2017

SANDIA NATIONAL LABORATORIES
HIGH PERFORMANCE COMPUTING

The 2017 High Performance Computing Annual Report is dedicated to John Noe and Dino Pavlakos.

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Building a foundational framework in high performance computing

Sandia National Laboratories has a long history of significant contributions to the high performance computing community and industry. Our innovative computer architectures allowed the United States to become the first to break the teraflop barrier—propelling us to the international spotlight. Our advanced simulation and modeling capabilities have been integral in high consequence US operations such as Operation Burnt Frost. Strong partnerships with industry leaders, such as Cray, Inc. and Goodyear, have enabled them to leverage our high performance computing capabilities to gain a tremendous competitive edge in the marketplace.

As part of our continuing commitment to provide modern computing infrastructure and systems in support of Sandia's missions, we made a major investment in expanding Building 725 to serve as the new home of high performance computer (HPC) systems at Sandia. Work is expected to be completed in 2018 and will result in a modern facility of approximately 15,000 square feet of computer center space. The facility will be ready to house the newest National Nuclear Security Administration/Advanced Simulation and Computing (NNSA/ASC) prototype platform being acquired by Sandia, with delivery in late 2019 or early 2020. This new system will enable continuing advances by Sandia science and engineering staff in the areas of operating system R&D, operation cost effectiveness (power and innovative cooling technologies), user environment, and application code performance.

We were also able to expand our existing computing base with the acquisition of another Commodity Technology System (CTS-1) cluster to be named "Eclipse." This system augments four existing CTS-1 platforms that were acquired in FY16-FY17.

The combination of Sandia institutional investment and the ASC program's commitment to Sandia will ensure a robust and effective research and development program, with cogent options for the DOE/NNSA Science-based Stockpile Stewardship Computational Simulation effort in support of the nation's defense needs.

Our computing resources and expertise allow Sandia to continue to provide exceptional service in the national interest by using sophisticated computational modeling for solutions to national scientific challenges. Sandia continues to invest in growing its critical capabilities, while establishing leadership as a nationally-recognized high performance computing facility. As the importance of high performance computing grows, it is critical to continue expanding our computing capabilities to remain on the cutting edge of innovation and discovery.

David White, Director of Cybersecurity and Mission Computing

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AUGMENTED REALITY APP

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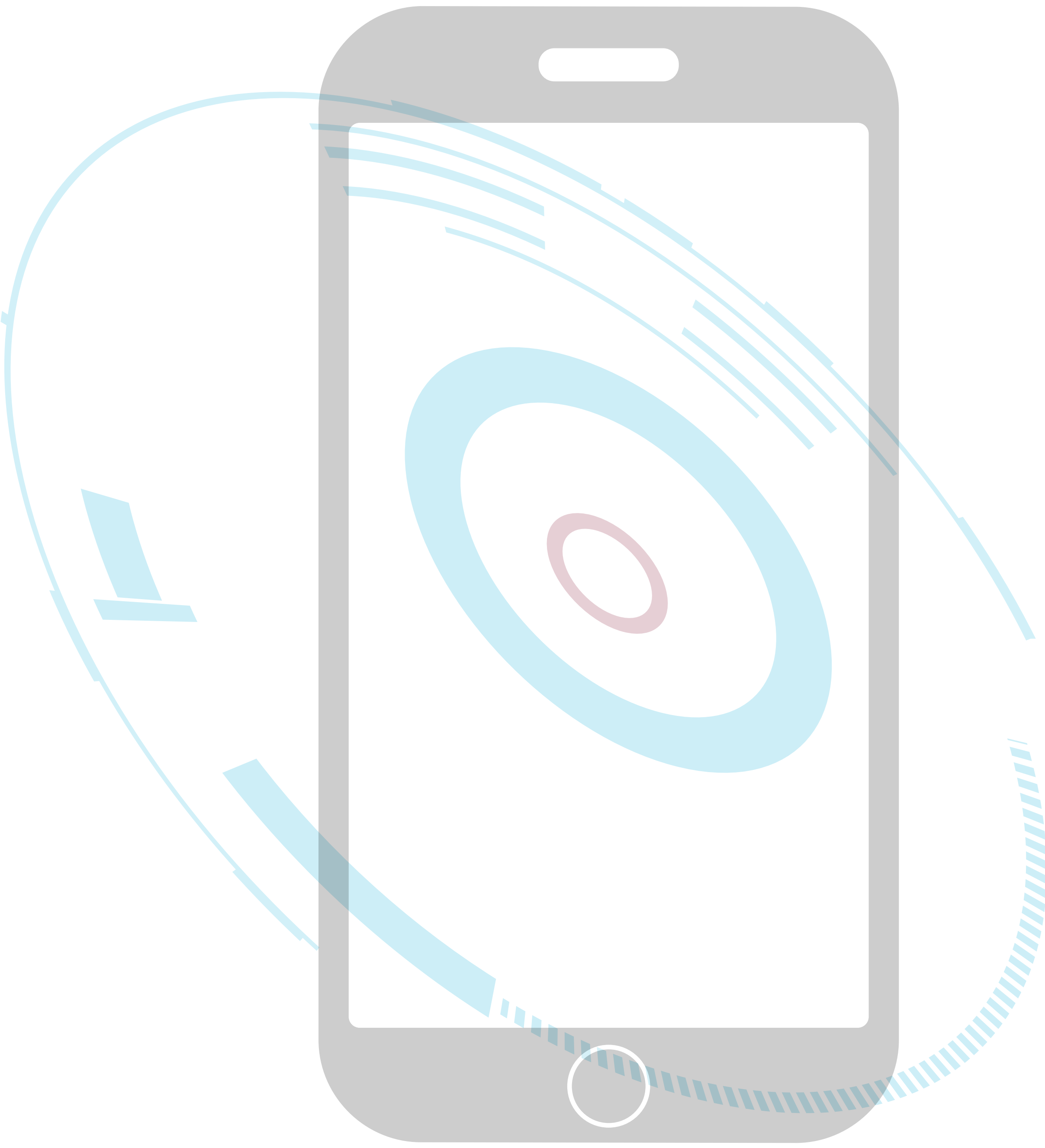



HPCs Then & Now

Established during the Atomic Era, high performance computing has expanded beyond Sandia National Laboratories and our national security mission to significantly impact many applications throughout industry, research, and academia.

In the 1940s, the United States began utilizing early supercomputers to solve complex nuclear physics problems and conduct analysis on data obtained during field testing. With the ability to solve complex calculations a thousand times faster than manual calculations, these early supercomputers played a critical role in the nation's development of our nuclear arsenal.

High performance computing's role evolved when the United States discontinued nuclear testing in 1992. The nation began to rely on sophisticated computational models instead of field tests to certify the safety and effectiveness of the nuclear stockpile. During this time, the United States made major investments throughout the national lab complex (Sandia National Laboratories, Los Alamos National Laboratory, and Lawrence Livermore National Laboratory) to expand upon existing computing capabilities. Early investments went toward building new supercomputers in partnership with industry such as Intel, IBM, and SGI, and advancing engineering physics integrated codes. The initial goal was to deploy systems with the processing power to create reliable high fidelity models and simulations to validate the nation's nuclear stockpile. The investment in this critical capability launched the United States as an international leader in high performance computing.

While still a critical capability to nuclear weapons, it has now become essential to all of Sandia's research areas. Sandia's researchers are leveraging HPCs to provide solutions to real-world challenges, such as climate change, disease transmission, and the impact of natural disasters. Sandia continues to advance this capability by expanding beyond traditional massively parallel scientific computing platforms and investing in data analytics, Emulytics platforms for deep learning, and working toward the exascale computing environment of the future. These continued investments will allow us to remain a national leader in computational science and engineering for years to come.

Sandia's HPC program has changed the industry and impacted the world. From demonstrating the effectiveness of massively parallel computing platforms to creating scalable computer architectures—Sandia is a leader in computational science and engineering.

High-Performance Computing

Advanced computer systems with the ability to solve complex computational problems through modeling, simulation, and data analysis that are too large or would take too long on standard computers

1950s–1960s

Data generated during nuclear weapons field testing necessitates need for high performance computing capabilities at Sandia and other defense laboratories across the nation.

1987

Sandia researchers win the inaugural Gordon Bell Prize for demonstrating that scientific applications could achieve thousand-fold speedups on massively parallel processors.

PAGE 2

1989

Sandia develops CTH codes, used for computer modeling of high-speed impacts and the effects of nuclear explosions. The code is selected as the Department of Defense's code of choice for solving high velocity impact problems.

PAGE 3

1991

Sandia and the University of New Mexico partner to develop SUNMOS, a new message passing scheme and high performance I/O on the nCUBE-2. SUNMOS and its many derivatives have been successfully deployed on many HPCs.

PAGE 4

1992

Sandia and Goodyear enter into a Cooperative Research and Development Agreement (CRADA) to apply advanced modeling and simulation capabilities to access the performance of new tire designs.

The United States discontinues underground nuclear testing, creating a new reliance on HPCs to validate and verify the US nuclear stockpile.

PAGE 6

1993

The Top500 list is established to rank the top performing supercomputers. Sandia's Intel XP/S 140 Paragon, the first massively parallel computing platform at Sandia, reaches number one on the 1994 Top500 list.

PAGE 8

1995

As part of the Science-based Stockpile Stewardship Program, the Accelerated Strategic Computing Initiative (ASCI) is established to advance computing capabilities to validate the nuclear stockpile using computational modeling and simulation.

PAGE 10

1996

ASCI Red, the first platform procured through the ASCI program, is delivered to Sandia.

The United States signs the Comprehensive Nuclear Test Ban Treaty, formalizing the United States' commitment to alternative methods for nuclear weapon verification.

1997

ASCI Red is No. 1 on Top500 List as the first teraflop/s computer with a Linpack performance of 1.068 teraflop/s.

1998

Sandia establishes the Massively Parallel Computing Research Lab, which pioneered massively parallel computing for solving complex problems in science and engineering.

2001

As part of the ASCI program, DisCom was established, creating a high speed network that connects Sandia, Los Alamos National Laboratories, and Lawrence Livermore National Laboratory—ensuring all HPC resources could be accessed remotely.

PAGE 12

2002

Sandia and Cray, Inc. enter into a contract to deliver Red Storm—the next HPC funded by the ASCI program.

2005

Thunderbird is sited at Sandia, representing Sandia's initial investment in large-scale HPCs as an institutional resource and expanding massively parallel high performance computing to research areas beyond nuclear weapons.

PAGE 14

2008

Calculations performed on Red Storm play an integral role in the successful execution of Operation Burnt Frost, a mission to intercept a defective US satellite.

PAGE 18

2008

The term *Emulytics* is coined at Sandia. The term describes the combination of emulative network computing and analytics used for various testing and cybersecurity purposes. This work continues today.

2009

Catamount, a lightweight kernel operating system based on SUNMOS, receives an R&D 100 Award.

PAGE 22

2010

Red Sky/Red Mesa is named one of 15 winners of Oracle's Eco-Enterprise award. Red Sky/Red Mesa represents a collaboration between Sandia and the National Renewable Energy Laboratory.

National Nuclear Security Administration dedicates the National Security Computing Center at Sandia, a Department of Energy (DOE) user facility for classified applications that require HPCs.

2012

Sandia establishes the Institutional Computing Program for the procurement and operation of HPC platforms to support the lab-wide demand for high performance computing capabilities for research beyond nuclear weapons.

PAGE 26

2014

DOE's ACME (Accelerated Climate Modeling for Energy) Project is established to develop a computationally advanced coupled climate-energy model to investigate the challenges posed by the interactions of weather-climate scale variability with energy related sectors.

Sky Bridge, Sandia's first water cooled machine, is sited at Sandia Labs.

PAGE 28

2015

Sandia's Born Qualified Grand Challenge uses HPCs to model additive manufacturing processes to predict process-structure-performance relationships.

President Obama signs the National Strategic Computing Initiative Executive Order, calling for the accelerated development of technologies for exascale supercomputers and funding research into post-semiconductor computing.

PAGE 30

2016

Sandia's high performance computing capabilities are used to validate physical testing on the B61-12 nose assembly as part of the B61-12 Life Extension Program.

PAGE 34

2017

Sandia invests in Synapse, the first machine learning/deep learning high performance platform at Sandia.

PAGE 36

2018

Expected completion of 725-E Expansion—Sandia's new home for high performance computing.

2019

ARM Test Beds to be completed and installed in Sandia's new HPC Center (725-E), which enable Sandia's research into advanced architectures to achieve exascale computing.

PAGE 38

2021–2023

DOE's Exascale Computing Project deploys its initial exascale systems. Sandia is among the core laboratories working together to achieve the project's ambitious goals.

LOOKING BACK

By the end of the last millennium, Sandia's high performance computing efforts had developed the first computer in the world to break the one teraflop barrier. Sandia achieved massively parallel platforms and made groundbreaking advances in modeling and simulation.

1989

A Legacy of Leading-Edge Codes

In the mid 1990s, the Advanced Scientific Computing Initiative (ASCI) was funded to take on a confluence of two major shifts in modeling and simulation: a need to support neuclear weapon stockpile stewardship in the post-underground test ban era, and a need to address a paradigm shift in high performance computing toward massively parallel distributed computing. Both of these needs were to have significant impact on the nature of computational simulation software.

ASCI invested in a modernization of numerical simulation capabilities—the ability to "virtually test" through modeling and simulation. At Sandia, the ASCI program funded the creation of the SIERRA engineering mechanics codes and the RAMSES electromagnetic radiation and circuit codes. These new leading-edge code capabilities emphasized modeling relevant physics applied to simulations for stockpile stewardship that made use of the newest, fastest HPC platforms fielded by the DOE ASCI program.

The complexity of the problems led to the concept of team-developed codes, a significant departure from the one-or two-person code teams developing single-purpose codes prior to ASCI. Code teams addressed the code programming changes needed to support (what was to be) the first round of HPC architecture changes.

Several years later, in 2004, the Advanced Scientific Computing program (ASC) took over where ASCI left off to put into production these new simulation capabilities for the weapon Life Extension Program (LEP) and major alterations (ALT) stockpile work.

Today, another momentous architecture shift is occurring in high performance computing to address energy efficient computing as the computation simulation community pushes toward exascale. Starting in about 2015, code teams are once again addressing programming changes needed to support these new platforms.

Sandia's collaborative efforts to develop science and engineering codes emerged to solve the problems unique to Sandia's national security mission. This work continues to develop as teams incorporate uncertainty quantification and consider how to transition 25 years of software to exascale architecture. For codes like SIERRA and RAMSES, which target engineering in extreme environments, being able to run effectively on HPCs is an important part of the future, something Sandia continues to anticipate and address.

1991

SUNMOS and the Creation of Lightweight Kernel Operating Systems

Sandia became an expert in computer system architecture and predicting ways to improve system performance. This led to the development of customized software environments based on lightweight compute node operating systems.

Sandia partnered with the University of New Mexico to develop SUNMOS, an operating system for message passing and process support that consumes a minimal amount of memory. The lightweight kernel operating systems maximizes CPU resources by reducing OS and runtime system overhead; maximizing memory resources, with a small memory footprint and large page support; maximizing network resources, with no virtual memory and physically contiguous address mapping; and increasing reliability, with a small code base and reduced complexity.

Originally developed for nCUBE-2 MIMD, SUNMOS was later successfully ported to Paragon after the OS provided by Intel failed to scale well. SUNMOS and its derivatives have been used on multiple Sandia HPCs. Catamount, one of its descendants, was successfully deployed on Red Storm and was later awarded a prestigious R&D 100 Award in 2009.

1992 Using Code to Design the Ideal Tire

Modeling and simulating tire performance is complicated and considers millions of material combinations, permutations, blending structural mechanics, and rigid body and fluid dynamics under varying temperature, pressure, and wear conditions. In 1992, Goodyear looked at Sandia's advanced computational mechanics software applications developed for nuclear weapons programs and saw that they could be applied to tires. Through a Cooperative Research and Development Agreement (CRADA) established in 1993, Goodyear was able to use Sandia computer codes to develop new tires for manufacture rather than building and testing three to five prototypes. Goodyear's time to manufacture was reduced by one-half or more.

The collaboration produced the Assurance TripleTred, a unique all-weather tire with a three-part tread pattern. Goodyear wanted a visually distinctive tire that would generate buzz and demonstrate its best technology and quality. Launched in 2004, the TripleTred was brought from concept to market in less than a year. Goodyear says the tire could not have been produced without modeling and predictive testing tools developed with Sandia.

This partnership, based primarily on adapting Sandia's computational mechanics codes to perform simulations of the mechanical performance of tires, has been highly acclaimed as perhaps DOE's best example of tech transfer between the national laboratories and private industry. Goodyear has used the technology transferred from Sandia to make computational simulation an integral part of their tire design process. In addition to many other awards, Goodyear and Sandia jointly received a R&D100 Award in 2005 for their use of computational simulation to bring Goodyear's Assurance line of tires to market in record time.

The CRADA has been renewed repeatedly since 1993 and Goodyear continues to produce innovative products developed in collaboration with Sandia. In addition to demonstrating the use of codes to advance and accelerate production, the CRADA is a prime example of a partnership that targets a strategic technical challenge. Goodyear and Sandia are jointly developing new capabilities, such as modeling tire performance under severe maneuvering, which helps Sandia with simulations for national security. Much of the research done under the CRADA has been applied to Sandia's science-based nuclear weapons stockpile stewardship mission.

2017 marks a 25-year partnership between Sandia and Goodyear Tire & Rubber Company. Since 1993, they have worked together to advance tire science along with computer modeling and simulation.

1993

TOP500 The List.

Defining High Performance

HPC performance data is valuable to manufacturers, users, and potential users. The Top500 list was established in 1993 to evaluate and rank the top supercomputers in the world. This twice yearly list allows the high performance computing community to track and identify industry trends. Rankings are based on the High Performance LINPACK (HPL) Benchmark. Sandia first appeared in the list in 1994 with Paragon and has made regular appearances on the list ever since the list was first created—with over 180 total appearances, including eight number one rankings. Following their partnership with Sandia on Red Storm, Cray Inc. has appeared repeatedly in the Top500 and have become an industry leader in system performance.

An Alternative Measure

In collaboration with the Innovative Computing Laboratory at the University of Tennessee, Sandia developed an alternative metric for performance evaluation—the High Performance Conjugate Gradients (HPCG) Benchmark. Designed to complement the HPL, HPCG exercises computational and data access patterns that more closely match a different and broad set of important applications, and provide incentive to computer system designers to invest in capabilities that will impact on the collective performance of these applications. HPCG results are now featured alongside HPL results in the Top500 list.

1994

June
Paragon (#1)
143.4 gigaflops

November
Paragon (#2)
143.4 gigaflops

1995

June
Paragon (#2)
143.4 gigaflops

November
Paragon (#2)
143.4 gigaflops

1996

June
Paragon (#3)
43.4 gigaflops

November
Paragon (#4)
143.4 gigaflops

1997

June
ASCI Red (#1)
1,068 gigaflops

November
ASCI Red (#1)
1,338 gigaflops

1998

June
ASCI Red (#1)
1,338 gigaflops

November
ASCI Red (#1)
1,338 gigaflops

1999

June
ASCI Red (#1)
2,121 gigaflops

November
ASCI Red (#1)
2,379 gigaflops

2000

June
ASCI Red (#1)
2,379 gigaflops

November
ASCI Red (#2)
2,379 gigaflops

2001

June
ASCI Red (#3)
2,379 gigaflops

November
ASCI Red (#4)
2,379 gigaflops

2002

June
ASCI Red (#7)
2,379 gigaflops

2005

November
Thunderbird (#5)
38.3 teraflops

Red Storm (#6)
36.2 teraflops

2006

June
Thunderbird (#6)
38.3 teraflops

November
Red Storm (#2)
101.4 teraflops

Thunderbird (#6)
53 teraflops

2007

June
Red Storm (#3)
101.4 teraflops

**All performance values represent actual performance on HPL*

1995

Accelerated Strategic Computing Initiative

Boon to High Performance Computing at Sandia and throughout the Nation

Since its creation, ASCI/ASC has delivered 10 supercomputers between the three laboratories—improving performance with each new machine.

1996: ASCI Red (Sandia)
1.068 teraflops,
3 teraflops in 1999

1998: ASCI Blue Pacific (LLNL) & ASCI Blue Mountain (LANL)
3 teraflops

2000: ASCI White (LLNL)
12.3 teraflops

2003: ASCI Q (LANL)
20 teraflops

2005: ASCI Purple (LLNL)
100 teraflops

2008: Roadrunner (LANL)
1 petaflop

2010: Cielo (LANL)
1.4 petaflop

2013: Sequoia (LLNL)
20 petaflops

2015: Trinity (LANL)
40 petaflops

Prior to 1992, the United States used full-scale nuclear field tests to assess weapon performance, safety, and reliability. In 1996, the United States signed the Comprehensive Test Ban Treaty, thereby formally ending our reliance on full-scale nuclear testing. Faced with an aging stockpile, the Department of Energy (DOE) established the Science-Based Stockpile Stewardship program (SSP) to develop new tools for ensuring the effectiveness of our nuclear deterrent. The SSP determined that weapons scientists and engineers must rely much more heavily on sophisticated computational models run on incredibly powerful computers that simulate the complexities of nuclear physics, weapons components, and the weapons system as a whole, to determine the impact of design changes and aging on the stockpile. To meet this challenge, the Accelerated Strategic Computing Initiative (ASCI, later known as Advanced Simulation and Computing—ASC) was established in 1995 to advance high performance computing capabilities at the DOE's three defense program laboratories: Sandia, Lawrence Livermore National Laboratory (LLNL), and Los Alamos National Laboratory (LANL).

Since the last nuclear field test in 1992, the United States' experience base was starting to decline, which meant that ASCI had to scale up computing capabilities rapidly to verify them against actual physical test designs and data. Computing resources at this time were inadequate to handle the high fidelity modeling and simulations required by the SSP, so ASCI and the participating labs worked with industry to accelerate development of supercomputers.

ASCI recognized Sandia's early demonstration in the effectiveness of massively parallel computing systems, which made Sandia an excellent candidate to receive the first ASCI platform. In 1996, ASCI Red was sited at Sandia. ASCI Red was the first supercomputer to break the teraflop barrier and was recognized as the fastest supercomputer in the world from 1997 to 2000.

Because of the ASCI/ASC program, the United States emerged as a leader in high performance computing and advances made through this program helped influence the HPC industry worldwide. Sandia leverages capabilities and expertise developed through the ASCI/ASC program to extend the availability of strategic computing to all of Sandia's mission programs, enabling Sandia to remain at the forefront of computational science and engineering.

ASC Program Elements

Integrated Codes: Funds the critical skills needed to develop, maintain, and interpret the results of large-scale integrated simulation codes that are needed to maintain and extend the lifespan of our stockpile.

Physics and Engineering Models: Funds the critical skills charged with the development, initial validation, and incorporation of new models into the Integrated Codes.

Verification and Validation: Provides assurance that the models in the codes produce mathematically correct answers and that the answers reflect physical reality.

Computational Systems and Software Environment: Provides users of ASC computing resources a stable and seamless computing environment for all ASC-deployed platforms.

Facility Operations and User Support: Provides necessary physical facility and operational support for reliable and effective use of tri-lab computing resources (Sandia, LANL, LLNL).

Advanced Technology Development and Mitigation: Addresses the need to adapt current integrated design codes and build new codes that are attuned to emerging computing technologies.

1996

ASCI Red

The World's First Teraflops Machine

Teraflops and beyond

FLoating-point **O**perations **P**er **S**econd=**FLOPS**

Gigaflop: one billion (10^9) flops

Teraflop: one trillion (10^{12}) flops

Petaflop: one thousand million million (10^{15}) flops

Exaflop: one billion billion (10^{18}) flops

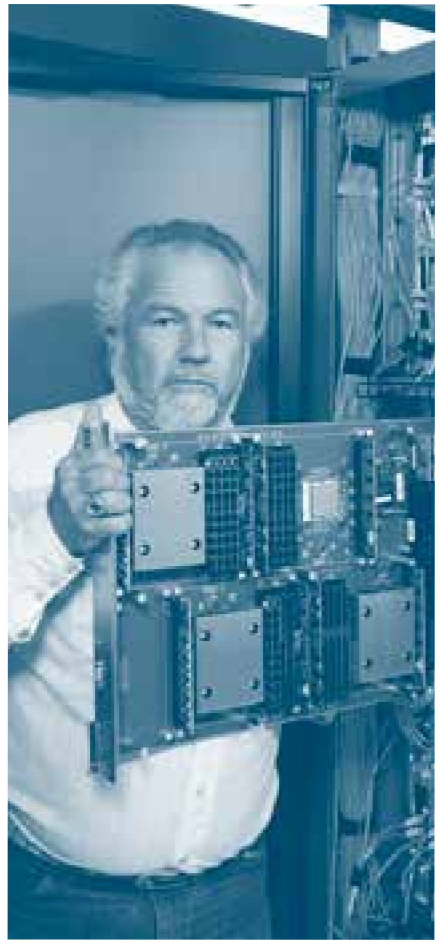
Starting in the late 1980s, Sandia demonstrated the viability of massively parallel processing systems, such as the nCUBE-10 and the Intel Paragon, to create advanced modeling and simulations to solve complex mission challenges. This demonstrated success led Sandia to become the recipient of ASCI Red—the first high performance computing platform funded through the Accelerated Strategic Computing Initiative (ASCI). ASCI Red represented a major leap in computer performance and ushered in an era of US dominance in the production and implementation of supercomputers.

ASCI Red's architecture was based on the successful Paragon platform that was in place at Sandia from 1993 to 1998. ASCI Red was a distributed memory MIMD (multiple instruction, multiple data) massively parallel machine consisting of 9,632 compute nodes with a peak performance of 1.3 teraflops. The system was organized into four partitions: Compute, Service, System, and I/O. To maximize performance, Cougar (Intel's port of Puma, a Sandia/University of New Mexico-developed operating system based on SUNMOS), a lightweight OS was run on the Compute partition for optimal performance. ASCI Red was number one on the Top500 list for over 3 years until it was replaced by ASCI White, another ASCI-funded HPC sited at Lawrence Livermore National Lab.

2002

Red Storm

Sandia's most influential supercomputer



In 2002, Cray Inc. signed a contract with Sandia to deliver Red Storm, a new high performance computing platform to replace the aging ASCI Red platform. Funding for this acquisition was secured through the Advanced Simulation and Computing (ASC, formerly ASCI) program with the requirement that the new HPC performed 7 times greater than ASCI Red. Cray built Red Storm based on a Sandia-designed architecture that allowed for future scalability to meet greater performance demands. Typically, design and construction of HPCs takes an average of 4-5 years, but Cray worked with Sandia to deliver Red Storm in a record-breaking 30-month time frame.

Compared to other supercomputers at the time, Red Storm was one of the most inexpensive at only $77.5 million. Red Storm was unique due to the design's utilization of off-the-shelf parts, making it cheaper and easier to maintain and upgrade. The only custom component was an interconnect chip that was developed to pass information more directly from processor to processor while applications were running. Operating costs were also low, energy usage was 2.2 megawatts—nearly half the amount of energy required to run similar supercomputers.

Red Storm's peak performance at installation was 41.5 teraflops, but its unique design allowed for future scalability. In 2008, Sandia and Cray embarked on a major upgrade that increased performance to 284.16—nearly 7 times more powerful than when it was first installed. The platform's ability to accommodate single-, dual-, and quad-core processors, made it possible to do these massive upgrades. Red Storm supported both classified and unclassified missions until July 2011.

The Incredible Scalability of Red Storm

Just like its predecessor (ASCI Red), Red Storm was designed to be scalable and was upgraded several times during its lifetime.

	teraflops	
2005	41.5	*10,368 processors*
2006	124.2	*25,920 processors*
2008	284.16	*38,400 processors*

Red Storm's success was a result of the experience Sandia gained through the development and use of previous supercomputing platforms, Paragon and ASCI Red. Sandia's experience allowed for the development of a clear design philosophy and sound operational judgment. Red Storm was not only a crowning achievement for Sandia, Cray also leveraged Red Storm's unique architecture as the blueprint for the XT3, one of Cray's most successful commercial supercomputers. Sandia continues to collaborate with Cray, Intel, IBM and other industry partners to scout a path for further HPC systems.

CRAY
THE SUPERCOMPUTER COMPANY

"Virtually everything we do at Cray—each of our four product lines—comes from Red Storm. It spawned a company around it, a historic company struggling as to where we would go next. Literally, this program saved Cray."

—Cray Inc. President and Chief Executive Officer Peter Ungaro

2008

Operation Burnt Frost

Intercepting an Errant Satellite

Burnt Frost Simulations Statistics

~25,000 processors, Red Storm Jumbo Mode

638 job launches on Red Storm in 5 weeks

6,200,000 node-hours of run time in 5 weeks

50 high-resolution CTH hydrocode runs completed (200 to 600 million computational zones for each simulation)

10 Hydro-structural simulations completed (Zapotec code: CTH/ Pronto Coupled Code)

In 2008, Sandia was called to support Operation Burnt Frost, an effort by the Missile Defense Agency to intercept an errant satellite using a US Navy interceptor. Using physics-based modeling and simulation on Red Storm and Sandia's knowledge in Missile Defense Lethality, Sandia provided crucial lethality requirements and debris prediction for a kill assessment. Sandia also assisted in the real-time assessment of the event during the operation at Schriever Air Force Base in Colorado.

The satellite had failed shortly after its launch in 2006 and by early 2008 its orbit had deteriorated to the point of reentry into the Earth's atmosphere. The malfunctioning satellite contained 1,000 pounds of toxic hydrazine fuel that posed a threat if the tank did not explode prior to reentry. Operation Burnt Frost had only a few months to model and simulate a successful interception of the defective satellite.

Red Storm was used to run simulations to intercept the defective satellite, which was traveling at 17,000 miles per hour, 153 miles above earth. For approximately two months preceding the event, Sandia personnel ran Red Storm simulations to assess and plan the complex mission, including hundreds of impact simulations in a matter of days and weeks. The impact simulations answered critical technical questions, affecting early decisions to go forward with the operation.

The team used the results to predict mission details and possibilities. The team also provided data confirming that the satellite was successfully intercepted.

Modeling and simulation by Sandia contributed to the early decision to proceed with the operation and helped the US Department of Defense (DoD) plan and execute the shot. The information also helped conduct analysis after the satellite was brought down. Operation Burnt Frost concluded on February 20, 2008 when a standard missile launched from the USS Lake Erie successfully intercepted the satellite.

Burnt Frost and the Creation of the National Security Computing Center

Red Storm proved itself in broadened applications when it was called into service to assist the DoD in planning Operation Burnt Frost, the highly successful engagement to safely shoot down an errant US satellite in 2008. Use of this facility was extended when the intelligence community recognized that simulations at the extreme scales afforded by Red Storm could uniquely contribute to solving additional national security challenges.

In January 2008, the NNSA asked Sandia to consider turning one of its nuclear weapons resources in to a broader resource for other challenges to national security. In May 2008, Sandia agreed to move forward with the conversion of Red Storm. By July 2009, the facility and associated resources became available for SCI use. This led to its dedication as the National Security Computing Center by the NNSA on February 25, 2010. At the time, Red Storm was listed among the top 15 fastest computers in the world.

Scan with SNLSimMagic App to watch history come to life.

CURRENT PROJECTS

Today, Sandia is utilizing high performance computing to meet complex challenges facing the nation. Applications include accelerated climate modeling, improved fidelity in modeling and simulation, the advent of Emultytics, and advances in additive manufacturing.

EMULYTICS

Emulate, analyze, and understand complex systems

Networked Information Technology systems play a key role supporting critical government, military, and private computer installations. Many of today's critical infrastructure systems have strong dependencies on secure information exchange among geographically dispersed facilities. As operations become increasingly dependent on the information exchange they also become targets for exploitation. The need to protect data and defend these systems from external attack has become increasingly vital while the nature of the threats has become sophisticated and pervasive making it a daunting challenge. Enter Emulytics!

The term "Emulytics" was coined at Sandia in 2008 when a need for two kinds of computing environments was noticed: information analytics and graph analytics. Emulytics is derived from the terms emulative network computing and analytics. Emulytics includes and seeks to include:

- Large-scale, vastly heterogeneous networked systems
- Integrated systems that can be configured and used both for controlled experimentation and interactive exploration of system behavior
- Components that may be real, emulated, or simulated
- Network(s) creation, management, and instrumentation
- Large HPC platform management and monitoring
- Data extraction and warehousing
- Analysis and result visualization.

Screenshot of the Supercomputing model, running in Sandia's Emulytics platform. This graph shows an abstraction of the network that we can compare to the model for first-order validation.

Sandia supports an open-source project "minimega" (minimega.org) to support creating virtualized models of computer-related networks. This is the core capability that enables much of the Emulytics program at Sandia. Key features allow:

- Scalable experiment development: design and test an experiment on a laptop, and then upload and run it on a large cluster to increase the number of nodes in the model
- Performance considerations: minimega orchestration can tear down and reprovision extremely large networks (on the order of 10,000 elements) in seconds, thus enabling many iterations of studies on a consistent model

The tool has been used by academic researchers and enables Sandia's cyber-range and operational systems testing analysis and training efforts.

Emulytics blends simulation, virtualized hardware and software, emulated devices, and the direct deployment of actual hardware and software to create live-virtual-constructive (i.e., real-emulated-simulated) environments. Emulytics enables rich analyses through scalable infrastructures while being deployable with great efficiency. Among its many applications, Emulytics provides cyber defender training, helps to characterize otherwise unmanageable systems, and has even been used to understand and provide quantitative evidence of potential cyber threat impacts on the performance of physical protection systems. Securing today's sophisticated information technology facilities involves not only creating secure system architectures and secure system configurations, but also heavily relies on well-trained defenders. Thus, there is a need for flexible cyber security training, testing, and analysis platforms that can replicate information systems with high levels of realism to enable training and analysis.

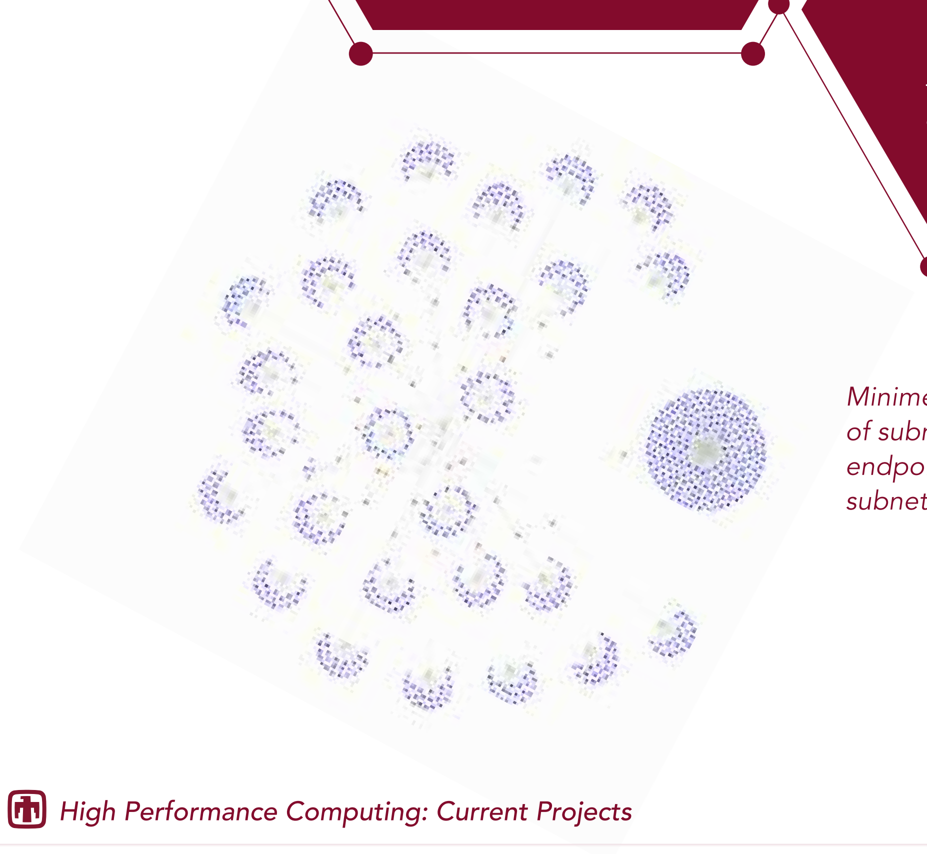
Minimega feeds thousands of emulated Android devices synthetic GPS locations to emulate users walking and driving around Livermore, CA as part of the MegaDroid LDRD.

Scan with SNLSimMagic App to see our work come to life.

Sandia has engaged in multi-year research projects to develop new strategies and methodologies that enable researchers to quickly and accurately model information systems' hosts and networks of interest for cyber analysis and training. Emulytics provides the capability to combine real, emulated, and simulated devices—i.e., live, virtual, and constructive—into a single controlled experiment to enable system-wide cyber training, while answering a wide variety of cyber-related questions. High performance computing capabilities enable the Emulytics platform to represent complex, large-scale, complicated system enterprises, such as government facilities like Sandia, or to model threats across the national power grid infrastructure like the recent Mirai internet-of-things botnet.

Sandia advises the Department of Homeland Security on policies and protections related to the cyber defense of civilian government networks (.gov). Emulytics is used to model portions of the nation's infrastructure to answer "what if" questions for technology, architecture, and policy changes. Sandia aims to be able to create models of the entire national infrastructure.

Information System: According to the *Business Dictionary*, an information system is "a combination of hardware, software, infrastructure and trained personnel organized to facilitate planning, control, coordination, and decision making in an organization."



Minimega models a simple enterprise network with dozens of subnets (represented in red) each containing dozens of endpoints (represented in blue). A core router connects the subnets to the outside world.

What's at Stake? The Importance of Emulytics Capabilities

Currently, cyber defender training and system analysis are performed on operational systems, on limited scale testbeds, or on simulated models of the system. However, each approach has some disadvantages.

- Operational systems: Analysis and training on operational systems is limited to the most benign levels because any disruption to the operational system has potentially severe consequences. While defenders gain experience with the actual system, this approach reduces operators' ability to test and analyze the system. The scale of operational systems can be the size of entire nations or even the global routing infrastructure (the Internet). Creating full-scale replicas for experimentation is not economically feasible, so operators turn to virtualization and modeling techniques.
- Testbeds: Testbeds for analysis and training are typically expensive, time-consuming to construct and deploy, single-purpose, and difficult to maintain due to fast-paced technological advances. Testbeds are also typically limited to small subsets of the larger system, which limits their realism.

Sandia's Emulytics solution provides: Networked endpoints (OS, virtual, HITL), instrumentation, data collection, and analysis backend capability. Sandia provides a platform capable of adequately representing the operational system for analysis and for cyber teams to exercise their techniques and develop tools, tactics, and procedures.

COOLING

Unlocking the Infrastructure for Continued High Performance Computing Advances

Sandia has been at the forefront of high performance computing cooling system advances. Among other benefits, improved cooling systems save energy, reduce water use, and decrease the footprint of computing systems.

In the early 1980s, a typical data center emphasized the machine with little consideration of the operations and infrastructure delivery or cost. At the time, systems were direct cooled with steam driven chillers where the critical factor was a low water temperature. The late 1980s to 1990s saw a shift to air-cooled racks and electric-driven centrifugal fans with raised Computer Room Air Conditioner (CRAC) units strewn throughout data center floors. At this point, environmental concerns such as water and refrigerant use were emerging and were further compounded by concerns about rising operational and energy costs.

When Sandia installed the 8,960-processor Thunderbird cluster—jointly designed by Sandia and Dell—data center operators took steps to address issues associated with costs and efficiencies. The infrastructure for Thunderbird used a then-new hot aisle/cold aisle configuration. A subfloor and cold side control complemented this approach. Because data centers cannot have combustible material, the cluster required a non-combustible enclosure above the units to trap the cooler air and prevent the bottom nodes from overheating. To solve this problem, the Sandia team resorted to innovation, using hot air balloon material, thereby developing and installing a first-of-its-kind cold air containment system.

When Red Storm was installed in 2005, it utilized plug fan cooling technologies for the first time in an HPC system in the United States. Plug fan cooling allowed the systems to omit belts, lowered the maintenance cost, and lowered operating costs. The system was among the first to utilize a pressure differential allowing all CRAC units to work as one based on the power consumption of the computer. It also first utilized a 100 amp, 208 volt power supply to each computer.

Since those initial steps, Sandia continues to collaboratively develop and support more efficient data center infrastructure.

Sandia partnered with the National Renewable Energy Laboratory and Johnson Controls to deploy the Thermosyphon Cooler Hybrid System, an integration of a dry heat rejection device, a thermosiphon cooler (TSC) and an open cooling tower. The improved heat rejection system, which combines equipment and controls, embraces the “smart use of water,” using evaporative cooling when advantageous thus saving water, and modulating toward increased dry sensible cooling as system operations and ambient weather conditions permit. Innovative fan control strategies ensure optimal balance between water savings and parasitic fan energy. TCHS has saved over one million gallons of water over the course of 10 months. The system is slated for installation at Sandia in 2018, realizing a savings of five million gallons of water annually.

DATA CENTER IMPROVEMENTS

ASCI Red

1996 design used **return-air utilization** (duct CRAC units to the ceiling to prevent short cycling)

Thunderbird

2 MW of power and 400 tons of cooling

Among the first HPCs with **hot aisle/cold aisle configuration**

First to use **cold-air containment** out of hot air balloon materials

Built-in subfloor contained air and the system utilized cold side control

Red Storm

First HPC in the United States to use **plug fan cooling** technologies

First time to use a **pressure differential:** CRAC units worked as one based on the computer's power consumption

First time utilizing **100 amp 208 power supply** to each computer

Red Sky/Red Mesa

NREL collaboration which installed first **240-volt system** with new power distribution units

First cooling door HPC system to use **134a liquid pumped refrigerant** and a laminar air flow configuration

Unique warm-air cooling system used entering air temperatures of 72°F, complemented by a **liquid-to-liquid heat-exchange system**

Pecos/Chama

Hot aisle containment system

Used the Thunderbird **air floor and power concept**, allowing minimal infrastructure cost to build out the system

Cayenne /Serrano

480 volt system with liquid cooling on the chip

Approximately **70 to 75°F entering water temperatures**

Valves in place for **energy reuse** from return water

Liquid cooling permits a small footprint

Sky Bridge

First HPC system to use **Asetek liquid cooling** on the chip (approximately 65 % of heat to direct internal cooling on the chip)

65 to 70°F entering water temperatures allowed for more free cooling (non-mechanical, no chillers) for an estimated 70% of the year.

First **480 volt system** with overhead buss system

Total operational annual **costs savings of up to 70%**

Total installation **cost savings of around 45%**

New cooling and power design decreased supporting infrastructure footprint by approximately **1000 sq. ft.** on the data room floor

ACME

Improving Predictive Climate Modeling on Evolving Computing Systems

The Accelerated Climate Modeling for Energy (ACME) project is a multi-lab effort to examine and attempt to answer impactful questions in three areas that drive climate change: the water cycle, biogeochemistry, and the cryosphere—the area of the earth where water exists as ice or snow. The goal of ACME is to develop and create a detailed climate and Earth system model. ACME addresses the most challenging and demanding climate change issues, such as how features important to the water cycle might affect river flow and watershed supplies. In addition, ACME will accelerate the development and application of fully coupled, state-of-the-science Earth system models for scientific and energy applications. In the development of Earth system and climate models, ACME seeks to provide leadership to the international scientific community.

Sandia's ACME team includes mathematicians, computer scientists, and software engineers who will lead the development of a comprehensive program for software engineering and computational performance of the system. Sandia will be applying a wide range of high performance computing approaches, including developing new algorithms specifically adapted to these architectures. Efficient computer use will enable users to model the many physical processes at the fidelity needed to answer ACME's questions.

One of the goals is to develop new features in the code by putting more software testing into place so that performance experts can make code modifications and be confident that they aren't changing the science in the process of optimizing the code. Sandia will incorporate computational mathematics libraries developed by DOE into ACME, such as those from the Trilinos project, for solving non-linear problems and performing load-balancing. Leveraging DOE's investment in these areas is one of ACME's strategies for obtaining the best possible performance on evolving computing systems to the exascale level.

As US computing capability moves toward exascale, ACME will improve predictive climate modeling and prepare the research community for a coming paradigm shift in computing architectures and programming models.

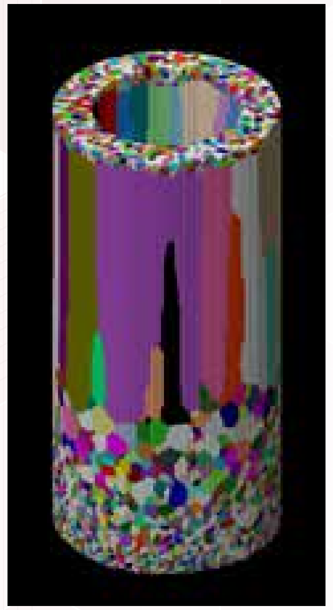
Uncertainty Qualification

Uncertainty Quantification is another specialty area where Sandia will contribute to ACME by identifying boundaries for uncertainties in prediction generated by land modeling, which focuses on the physical characteristics of vegetation, soil, and other terrestrial features at risk from climate change.

Advancing Exascale Computing

ACME's key computational mission is to develop an Earth system modeling capability that runs efficiently on DOE's upcoming pre-exascale and exascale supercomputers scheduled to be deployed at the two DOE Office of Science Leadership Computing Facilities—Oak Ridge National Laboratory and Argonne National Laboratory. The roadmap for these new computing architectures remains uncertain, but it is clear that each compute node will contain ever more processing elements with a more complex memory hierarchy requiring increased vectorization to improve performance. Adapting a complex model such as ACME to these new architectures requires a combination of changes such as new data structures, code refactoring, and new algorithms.

New subcomponents being developed for ACME are typically written in C++, which opens up more powerful abstractions for performance portability and code maintainability and a larger set of tools and libraries that can be leveraged for performance. A current example is the development of multi-moment semi-lagrangian transport scheme for both ocean and atmosphere, using Kokkos and Legion. Kokkos is a C++ array class that abstracts both the execution model and data layout. Legion is a programming model that facilitates task-based parallelism. These approaches will allow scientists and software engineers to more quickly adapt to new computing architectures, allowing them to focus more on how to translate ideas into software and less on the details of fast-changing computer hardware.



Scan with SNLSimMagic App to see our work come to life.

Predicted microstructure for a stainless steel cylinder fabricated using the Laser Engineered Net Shape Additive Manufacturing process demonstrating a transition from equiaxed to columnar grains. The thermal history was simulated in the Sierra multiphysics finite-element software suite and used as input for the microstructure prediction in SPPARKS, a kinetic Monte Carlo simulation code.

AM

Born Qualified: Process and Performance Modeling for Additive Manufacturing

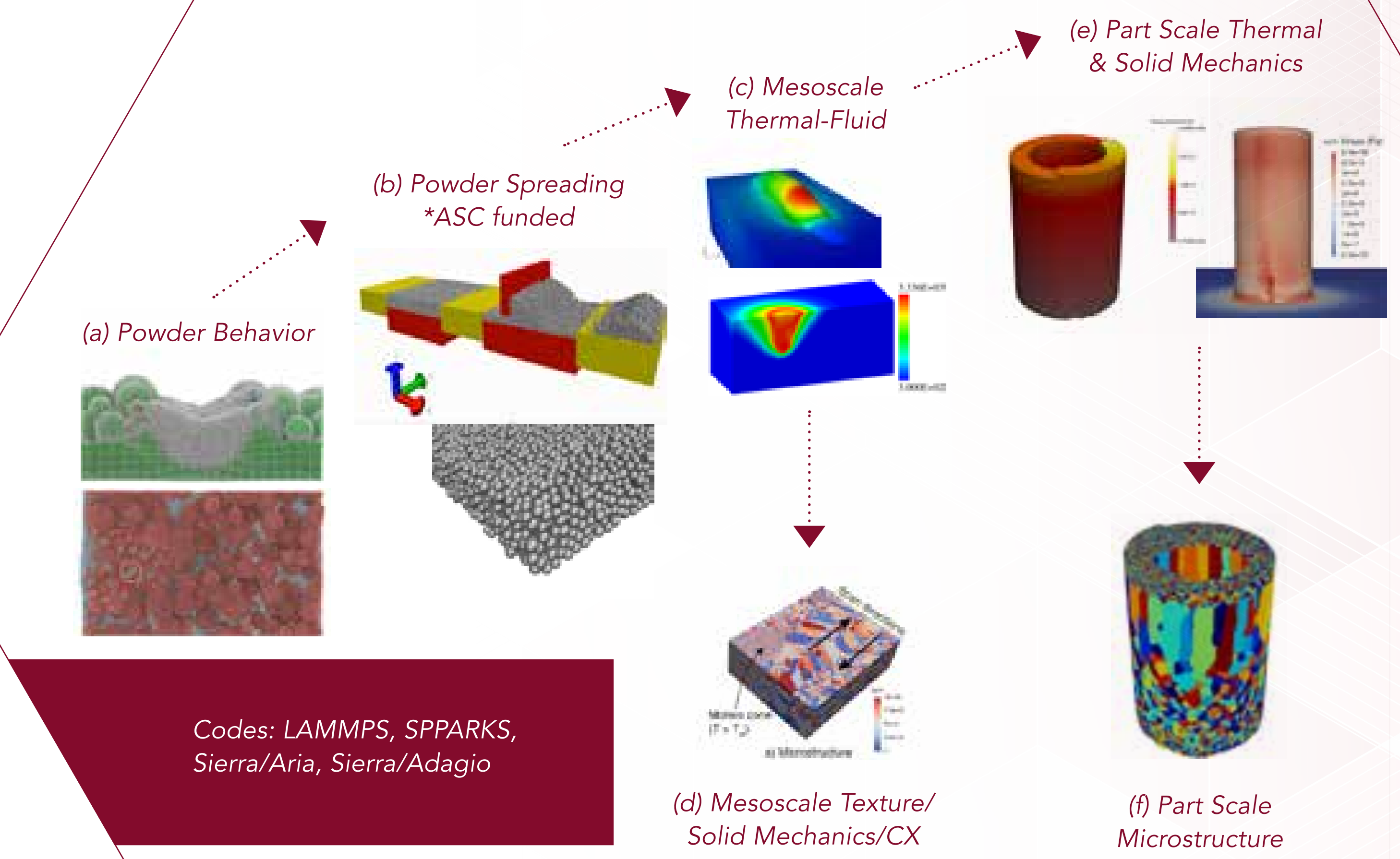
Additive Manufacturing (AM), sometimes referred to as 3D Printing, is a broad term that describes the fabrication of parts by the addition of material. Within the realm of metal AM, metal powder is typically melted by a laser heat source in a layer-by-layer fashion until the part is complete.

Born Qualified, an ongoing Laboratory Directed Research and Development (LDRD) Grand Challenge, revolutionizes component engineering design, manufacture, and qualification paradigms through the use of AM. The vision for this change lies in the development of a deep understanding of materials and processes by integrating validated, predictive capability with real-time and ex-situ diagnostics to realize uncertainty quantification-driven qualification of design and processes. Component level predictive modeling plays a crucial role in developing an understanding of the behavior in complex AM materials.

Modeling the metal AM process is challenging due to the long build times, high thermal gradients, and rapid, transient nature of the laser heat source. However, accurately modeling the AM process is key to predicting the process-structure-property-performance relationships necessary in a science-based qualification strategy. Sandia researchers have been able to model the thermal and mechanical history and resulting residual stress field in metal AM part production using the massively parallel SIERRA multiphysics software. The thermal results are also being used to predict grain structure and morphology in microstructure simulations performed in SPPARKS, a Kinetic Monte Carlo tool for predicting grain evolution. High performance computing capabilities at Sandia have allowed these simulations to be performed in a matter of hours rather than weeks, months, or even longer time periods that are problematic for conventional computing resources.

The goal for future work is to further increase modeling efficiency for larger parts and to use predictive modeling for process optimization to reduce defects and provide closed-loop feedback control for AM machines. This type of optimization will lead to improved part quality and reduced production time. With future next-generation platforms, models will likely become faster than real time part production and will accelerate part design, production, and qualification.

The AM Process



The AM process is being simulated at multiple length scales. (a and b) At the powder scale, molecular dynamics and discrete element methods are used to study powder particle flow and physical properties. (c and d) At the mesoscale, combined thermal-fluid simulations provide detailed meltpool information and surface shape. Microstructure simulations also give insight to solidification grain structures. (e and f) At the macroscale, simulations of full parts provide thermal histories and residual stress fields, along with microstructural effects on part performance.

B61-12

Using Modeling and Simulation to Complement Testing for Increased Understanding of Weapon Subassembly Response

As part of Sandia's nuclear deterrence mission, the B61-12 Life Extension Program aims to modernize the aging weapon system. Modernization requires requalification and Sandia is using high performance computing to perform advanced computational simulations to better understand, evaluate, and verify weapon system performance in conjunction with limited physical testing.

The Nose Bomb Subassembly (NBSA) of the B61-12 is responsible for producing a fuzing signal upon ground impact. The fuzing signal is dependent upon electromechanical impact sensors producing valid electrical fuzing signals at impact. Computer generated models were used to assess the timing between the impact sensor's response to the deceleration of impact and damage to major components and system subassemblies. The modeling and simulation team worked alongside the physical test team to design a large-scale reverse ballistic test to not only assess system performance, but to also validate their computational models. The reverse ballistic test conducted at Sandia's sled test facility sent a rocket sled with a representative target into a stationary B61-12 NBSA to characterize the nose crush and functional response of NBSA components. Data obtained from data recorders and high-speed photometrics were integrated with previously generated computer models to refine and validate the model's ability to reliably simulate real-world effects. Large-scale tests are impractical to conduct for every single impact scenario. By creating reliable computer models, we can perform simulations that identify trends and produce estimates of outcomes over the entire range of required impact conditions.

Sandia's HPCs enable geometric resolution that was unachievable before, allowing for more fidelity and detail, and creating simulations that can provide insight to support evaluation of requirements and performance margins. As computing resources continue to improve, researchers at Sandia are hoping to improve these simulations so they provide increasingly credible analysis of the system response and performance over the full range of conditions.

Scan with SNLSimMagic App to see our work come to life.

LOOKING FORWARD

The future of high performance computing at Sandia will bring innovation and scientific discovery to fruition through deep learning and exascale computing. A new facility will bring online more resources to meet increasing demand.

SYNAPSE

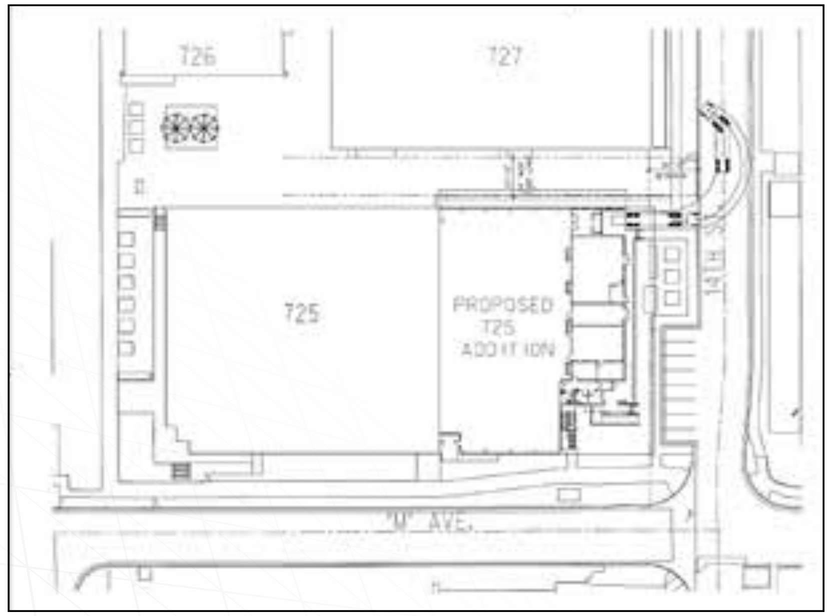
Sandia has recently invested in a new deep learning computing platform—adding a new capability to our institutional high performance computing program

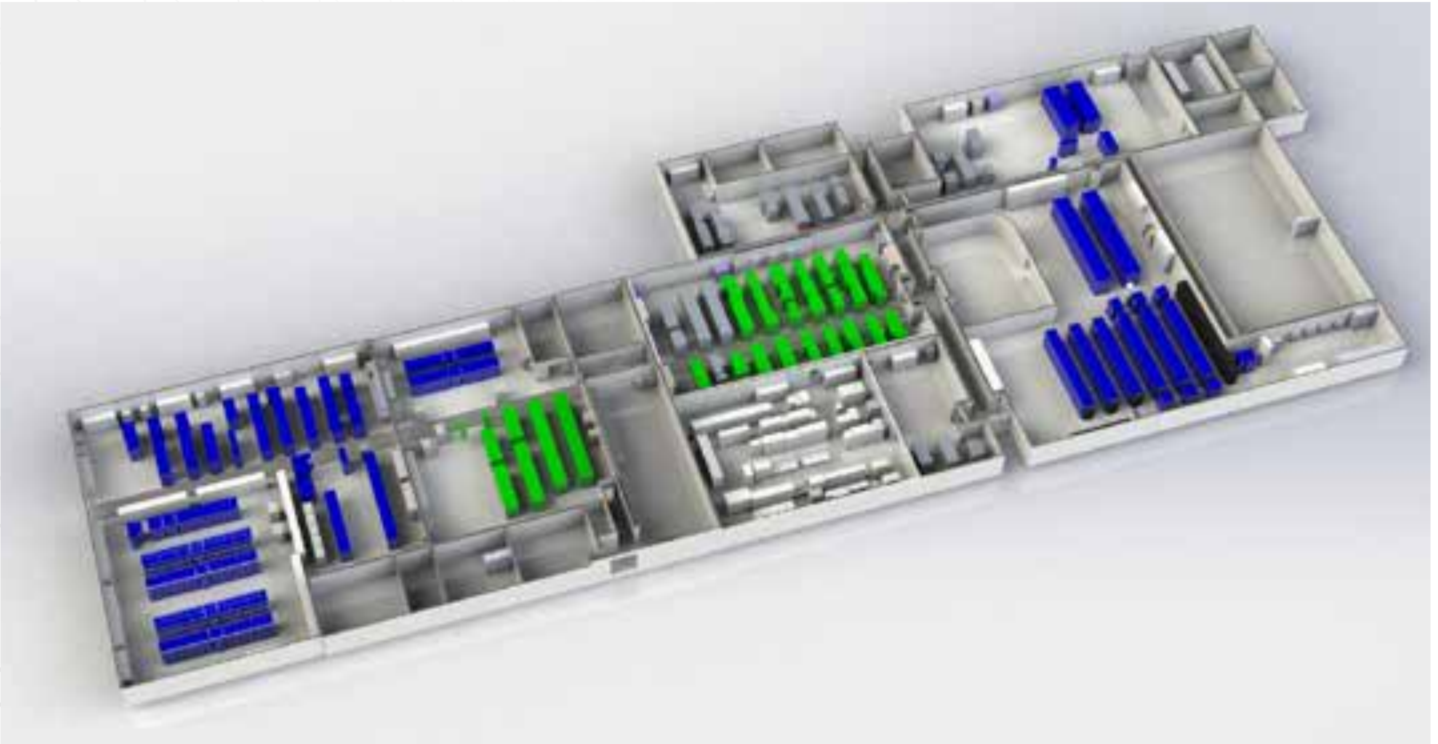
Whether it is voice recognition on your smartphone or recommendations based on recent purchases, machine learning and deep learning have become ubiquitous in our daily lives. Researchers at Sandia are developing deep neural networks to conduct analysis on large data sets from sensors, images, audio, and video to address national security challenges and high consequence decision making. For instance, researchers are developing deep learning models for high confidence identification of threats in radar imagery or for automatic detection of computer network anomalies. To support these research efforts, Sandia recently invested in Synapse, a new data analytics platform consisting of six NVIDIA DGX-1 nodes, as an institutional high performance deep learning solution.

Sandia's recent investment provides a powerful deep learning platform, with a total 48 Tesla V100 GPUs across six nodes. Prior to Synapse, deep learning research at Sandia was being conducted on modified desktops with one to two GPUs. With 48 GPUs in a single platform, Synapse increases productivity by speeding up the iterative process of training and developing deep learning models. Synapse supports several open source deep learning frameworks, including TensorFlow, Theano, CNTK, and others—allowing users to select the framework that best suits their model. Once a deep learning model is developed and refined on Synapse, it can be moved over to one of Sandia's data analytics clusters, Ray or Longfin, to conduct verification on large data sets.

By investing in Synapse, Sandia aims to broaden the impact of deep learning on our research and national security mission.

Synapse is currently being used to support Sandia's Open Threat Assessment Platform project, aimed at developing and demonstrating an open architecture baggage-screening prototype in support of Transportation Security Administration. Researchers applied convolutional neural networks to detect conventional explosives in luggage. Unlike other weapons, explosives can take on a variety of different shapes and are much harder to identify. Researchers used the material's response to x-rays to develop a threat recognition algorithm and then trained it to automatically identify threats from a database of x-ray images of luggage. Synapse enabled researchers to fully train and model in as little as 45 minutes—increasing their productivity and quickly delivering a model that could potentially improve the safety of commercial air travel.





BUILDING 725-E

Sandia's New Home for High Performance Computing

In 2012, Sandia established an Institutional Computing Program for procurement and operation of HPC platforms to support the rapidly growing labs-wide demand for high performance capabilities for research beyond nuclear weapons. Currently, the Sandia New Mexico site is home to a dozen HPC platforms, half of which were procured through the Institutional Computing Program. These platforms are currently housed alongside our enterprise resources and have shared infrastructure, such as cooling, networking, and power. Advanced HPC architectures have led to increased weight and power densities, more complex cooling requirements, and higher performing network and storage requirements. As the current building reaches capacity and resources become strained, it is becoming increasingly difficult to site new HPC platforms. To continue providing a reliable Labs-wide resource, it has become necessary to provide a separate dedicated facility for HPC platforms.

In 2017, Sandia broke ground on a new purpose-built high performance computing facility. The new building will sit next to the DOE's National Security Computing Center and will feature an inexpensive, flexible layout that can be easily extended to meet future needs. The new facility will feature a state-of-the-art liquid cooling system designed in partnership with the National Renewable Energy Laboratory, resulting in one of the most energy efficient facilities in use throughout DOE. The reapplication of excess power and cooling from the adjacent building will reduce construction costs. The new HPC center will have improved high-speed networking and remote access architectures, improving reliability for remote users.

725-East will house the first ASC ARM Exascale Prototype platform. Operational experience with this Vanguard system will inform Sandia, DOE/NNSA's ASC program, and the high performance computing community in general of the viability of an ARM exascale platform. The exascale prototype will be the largest computer ever sited at Sandia with expected performance around 20 Petaflops.

This new investment is another way in which Sandia's Institutional Computing Program is meeting the increased demands for high performance computing resources throughout Sandia and ensuring operational reliability and efficiency.

EXASCALE RISING

Exascale, the next challenge in high performance computing systems: machines capable of at least a billion, billion calculations per second or 50 to 100 times faster than the most powerful supercomputers in use today. The Exascale Computing Project (ECP) was established with the goals of maximizing the benefits of high performance computing, and accelerating the development of a computing ecosystem, encompassing applications, system software, hardware technologies, and architectures, and workforce development to meet the scientific and national security mission needs of the DOE by the early- to mid-2020s. ECP is chartered with breakthrough modeling and simulation solutions to address the most critical challenges in scientific discovery, energy assurance, and national security. The power of this new class of systems will be measured in exaflops, i.e., 10^{18} floating point operations per second, or a thousand times more powerful than today's petaflop machines.

The ECP's multi-year mission is to exploit the benefits of high performance computing, and to bolster US economic competitiveness, national security, and scientific discovery. ECP is not just a project to build extremely fast, large capacity computers: the project will foster innovation in hardware, software, platforms, and workforce development, essential to the effective development and deployment of future exascale systems.

ECP

EXASCALE COMPUTING PROJECT

Exascale at Sandia

Improved computer climate models of Earth's clouds and more accurate simulations of the combustion engine are goals for two projects led by Sandia funded in the first round of project awards from DOE's break-out $39.8 million Exascale Computing Project (ECP). Sandia will also conduct research with other laboratories on exascale projects whose goals range from developing physics models for more efficient wind energy production to improving understanding of materials at the molecular level, and simulating quantum mechanical effects in materials.

Sandia is providing ECP with leadership of the hardware technology investment strategy. These ECP investments are made with companies that support the US computing eco-system and are focused on architecture R&D at the node and system level with enough time to support co-design of future hardware designs. In June 2017, the DOE announced $258 million of architecture R&D contracts with AMD, Cray Inc., Hewlett Packard Enterprise, IBM, and Intel. These R&D contracts provide an opportunity for ECP's application development and software technology projects to impact future commodity computing components through collaborative co-design.

Sandia National Laboratories

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