

Advanced Simulation and Computing Campaign

Funding Schedule by Subprogram

	(dollars in thousands)		
	FY 2009 Actual	FY 2010 Current	FY 2011
	Appropriation	Appropriation	Request
Advanced Simulation and Computing Campaign			
Integrated Codes	138,917	140,882	165,947
Physics and Engineering Models	49,284	61,189	62,798
Verification and Validation	50,184	50,882	54,781
Computational Systems and Software Environment	156,733	159,022	175,833
Facility Operations and User Support	161,007	155,650	156,389
Total, Advanced Simulation and Computing Campaign	556,125	567,625	615,748

Outyear Funding Profile by Subprogram

	(dollars in thousands)			
	FY 2012	FY 2013	FY 2014	FY 2015
Advanced Simulation and Computing Campaign				
Integrated Codes	167,327	163,752	163,887	168,143
Physics and Engineering Models	66,541	65,019	64,626	66,438
Verification and Validation	54,168	52,879	52,300	53,835
Computational Systems and Software Environment	175,833	175,833	175,833	180,912
Facility Operations and User Support	159,071	158,774	158,774	163,806
Total, Advanced Simulation and Computing Campaign	622,940	616,257	615,420	633,134

Mission

The goal of the Advanced Simulation and Computing (ASC) Campaign is to provide leading edge, high-end simulation capabilities to meet weapons assessment and certification requirements including weapon codes, weapons science, computing platforms, and supporting infrastructure. The ASC Campaign serves as the computational surrogate for nuclear testing to determine weapon behavior.

As such, ASC simulations are central to our national security. Our ability to model the extraordinary complexity of nuclear weapons systems is essential to establishing confidence in the performance of our aging stockpile. The ASC tools enable comprehensive understanding of the entire weapons lifecycle, from design to safe processes for dismantlement. The ASC simulations play an essential role in simulating device performance to ensure that systems in the stockpile meet all specifications in the “stockpile-to-target sequence.” In the absence of testing, only through ASC simulations can the National Nuclear Security Administration (NNSA) determine the effects of changes to current systems, as well as calculate confidence levels of future untested systems.

The ASC tools are also used to address areas of national security beyond the U.S. nuclear stockpile. Through coordination with other government agencies, ASC plays an important role in supporting nonproliferation, emergency response, nuclear forensics and attribution activities. Resources have been used to characterize special nuclear material (SNM) and devices. The ASC simulation capabilities have been used by Department of Homeland Security (DHS) to assess various mitigation strategies, and the results have been published in peer-reviewed journals. There is a growing effort to enhance the

capabilities of these tools, such as the identification of a perpetrator or supporting state through forensic analysis of post-explosion radionuclide debris.

Benefits

The ASC Campaign is comprised of five subprograms that support activities in the areas of weapon codes, weapon science, computational infrastructure, and computing center operations. Each subprogram is a unique contributor to Governmental Performance and Results Act (GPRA) Unit Program Number 30.

The ASC Program's primary customer is Directed Stockpile Work (DSW). ASC codes and computing infrastructure are the means by which DSW work such as design, analysis, baselining, and Significant Findings Investigations (SFI) closure are performed. Stockpile work, science and simulation are bound together through the Predictive Capability Framework. In the context of simulation, predictive capability can best be understood in contrast to Baseline models that were based on the underground test results and which employed sophisticated approaches to interpolation within the underground data or minimal extrapolation. A predictive capability enables accurate simulations of device behavior outside the parameter space spanned by the underground test data. Historically, the codes were carefully calibrated to give results consistent with the diagnostics fielded in Nevada. As long as the calculated configurations were close to the as-tested regime, one could be confident in the results. When aging or flaws in the as-built reality are added into the mix, the simulations must depart from the parameter space spanned by the baseline. Then we must have recourse to models and numerical representations of the physics and engineering that capture reality. We must be able to simulate behavior, to predict responses and performance outside the range of the test data, the last of which were collected in 1992.

As an example of how ASC, the Campaigns and DSW work in a collaborative fashion to tackle problems of the national security enterprise (NSE) was when a significant fraction of the Red Storm compute time in FY 2008 was instrumental in planning a Navy operation to destroy an errant satellite, which posed a terrestrial threat if allowed to reenter the Earth's atmosphere in an uncontrolled manner. ASC provided the computational simulation technology and compute resources. The Engineering Campaign provided phenomenology experiments and diagnostics for sub-scale validation tests. DSW/STA funded the test hardware. Critical contributions from each of these programs resulted in a successful proof of concept, with rapid design and fabrication of prototype hardware. Conceptual design and testing of this hardware is now underway.

The Predictive Capability Framework (PCF) is an integrated roadmap that reflects the responsive scientific capabilities needed to deliver a predictive capability to the nuclear security enterprise. Participants of the PCF include Defense Science, ASC, Engineering, DSW Research & Development, and Inertial Confinement Fusion Ignition and High Yield Campaign. The PCF identifies a list of long-term integrated goals and links the progress in the predictive capabilities to the progress in the five enabling capabilities, four of which (theory/model capabilities, code/algorithm capabilities, computational facilities, and Quantification of Margins and Uncertainties (QMU) and Verification & Validation (V&V) capabilities) are developed by the ASC program. With the pending completion of major new experimental facilities and entry into peta-scale high performance computing, the PCF represents a new phase of science-based stockpile stewardship – one better aligned to the challenges of an aging and changing stockpile.

Additionally, the ASC program and the Office of Science recognize their common interests in computing and the need to begin exploration into the path toward exascale computing. Federal program managers have commissioned a Federal executive board and laboratory steering committee to develop a common plan on what it will take to achieve exascale computing by the end of the decade. Like the NSE laboratories, the Office of Science laboratories are key players in developing tools to make high-performance computing systems more usable and efficient. Therefore, the two organizations seek to form two institutes, the Institute for Advanced Architectures with Sandia and Oak Ridge, and the ABLE (Argonne, Berkeley, Livermore Exascale) Institute to capitalize on the expertise across the complex in advanced systems and computational sciences. The ASC program is also engaged in the SciDAC (Scientific Discovery through Advanced Computing) program to capitalize on the Office of Science investments in new science advanced by academia and other laboratories.

Annual Performance Results and Targets

(R = Results; T = Target)

Performance Indicators	FY 2006 Results	FY 2007 Results	FY 2008 Results	FY 2009 Results	FY 2010	FY 2011	FY 2012	FY 2013	FY 2014	FY 2015	Endpoint Target
<p>Secretarial Goal: Security: Reduce nuclear dangers and environmental risks GPRA Unit Program Number: 30, Advanced Simulation and Computing Campaign</p>											
<p>Adoption of ASC Modern Codes: The cumulative percentage of simulation runs that utilize modern ASC-developed codes on ASC computing platforms as measured against the total of legacy and ASC codes used for stockpile stewardship activities. (Long-term Outcome)^a</p>	R: 50%	R: 63% T: 63%	R: 72% T: 72%	R: 80% T: 80%	T: 85%	T: 90%	T: 95%	T: 100%	N/A	N/A	By 2013, ASC-developed modern codes are used for all simulations on ASC platforms. Adoption of Modern ASC Codes will enable a responsive simulation capability for the nuclear security enterprise. This measure is meant to show how quickly ASC codes are being adopted by the user community in place of legacy codes.
<p>Reduced Reliance on Calibration: The cumulative percentage reduction in the use of calibration “knobs” to successfully simulate nuclear weapons performance. (Long-term Outcome)^a</p>	R: 2%	R: 8% T: 8%	R: 16% T: 16%	R: 25% T: 25%	T: 30%	T: 35%	T: 40%	T: 45%	T: 50%	T: 55%	By 2024, several major calibration knobs affecting weapons performance simulation have been replaced by science-based, predictive phenomenological models. Reduced reliance on calibration will ensure the development of robust ASC simulation tools, These tools are intended to enable the understanding of the complex behaviors and effect of nuclear weapons, now and into the future, without nuclear testing.
<p>ASC Impact on SFI Closure: The cumulative percentage of nuclear weapon Significant Finding Investigations (SFIs) resolved through the use of modern (non-legacy) ASC codes, measured against all codes used for SFI resolution. (Long-term Outcome)^a</p>	R: 10%	R: 25% T: 25%	R: 37% T: 37%	R: 50% T: 50%	T: 60%	T: 65%	T: 70%	T: 80%	T:85%	T:100%	By 2015, ASC codes will be the principal tools for resolution of all SFIs. This demonstrates how valuable the ASC tools are for meeting the needs of the weapon designer’s analysts by documenting the impact on closing SFIs.

Performance Indicators	FY 2006 Results	FY 2007 Results	FY 2008 Results	FY 2009 Results	FY 2010	FY 2011	FY 2012	FY 2013	FY 2014	FY 2015	Endpoint Target
<u>Code Efficiency: The cumulative percentage of simulation turnaround time reduced while using modern ASC codes. (Efficiency)^a</u>	R: 6%	R: 7% T: 7%	R: 13% T: 13%	R: 13% T: 13%	T: 15%	T: 20%	T: 27%	T: 34%	T: 42%	T: 50%	<u>By 2015, achieve a 50% reduction in turnaround time, as measured by a series of benchmark calculations, for the most heavily used ASC codes. To show code efficiency by demonstrating that simulation time decreases as the ASC codes mature.</u>

FY 2009 Accomplishments

Predictive Capability

- There has been a consistent annual increase in the cumulative percentage of simulation runs that utilize modern ASC-developed codes on our computing platforms as measured against the total of legacy codes used for stockpile stewardship activities. Current target is for 80 percent of these problems to be run with modern codes.
- An ASC tri-lab team completed a multiyear effort to identify and develop verification test problems to assess the numerical performance of models and algorithms implemented in ASC codes to demonstrate whether the numerical results of the discretization algorithms in physics and engineering simulation codes provide correct solutions of the corresponding continuum equations.
- Large, fully resolved simulations of turbulence mixing have exercised the ASC Program's scientific and computational science capabilities, revealing new and unexpected physics in the study of mixing.

Simulation for the Stockpile

- The ASC program's Red Storm supercomputer at SNL was instrumental in planning a Navy operation to destroy an errant satellite, which posed a terrestrial threat if allowed to reenter Earth's atmosphere in an uncontrolled manner.
- The Los Alamos forensics team successfully identified a device in a blind nuclear forensics exercise organized by Nuclear Weapons Incidence Response's Office of Emergency Response and the Defense Threat Reduction Agency in October 2008. This success was enabled by use of validated Los Alamos ASC codes and new metrics to guide identification of the device technology.
- Sandia's SIERRA software was used to simulate the first ever T-bone crash at 55mph involving two Safe Guards Tractor/Armored Trailer vehicles. This study leveraged ASC computers and codes to study a broader class of National Security applications beyond traditional weapons performance assessments.

High-Performance Computer Platforms

- DAWN, the initial delivery system of the Sequoia contract, was delivered to Livermore on March 27. The equipment for this 500 teraflop BlueGene/P system was fully delivered, installed, configured, and executed via a synthetic workload all in well under 3 months.
- The ROADRUNNER petascale machine was delivered to LANL in 2008, becoming the first supercomputer capable of sustained 1 petaFLOPS performance. In 2009, 10 Open Science projects were chosen from 29 proposals to use Roadrunner during system and code stabilization phase.

ASC Collaborations

- ASC and the Advanced Scientific Computing Research (ASCR) program in the Office of Science are currently working out a research, development and engineering collaboration to usher in Exascale computing at the end of the new decade.
- ASC established the NNSA Alliance for Computing at Extreme Scale (ACES) institute between LANL and SNL, devoted to providing high performance capability computing assets required by NNSA's stockpile stewardship mission. SNL and ORNL are also collaborating through the Institute for Advanced Architectures and Algorithms (IAA), aimed at maintaining our global leadership in Science and Technology, and future competitiveness.

Major Out-year Priorities and Assumptions

The outyear projections for the Advanced Simulation and Computing (ASC) Campaign total \$2,487,751,000 for FY 2012 through FY 2015. Simulation is pervasive throughout the nuclear weapons enterprise. ASC will continue to support annual assessments, certification, and SFI resolution through provision of simulation codes and high-performance computing resources. Replacement of older institutional models with more physics-based representations will take place. The laboratories will continue incorporation of verification and validation activities into software development and simulation that will move the existing culture toward an environment that considers Quantification of Margins and Uncertainties. Final deliveries of existing platforms procurements will take place.

The out-year funding profile will enable a stronger simulation program and inject a renewed scientific rigor back into the program essential to supporting the implementation of the Comprehensive Test Ban Treaty (CTBT). Developing robust peer review among the national security laboratories as we move away from the test base is essential to the continued pursuit of CTBT. Comprehensive uncertainty quantification calculations in 3D will provide the confidence necessary to make reliable progress toward the predictive capability necessary to address stockpile aging issues. In the next decade, predictive capability and DSW simulation deliverables will demand ever more powerful and sophisticated simulation environments. This request will position the national security laboratories to take advantage of future platform architectures to more efficiently steward the stockpile.

Detailed Justification

(dollars in thousands)

FY 2009	FY 2010	FY 2011
138,917	140,882	165,947

Integrated Codes (IC)

This subprogram primarily addresses the improvement of weapons system simulations to predict, with reduced uncertainties, the behavior of devices in the stockpile. It also enables analysis and design for future warhead modifications and stockpile options. The products of this subprogram are the large-scale integrated simulation codes that are needed for Stockpile Stewardship Program (SSP) maintenance, the Life Extension Program (LEP), Significant Finding Investigation (SFI) closure, and a host of related requirements, including dismantlements. Specifics include the maintenance of the legacy codes; continued research into engineering code applications and manufacturing process codes; investigation and development of future non-nuclear replacement components; algorithms, computational methods and software architectures; advancement of key basic research initiatives; and explorations into emerging code technologies and methodologies. This subprogram also includes university partnerships that foster continued collaborations such as the Predictive Science Academic Alliances Program (PSAAP) and Computational Science Graduate Fellowship (CSGF) Program. The functional and performance requirements of this subprogram are established by designers, analysts, and code developers. It also relies upon the Physics and Engineering Models subprogram for the development of new models to be implemented into the modern codes. The subprogram also engages the Verification and Validation (V&V) subprogram in assessing the degree of reliability and level of uncertainty associated with the outputs from the codes.

The FY 2011 activities include the following: develop coupled multi-physics capabilities for device simulation based on scientific representation of device behavior with a reduced reliance on calibration to underground test data; produce more accurate numerical methods for treating complex geometries in 2-D and 3-D computer codes; develop the capability to simulate effects of replacement components and analyze various Stockpile-to-Target Sequence scenarios and modifications; accelerate code performance through more powerful numerical algorithms and improved approximations; maintain interactions with academic colleagues in computer science, computational mathematics, and engineering; conduct basic research relevant to the ASC Campaign in computer science, scientific computing, and computational mathematics; and continued support of the CSGF program.

The request supports the code development at the level needed for robust peer review as we move to support the implementation of the Comprehensive Test Ban. The request assures viable programs at both physics labs to fully support peer review for refurbishments, SFIs, modifications, and annual assessments as deemed necessary by the Subject Matter Experts (SMEs). It also positions the code developers to efficiently and effectively execute the ASC Code strategy for a rich, sustainable portfolio of simulations codes for the Complex.

The age of our stockpiled weapons and the dearth of designers with test experience in the NSE make it a National imperative that we maintain the technical expertise, apply scientific rigor to the code development process, and understand the physical processes that are being modeled.

(dollars in thousands)

FY 2009	FY 2010	FY 2011
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Physics and Engineering Models (PEM)

49,284 61,189 62,798

This subprogram develops microscopic and macroscopic models of physics and material properties, improved numerical approximations of transport, and models for the behavior of other critical phenomena. This subprogram is charged with the development, initial validation, and incorporation of new models into the Integrated Codes. Therefore, it is essential that there be a close interdependence between these two subprograms. There is also extensive integration with the experimental programs of the SSP, mostly funded and led by the Science Campaign.

The FY 2011 activities include: develop and implement the Equation of State and constitutive models for materials within nuclear devices; improve understanding of phase diagrams and the dynamic response of materials; continue physics-based modeling for plutonium aging; explore fundamental chemistry models of high explosives; improve representation of corrosion, polymer degradation, and thermal-mechanical fatigue of weapons electronics; improve models of melting and decomposition of foams and polymers in safety-critical components; support of the Stockpile-to-Target-Sequence requirements by improving models of microelectronic and photonic materials in hostile environments.

The request supports a model development portfolio for scientific exploration in key areas towards achieving predictive simulation capability including: plutonium aging, nuclear physics, atomic physics, equation of state, materials, high explosives, mix and burn, engineering performance.

Verification and Validation (V&V)

50,184 50,882 54,781

This subprogram provides a rigorous, defensible, scientifically based measure of confidence and progress in predictive simulation capabilities. The V&V subprogram applies systematic measurement, documentation, and demonstration of the ability of the codes and the underlying models in various operational states and functional regimes to predict behavior. V&V is developing and implementing Uncertainty Quantification (UQ) methodologies as part of the foundation to the QMU process of weapons assessment and certification. V&V also drives software engineering practices to improve the quality, robustness, reliability, and maintainability of the codes that evaluate and address the unique complexities of the stockpile.

In FY 2011, V&V will focus on UQ assessments that include: integral V&V assessment; catalog of Top Adjustable Parameters in Weapons Physics Simulations; expansion of the Primary Metric Project test suites to include more relevant Nevada Test Site events; and development of first events of the Secondary Calculational Assessment Methodology Project.

In light of the QMU methodology put forth by the NNSA to be applied to annual assessments, we must have a healthy V&V program to perform UQ. More generally, as nuclear test data is becoming less relevant with an aging stockpile and as weapons designers with test experience leave the complex, it becomes increasingly important that the codes of the complex are verified and validated so future generations of designers are comfortable relying on these foundational tools.

(dollars in thousands)

FY 2009	FY 2010	FY 2011
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Computational Systems and Software Environment (CSSE)

156,733 159,022 175,833

CSSE builds integrated, balanced and scalable computational capabilities to meet the predictive simulation requirements of the NNSA. It strives to provide users of ASC computing resources a stable and seamless computing environment for all ASC-deployed platforms. The complex and diverse demands of the ASC performance and analysis codes and the scale of the required simulations require the ASC Campaign to be far in advance of the mainstream high-performance computing community. To achieve its predictive capability goals, the ASC Campaign must continue to invest in and consequently influence the evolution of computational environments. The CSSE provides the stability that ensures productive system use and protects the large investment in simulation codes.

A balanced and stable computational infrastructure is a key enabling technology for delivering the required computing capabilities. Along with the powerful capability, capacity and advanced systems that the campaign fields, the supporting software infrastructure that is deployed on these platforms include many critical components, from system software and tools, to Input/Output (I/O), storage and networking, post-processing visualization and data analysis tools, to common computing environments. The immediate focus areas include moving toward a more standard user environment and improving its usability, deploying more capacity computational platforms, planning for and developing peta-scale computing capability, and making strategic investments to meet program requirements at an acceptable cost.

The FY 2011 activities include continuing acquisition of Sequoia at LLNL and Zia at LANL (with SNL) and beginning acquisition of capacity systems through TLCC II. Maintenance will continue on LANL's Roadrunner and the Sequoia Initial Delivery (ID) system at LLNL. ASC will continue to operate high-performance capacity computing scalable units to meet growing demands especially in the area of modern (QMU-based) weapons certification and assessment. CSSE will also maintain a common, usable, and robust application-development and execution environment for ASC-scale applications and platforms; produce an end-to-end, high-performance I/O, networking-and-storage archive infrastructure encompassing ASC Campaign platforms and operating systems, large-scale simulations, and data-exploration capabilities. ASC will provide a reliable, available, and secure environment for distance computing through system monitoring and analysis, modeling and simulation, and technology infusion. Development and deployment will continue on high-performance tools and technologies to support visual and interactive exploration of massive and complex data. The Campaign will provide system management of the ASC Campaign computers and their necessary networks and archival storage systems. This includes the deployment of effective data management, extraction, delivery, and archiving, as well as efficient remote or collaborative scientific data exploitation. Continued development and deployment of scalable data manipulation and rendering systems that leverage inexpensive, high performance commodity graphics hardware will continue. Additionally, ASC will stimulate research and development efforts through advanced architectures that explore alternative computer designs, promising dramatic improvements in performance, scalability, reliability, packaging, and cost.

(dollars in thousands)

FY 2009	FY 2010	FY 2011
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The request will permit the acquisition of 25 percent to 30 percent more computational resources to be applied to capability class problems, jobs that use a major portion of the system. Similarly, demand for capacity class resources, those problems which require smaller jobs but a higher number of runs, has exceeded planned capacity platform acquisitions. The request will be used to procure an additional 15 percent to 20 percent more computing resource capacity.

Facility Operations and User Support **161,007** **155,650** **156,389**

This subprogram provides necessary physical facility and operational support for reliable production computing and storage environments as well as a suite of services enabling effective use of ASC Tri-Laboratory computing resources. Facility operations include planning, integration and deployment, continuing product support, software license and maintenance fees, procurement of operational equipment and media, quality and reliability activities and collaborations. Facility Operations also covers physical space, power and other utility infrastructure, and Local Area Network/Wide Area Networking for local and remote access, as well as requisite system administration, cyber-security and operations services for ongoing support and addressing system problems.

The scope of the User Support function includes planning, development, integration and deployment, continuing product support, and quality and reliability activities collaborations. Projects and technologies include computer center hotline and help-desk services, account management, web-based system documentation, system status information tools, user training, trouble-ticketing systems, and application analyst support.

The FY 2011 activities maintain continuous and reliable operation and support of production computing systems and all required infrastructure to operate these systems on a 24-hour a day, 7-day a week basis, with an emphasis on providing efficient production quality stable systems. Facility Operations operate laboratory ASC computers and support integration of new systems ensuring that the physical plant has sufficient resources, such as space, power, and cooling, to support future computing systems. User Support provides the authentication and authorization services used by applications for the purposes of remote access and data movement across ASC-related locations. ASC will also develop and maintain a wide-area infrastructure (e.g., links and services) that enable remote access to ASC applications, data, and computing resources, to support computational needs at the plants permitting distant users to operate on remote computing resources as if they were local. The subprogram will provide analysis and software environment development, support for ASC laboratory computers and provide user services and helpdesks for ASC laboratory computers.

Total, Advanced Simulation and Computing Campaign **556,125** **567,625** **615,748**

Explanation of Funding Changes

FY 2011 vs. FY 2010 (\$000)

Integrated Codes

The increase funds code development for robust peer review as we move away from the test base. This is necessary to assure viable programs at both physics labs to support adequate peer review.

+25,065

Physics and Engineering Models

The increase supports a model development portfolio for scientific exploration in key areas - including plutonium aging, nuclear physics, atomic physics, equation of state, materials, high explosives, mix and burn, engineering performance - towards achieving predictive simulation capability.

+1,609

Verification and Validation (V&V)

The increase will address uncertainty quantification (UQ) and individually addressing the key factors contributing to simulation uncertainties.

+3,899

Computational Systems and Software Environment

The increase supports capability and capacity computing to restore predictive simulation and computing capabilities necessary for viable, stockpile programs at both physics laboratories.

+16,811

Facility Operations and User Support

The slight funding increase will ensure continued reliable operation and support of production computing systems and all required infrastructure to operate these systems on a 24-hour a day, 7-day a week basis, with an emphasis on providing efficient production quality stable systems.

+739

Total Funding Change, Advanced Simulation and Computing Campaign

+48,123

Capital Operating Expenses and Construction Summary

Capital Operating Expenses^b

(dollars in thousands)

	FY 2009	FY 2010	FY 2011
General Plant Projects	4,388	4,485	4,584
Capital Equipment	47,395	48,438	49,504
Total, Capital Operating Expenses	51,783	52,923	54,088

Outyear Capital Operating Expenses

(dollars in thousands)

	FY 2012	FY 2013	FY 2014	FY 2015
General Plant Projects	4,685	4,788	4,893	5,001
Capital Equipment	50,593	51,706	52,844	54,007
Total, Capital Operating Expenses	55,278	56,494	57,737	59,008

