has responsibility for weapon system integration and non-nuclear components design, qualification and production, and full life-cycle assessment.

To meet our nuclear weapons mission responsibilities, Sandia has a broad suite of engineering and physics simulation codes, including the SIERRA suite of structural, thermal, aero, and fluid mechanics capabilities, and the RAMSES suite of radiation, electromagnetic and electrical codes. We also steward capabilities for shock physics and multi-physics, including CTH and Alegra codes, and advanced phenomenological models for our codes that encompass a wide range of physics. These capabilities are founded on scalable parallel algorithms and libraries in Trilinos, and enabled through state-of-the-art meshing capabilities in Cubit and the workflow capabilities of WorkBench and CompSimUI. These application suites are integrated with phenomenological modeling and verification and validation studies through cross-cutting focus areas (radiation and electrical sciences, assured safety and security, delivery, and component performance) that guide prioritization and stockpile impact.

In the past year, computational simulation work has guided design, environments definition, and qualification activities for major modernization programs, including the B61 Life Extension Program and the W88 ALT 370 Program. The computational simulation capabilities developed by NNSA Advanced Simulation and Computing (ASC) have been successfully leveraged across all of Sandia's mission areas, and have had significant impact, through cooperative research and development agreements and academic alliances, with U.S. industries and universities.

Looking to the future, Sandia is embarking on a range of research and development activities to address the emergent challenges of advanced computing technologies at extreme scale. This includes simulation work, that will make use of the coming ASC Advanced Technology System, Trinity. Trinity is being jointly developed by Sandia and Los Alamos National Laboratory through the Alliance for Computing at Extreme Scales, and will be deployed late next year.

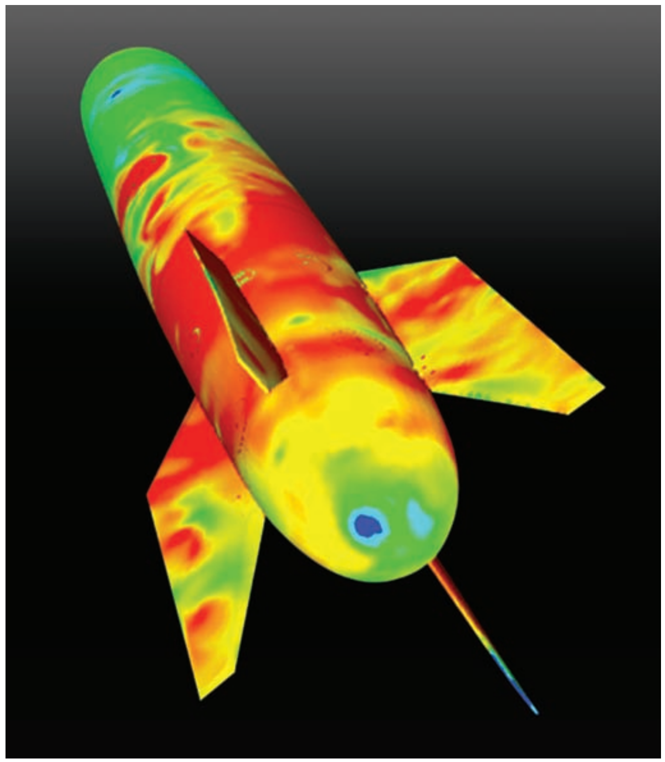
Ken Alvin
Senior Manager for Advanced Simulation & Computing

CAPTIVE CARRIAGE LOADS AND RESPONSE MODELING ON HPC PLATFORMS

One of Sandia's ongoing missions is the National Nuclear Security Administration (NNSA) B61-12 Life Extension Program (LEP). The overarching goal of this stockpile stewardship program is to address stockpile aging, ensure extended service life, and improve the security and reliability of the B61-12 weapon. Sandia's Engineering Sciences Center is developing and applying advanced computational modeling methods to support environmental specifications for the B61 LEP when the weapon is carried on aircraft prior to release (captive carriage). In captive carriage inside a weapons bay, the weapon is subjected to potentially large aero-acoustic pressure loadings because of the unsteady, turbulent flow within the weapons bay.

Simple models are unable to predict the amplitude and dominant modes of the fluid loading, so computational fluid dynamics models are used for the analysis. This is especially critical for the new platforms on which the B61-12 will be deployed, such as the F-35 aircraft. With the advent of the high performance computing Capability Computing Campaigns, computing resources have become available to tackle this challenging problem with high-fidelity simulation. These simulations utilize a coupled large eddy simulation (LES)/structural dynamics model to predict both the flow through the bay as well as the structural response of the weapon to flow-field pressure fluctuations. The flow field and the pressure loading are predicted using a high-fidelity time-accurate hybrid Reynolds-averaged Navier-Stokes/LES method and the response of the structure to this loading is computed using Sandia-developed Sierra-SD (structural dynamics) solver.

These simulations take several weeks to execute on several thousand cores, and multiple simulations at different flight conditions are carried out to populate the environment that the weapon is subjected to. The simulation framework, methods, and models are validated through detailed and systematic simulations of laboratory scale experiments carried out at Sandia expressly for this purpose. The result of this effort is accurate, reliable predictions of the vibration loading and response in a potentially critical environment for the B61-LEP.



The image shows the pressure loads and the resulting structural deflections (note the fin deflections) on a B61-3/4 weapon while being carried in a modern internal weapons bay.

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3,575,557

LARGE-SCALE REACTIVE MOLECULAR DYNAMICS SIMULATION OF INITIATION IN ENERGETIC MATERIALS

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Tzu-Ray Shan

Ryan R. Wixom

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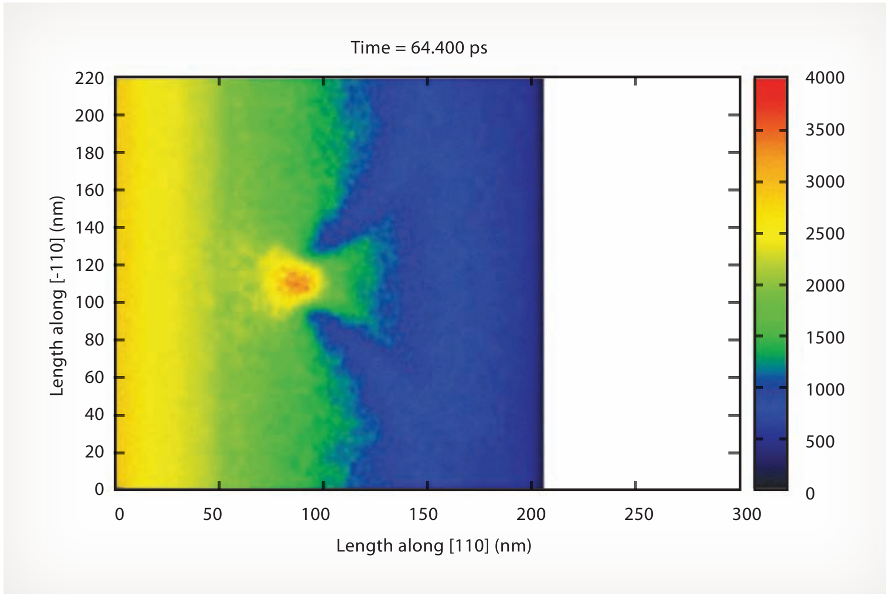
11,923,026

Quantifying margins of operation for detonators used in the weapons stockpile requires a detailed scientific understanding of how detonation is initiated in energetic materials. The response to shock impact of high explosive molecular crystals such as pentaerythritol tetranitrate (PETN) depends strongly on the material microstructure. A defect-free single crystal requires a higher initiation pressure than a polycrystalline powder of the same substance.

While the basic physics of how voids and other defects localize energy leading to initiation is understood, much remains to be learned. For example, what size of void has the greatest effect? Large-scale reactive molecular dynamics simulation provides a unique tool for studying hot spot formation and growth, without making strong assumptions about the material properties. Instead, the observed behavior emerges from the collective interaction of millions of atoms, as they exchange momentum and energy, compress to high density, and participate in exothermic chemical reactions.

Using the power of the LAMMPS molecular dynamics code and Sandia computing resources, Sandia researchers have been able to push the time and length scales of these simulations out farther than ever before, observing a variety of phenomena that help provide a better understanding of the behavior of explosives used in stockpile devices. Advancing this understanding of energy transfer mechanisms may enable the use of more insensitive materials in detonators, which has great implications for safety.



Spatial variation of temperature in an 8-million atom reactive molecular dynamics simulation of a supported shockwave passing through a PETN crystal initially containing a 20-nanometer cylindrical void. The image was taken 64 picoseconds after the initial impact. The yellow and red region is a nascent hot spot forming at the location of the collapsed void. The green layer is moderately warm material created when bulk PETN is compressed by the shockwave. The blue region on the right is uncompressed PETN lying ahead of the shockwave. The green region protruding to the right is a secondary shockwave emanating from the collapsed void.

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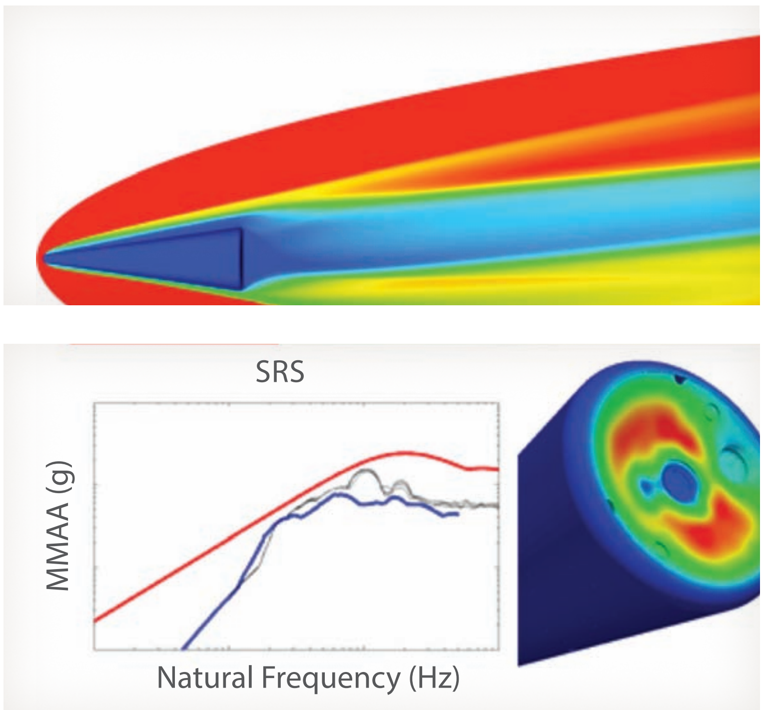
MECHANICAL ANALYSIS OF W78/88-1 LIFE EXTENSION PROGRAM WARHEAD DESIGN OPTIONS

The W78/88-1 Life Extension Program (LEP) encompasses the modernization of two major nuclear weapon reentry systems into an interoperable warhead. Several design concepts exist to provide different options for robust safety and security themes, maximum non-nuclear commonality, and cost. Simulation is one capability used to evaluate the mechanical performance of the designs in various operational environments, plan for system and component qualification efforts, and provide insight into the survivability of the warhead in environments that are not currently testable. The simulation efforts use several Sandia-developed tools through the Advanced Simulation and Computing program, including Cubit for mesh generation, the DART Model Manager, SIERRA codes running on the HPC TLCC2 platforms, DAKOTA, and ParaView. Several programmatic objectives were met using the simulation capability including: (1) providing early environmental specification estimates that may be used by component designers to understand the severity of the loads their components will need to survive, (2) providing guidance for load levels and configurations for subassembly tests intended to represent operational environments, and (3) recommending design options including modified geometry and material properties. These objectives were accomplished through regular interactions with component, system, and test engineers while using the laboratory's computational infrastructure to effectively perform ensembles of simulations.



Flight and radiation environment contour plots are shown along with a calculated shock response spectrum used for environmental specifications.

Because NNSA has decided to defer the LEP program, simulation results are being documented and models are being archived for future reference. However, some advanced and exploratory efforts will continue to mature key technologies, using the results from these and ongoing simulations for esign insights, test planning, and model validation.

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5,081,411


WE FOCUS ON YOUR SUCCESS THROUGH DELIVERING DIFFERENTIATING COMPUTING RESOURCES

Each mission area has, associated with its strategic goals, a diverse range of projects that can benefit from large-scale computing, as evidenced in part by the work presented in this publication. As stewards of the Institutional Computing Program, we strive to deliver the maximum return for your investment. We are implementing new approaches to better understand and address your computing needs and to identify strategic and tactical investments necessary to expand our coverage of Sandia programs. Our traditional scientific computing systems are being augmented by cloud systems, big data platforms, Emulytics clusters, and database accelerators. Other innovative test bed systems are available for experimentation and exploring the impact of future computer system architectures. We have personnel who excel in helping adapt and optimize codes on new systems, and who can help accelerate your move onto new capability systems at Los Alamos and Lawrence Livermore National Laboratories, as well as help improve your computing experience on Sandia systems.

The Mission Computing Council (MCC) was established this year to provide a forum for this partnership and we appreciate the strong support we have been given to understand mission area priorities and adjust policies to improve our impact and service. Each of the Program Management Units has representation on our council; if you have ideas or questions about services or capabilities that might be available to help you pursue your mission, please contact them. Your requests will help us–and your representatives on the MCC–understand the vast array of needs represented throughout Sandia.

Our major investment in fiscal year (FY) 2014 will result in the most computationally powerful computing platform ever fielded at Sandia. The new system, named “Sky Bridge,” was delivered in September, and will be in general availability by the end of the first quarter of FY 2015. It uses a hybrid cooling concept of liquid and air that will result in significant energy savings over the system’s lifetime. This computer will not require any modifications or conversions to Sandia codes that run on our current TLCC2 platforms.

I hope you enjoy reading about the diverse projects supported on our computer systems, and that you will engage us and the Mission Computing Council representatives in meaningful dialogue to build our understanding of what future investments will benefit Sandia most.

Tom Klitsner
Senior Manager, Computing Systems and Technology Integration

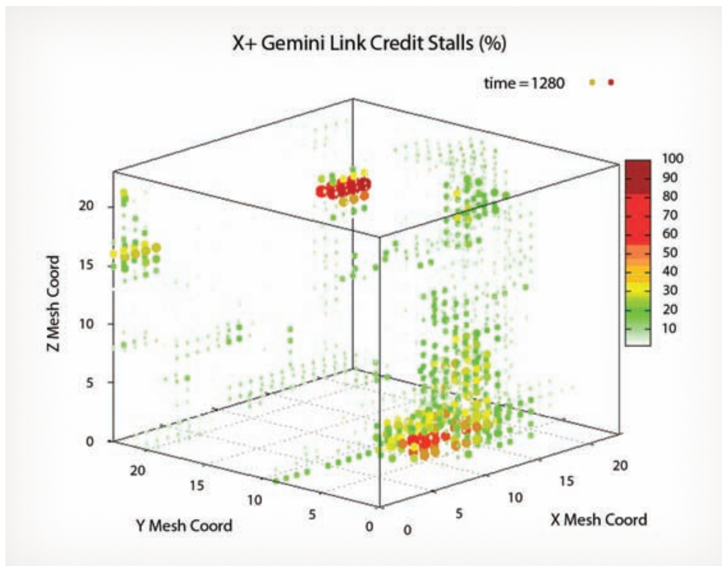
EXTREME-SCALE HPC MONITORING

Improving and ensuring computational performance is essential to enable the large-scale, high fidelity numerical simulations that are core to Sandia's mission. Continued performance scaling of HPC platforms is being achieved through increases in the number of compute elements and their connectivity bandwidth. The increase in raw compute power can only be taken advantage of through increases in application parallelism and/or platform sharing by many concurrent applications. As a result, HPC problem diagnosis and performance tuning is extremely difficult, if not impossible, without reasonably high fidelity system wide information at the per-component level.

Sandia's Lightweight Distributed Metric Service (LDMS) is the state-of-the-art in extreme-scale HPC monitoring. It enables collection, transport, and storage of resource state data from extreme-scale systems at fidelities and timescales necessary to provide understanding of application and system performance with no statistically significant adverse impact on application performance.

LDMS is installed on Sandia HPC systems to provide continuous monitoring of applications and system resource utilization. This data is being used to discover issues in both platform and application performance and to analyze applications' resource requirements to drive future system acquisitions. LDMS monitoring data is also being used in Sandia research work to enable mapping of applications to resources, based on dynamic evaluation of network and other resource contention.

On NCSA's Blue Waters platform, network monitoring using LDMS is being used to enable understanding of where and how congestion evolves in the network and thus understand related application performance issues and enable mitigating response. Blue Waters is an extreme-scale HPC platform, consisting of 27,648 compute and service nodes. It is a similar architecture to the ACES Cielo platform located at Los Alamos, the precursor architecture to the upcoming ACES Trinity platform.



Congestion in NCSA's Blue Waters platform high speed network shown in terms of percent of time spent stalled. The entire network for the machine is shown within the dimensions of the box. The network is a 3D torus of dimension 24 x 24 x 24 with links in each direction in X, Y, and Z including wrap around (e.g., from X=23 to X=0). High demand for the shared network resources among applications can result in communication slowdown and thus overall application slowdown.

Contact: Ann Gentile
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TEAM MEMBERS
Ann Gentile
James Brandt

HPC USER SUPPORT

Sandia's user support team for High Performance Computing (HPC) provides "OneStop" service. A tiered support system of knowledgeable professionals provides responsive, as-needed, support that emphasizes helping users to be successful, and providing quality support. Services include an HPC help desk; HPC account services; a OneStop web portal, and email notifications that deliver a wealth of information regarding platforms, systems status and outages, applications, how-to's, user-specific job information, and access to support professionals. Our team provides customized in-depth support when needed to explore issues related to code porting, performance analysis, handling of large data, visualization — whatever it takes to help users get their HPC work done, particularly when help is needed for complex runs or for managing complicated workflows.

OneStop HPC support is implemented using Information Technology Infrastructure Library® (ITIL) as a framework for IT service management. This framework addresses the full life cycle of support from incident management, change management, and knowledge management through best practices. ITIL is also the foundation of ISO/IEC 20000 (previously BS15000), the International Service Management Standard for organizational certification and compliance.

The HPC OneStop portal is accessible on the Sandia Restricted Network at https://computing.sandia.gov. The OneStop service desk is available Monday through Friday from 8:30 a.m. to 4:30 p.m. MDT. The service desk can also be reached through the phone or email.

COMMON ENGINEERING ENVIRONMENT COMPUTING RESOURCES

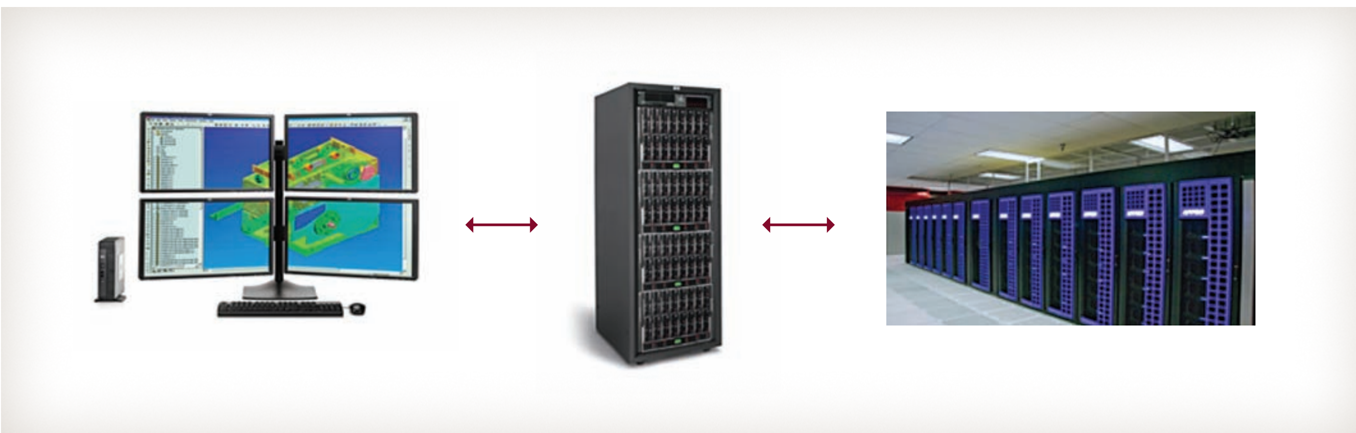
Sandia's Common Engineering Environment (CEE) is a "set" of preferred engineering tools and software, support services, best practices, processes, and training for all engineers and scientists. The CEE is a major component of Sandia's strategic efforts to excel in the practice of engineering. The CEE includes a rich set of technical computing resources that, together with integrated high performance computing (HPC), provides a complete end-to-end environment for computational science and engineering. CEE computing resources are available in the form of subscription-based services, dedicated software licenses, and HPC.

CEE's subscription-based services are cloud-like in that customers simply request services on line, services are provisioned behind the scenes, and then the customer connects to the services to use them. Subscription-based services include access to: commercial applications through shared-license pools, in-house applications, virtual engineering desktops through centralized workstations with remote high performance graphics, large memory compute servers, and some special-purpose HPC.

Dedicated individual and group licenses are available for many CEE applications for those who need to own a license. These dedicated software licenses are requested through Sandia's Software Asset Management System.

For those who need to solve large, complex, computational science and engineering problems, the HPC resources central to this report exemplify Sandia's CEE technical computing environment.

For more information or access to Sandia's CEE services, visit: https://computing.sandia.gov



Abaqus
Dakota
Matlab
ProE
Pspice
RAMSES
SIERRA
SolidWorks

MISSION COMPUTING SYSTEMS

CHAMA

USAGE: HPC **PROGRAM:** NW/ASC
TFLOPS: 392 **NODES:** 1,232
CORES: 19,712
MEMORY/CORE: 4.0 GB
PROCESSOR HOURS/YR: 172,677,120

Chama, along with Pecos, is a NW/ASC HPC system deployed in 2012 as part of the DOE/NNSA Tri-Labs TLCC–2, procurement. At 392 Teraflops, Pecos is a primary resource for NW/ASC users. In October 2013, Chama, and its companion cluster Pecos, were upgraded to double its available memory on every compute node. This upgrade improved job throughput and reduced compute times by allowing applications to run more compactly within the same overall memory footprint.

CIELO DEL SUR

USAGE: HPC **PROGRAM:** NW/ASC
TFLOPS: 86 **NODES:** 556
CORES: 8,896
MEMORY/CORE: 2.0 GB
PROCESSOR HOURS/YR: 77,928,960

Cielo del Sur is a Cray XE6 system, similar to the Cielo platform at Los Alamos National Laboratory.

DARK BRIDGE

USAGE: HPC **PROGRAM:** NW/ASC
TFLOPS: 588 **NODES:** 1,848
CORES: 29,568
MEMORY/CORE: 4.0 GB
PROCESSOR HOURS/YR: 259,015,680

Dark Bridge, a TLCC–2 class system (like Chama and Pecos), doubled in size this year to 588 TeraFlops.

DARK NEBULA

USAGE: Cloud **PROGRAM:** Institutional
TFLOPS: NA **NODES:** 100
CORES: 1,600
PROCESSOR HOURS/YR: 14,016,000

Dark Nebula is an Institutional Cloud system that was acquired at the end of FY13 for use as a research cloud in FY14. The system is comprised of Dell nodes having local disk and bound together with a highly configurable Ethernet fabric. An OpenStack cloud environment supports multiple research groups who are experimenting with “Infrastructure as a Service.”

DARK SAND

USAGE: HPC **PROGRAM:** Institutional
TFLOPS: 294 **NODES:** 924
CORES: 14,784
MEMORY/CORE: 4.0 GB
PROCESSOR HOURS/YR: 129,507,840

Dark Sand is a TLCC–2 class system (like Chama and Pecos) that supports Institutional users.

GILA

USAGE: HPC **PROGRAM:** Institutional
TFLOPS: 10 **NODES:** 48
CORES: 768
MEMORY/CORE: 4.0 GB
PROCESSOR HOURS/YR: 6,727,680

Gila is a small Institutional HPC system.

GLORY

USAGE: HPC **PROGRAM:** Institutional
TFLOPS: 38 **NODES:** 272
CORES: 4,352
MEMORY/CORE: 2.0 GB
PROCESSOR HOURS/YR: 38,123,520

Glory is a NW/ASC HPC system deployed in 2009 as part of the DOE/NNSA Tri-Labs TLCC–1 procurement. Now supplanted by the TLCC–2 systems, Glory transitioned to Institutional usage in FY14.

JEMEZ

USAGE: HPC **PROGRAM:** Institutional
TFLOPS: 95 **NODES:** 288
CORES: 4,608
MEMORY/CORE: 2.0 GB
PROCESSOR HOURS/YR: 40,366,080

Jemez is a new Institutional HPC system deployed during FY14. At 96 TFlops peak, this system is a cost-effective addition to the Institutional resources. Jemez received an upgrade to 4GB per core in FY14.

MINI SEQUOIA

USAGE: HPC **PROGRAM:** NW/ASC
TFLOPS: 107 **NODES:** 512
CORES: 8,192
MEMORY/CORE: 1.0 GB
PROCESSOR HOURS/YR: 71,761,920

Mini Sequoia is a small version of the Sequoia system recently deployed at LLNL. The purpose of Mini Sequoia is to provide local code-development and checkout system for the application teams that support Sandia users on Sequoia.

MUZIA

USAGE: HPC **PROGRAM:** NW/ASC
TFLOPS: NA **NODES:** 20
CORES: 320
MEMORY/CORE: 2.0 GB
PROCESSOR HOURS/YR: 2,803,2000

Muzia is a small-scale Cray XE6 system that was acquired as part of the Sandia/LANL partnership that manages the Cielo platform at LANL.

PECOS

USAGE: HPC **PROGRAM:** NW/ASC
TFLOPS: 392 **NODES:** 1,232
CORES: 19,712
MEMORY/CORE: 4.0 GB
PROCESSOR HOURS/YR: 172,677,120

Pecos is a NW/ASC HPC system deployed in 2012 as part of the DOE/NNSA Tri-Labs TLCC–2 procurement. At 392 Teraflops, Pecos is a primary resource for NW/ASC users. In October 2013, Pecos was upgraded to double its available memory on every compute node. This upgrade improved job throughput and reduced compute times by allowing applications to run more compactly within the same overall memory footprint.

PLATO

USAGE: Analytics **PROGRAM:** Institutional
TFLOPS: NA **NODES:** 51
CORES: 816
MEMORY/CORE: 6.0 GB
PROCESSOR HOURS/YR: 7,148,160

Plato is a newly deployed Hadoop cluster that entered production in FY14. The HP-based system runs out-of-the box Cloudera's CDH 5 enterprise product.

RED MESA

USAGE: HPC **PROGRAM:** Institutional
TFLOPS: 180 **NODES:** 1,920
CORES: 15,360
MEMORY/CORE: 1.5 GB
PROCESSOR HOURS/YR: 134,553,600

Red Mesa is an Institutional HPC system based on the Red Sky architecture. In FY14, Red Mesa transitioned into wider use by EC and other Partners.

RED SKY

USAGE: HPC **PROGRAM:** Institutional
TFLOPS: 264 **NODES:** 2,823
CORES: 22,584
MEMORY/CORE: 1.5 GB
PROCESSOR HOURS/YR: 197,835,840

Deployed in 2010, Red Sky and Red Sky (C) have been the workhorses of Institutional HPC computing. Red Sky was developed in collaboration with Sun Microsystems, and is the first large-scale HPC system to deliver an Infiniband interconnect based on a Torus network topology.

SKY BRIDGE

USAGE: HPC **PROGRAM:** Institutional
TFLOPS: 588 **NODES:** 1848
CORES: 29,568
MEMORY/CORE: 4.0 GB
PROCESSOR HOURS/YR: 259,015,680

Sky Bridge was acquired late in FY14, for production early in FY15. It is a water-cooled Cray CCS (formerly Appro) cluster, and at 588 TF peak, will provide a significant new computing resource for all of Sandia's Mission Computing Partners.

TWINFIN

USAGE: Analytics **PROGRAM:** Institutional
TFLOPS: NA **NODES:** NA

Twinfin is an IBM/Netezza appliance for structured- and semi-structured search. Twinfin came online for friendly users early in FY13, and is now moving to full production. The system integrates proprietary hardware and software to accelerate structured search integrated with data analytics.

UNITY

USAGE: HPC **PROGRAM:** Institutional
TFLOPS: 38 **NODES:** 272
CORES: 4,352
MEMORY/CORE: 2.0 GB
PROCESSOR HOURS/YR: 38,123,520

Unity is a NW/ASC HPC system deployed in 2009 as part of the DOE/NNSA Tri-Labs TLCC–1 procurement. Now supplanted by the TLCC–2 systems, Unity transitioned to Institutional usage in FY14.

UNO

USAGE: HPC **PROGRAM:** NW/ASC
TFLOPS: 8.64 **NODES:** 25
CORES: 400 **MEMORY/CORE:** 8.0 GB
PROCESSOR HOURS/YR: 3,504,000

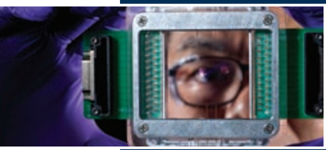
Uno is the first high-throughput cluster deployed at Sandia. Based on a Dell compute node, Uno is designed to provide high-throughput and fast turnaround for single-node jobs. Systems designed to run large jobs have to provide a high-bandwidth, low-latency interconnect, and need to keep every node as similar as possible. These requirements stem from the fact that parallel jobs run at the speed of their slowest component.

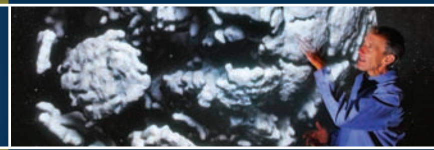
In contrast, Uno provides a variety of heterogeneous nodes (small and large memory, processors and accelerators) with its interconnect and file systems tuned for singe-node activities.

WHITNEY

USAGE: HPC **PROGRAM:** Institutional
TFLOPS: 38 **NODES:** 272
CORES: 4,352
MEMORY/CORE: 2.0 GB
PROCESSOR HOURS/YR: 38,123,520

Whitney, located at Sandia California, is a NW/ASC HPC system deployed in 2009 as part of the DOE/NNSA Tri-Labs TLCC–1 procurement. Whitney transitioned into alternative use in FY14.





SANDIA MISSION
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ON THE COVER: Turbulent hydrogen-air flame from a simulation created by a research team at Sandia's Combustion Research Facility. The 3-D rendering shows (in gold) areas where ideal proportions of fuel and oxygen are present and (in colors) areas where autoignition is taking place. The Sandia group, led by Jackie Chen, recently was awarded six million hours of supercomputing time by DOE's Office of Science to simulate flame stabilization, extinction, ignition, soot formation, and other processes in turbulent flames. Data produced in the project are being used to develop and validate predictive models that could help engineers design future fuel-efficient combustion engines for vehicles and lean power generators. The simulation, with one billion grid points and detailed hydrogen-air chemistry requiring 2.5 million processor hours on the Cray XT3 supercomputer at Oak Ridge National Lab, is the world's largest combustion simulation. The volume rendering was performed by researchers at DOE's Science Discovery through Advanced Computing (SciDAC) Institute for Ultrascale Visualization.

Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration