2015
BUSINESS PLAN
ADVANCED SIMULATION AND COMPUTING

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2015 BUSINESS PLAN

ADVANCED SIMULATION AND COMPUTING

ACKNOWLEDGEMENTS

Senior advisors to the ASC Program are expected to have a deep knowledge and understanding of the program, and Hans Ruppel and Charlie Slocomb certainly have that. Their wisdom and insight into the various aspects of the ASC Program were instrumental in the drafting of both the *ASC Business Model 2005* and *Business Plan 2015*. Besides their technical expertise, they lent diligence, attention to detail, and a strong desire to complete a useful product. They were a pleasure to work with and their contribution to this project and the ASC Program as a whole is greatly appreciated.

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EXECUTIVE SUMMARY

For as long as nuclear weapons exist, the U.S. will maintain a stockpile that is safe, secure, and effective. To do so, it will need a credible program to assess the systems in the stockpile and certify that they will work as expected. The Advanced Simulation and Computing (ASC) Program—referred to as the ASC Program—has the responsibility to provide the simulation tools that make possible the nation's nuclear deterrence in the absence of full-system nuclear weapons tests. This document describes the structure of the ASC Program and the relationship between its components. At its core, the ASC Program is a science-based endeavor that has integrated successfully a deep understanding of the details of nuclear weapons safety and performance with surrogate numerical experiments enabled by a powerful computing infrastructure.

To maintain a credible nuclear weapons program, the National Nuclear Security Administration's (NNSA's) Office of Defense Programs (DP) needs to make certain that the capabilities, tools, and expert staff are in place and are able to deliver validated assessments. This requires a complete and robust simulation environment backed by an experimental program to test ASC Program models. This *ASC Business Plan* document encapsulates a complex set of elements, each of which is essential to the success of the simulation component of the Nuclear Security Enterprise. The *ASC Business Plan* addresses the hiring, mentoring, and retaining of programmatic technical staff responsible for building the simulation tools of the nuclear security complex. The *ASC Business Plan* describes how the ASC Program engages with industry partners—partners upon whom the ASC Program relies on for today's and tomorrow's high performance architectures. Each piece in this chain is essential to assure policymakers, who must make decisions based on the results of simulations, that they are receiving all the actionable information they need.

The ASC Program nurtures its staff and encourages innovation; continues to improve its understanding of the archival test data; fully supports small-scale experimental efforts; enhances its alliances with the larger scientific community; and plans for and influences the development of computing technologies of the future, including meeting future power needs and providing supporting facilities.

The ASC Program continually works to meet national needs—economically, efficiently, and within the bounds set by Congress—to assure those who provide the resources that their funds are well invested. The *ASC Business Plan* explicitly details the way the elements of the ASC Program fit together to ensure a continued successful response to a critical national security need.

FOUNDATION

ASC DELIVERS TOOLS AND CAPABILITIES

The *ASC Business Plan* articulates the programmatic design for the successful delivery of the tools and capabilities required to simulate the behavior of a nuclear device in the absence of full-scale testing, thus meeting the requirements of the user community and DP's overall nuclear security needs. The plan includes the components and functions of the Nuclear Security Enterprise and reflects changes to the funding profile as set by the Administration and Congress.

The *ASC Business Plan* identifies the context in which the ASC Program exists and derives its mission and the customers it seeks to support. It highlights the management structure, the roles and responsibilities of those making decisions and allocating NNSA Headquarters' (HQ) resources, and the technical management and execution of work plans at the three NNSA national security laboratories (Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Sandia National Laboratories (SNL).

The *ASC Business Plan* ensures those who contribute to the ASC Program, from HQ to site offices to national laboratories and plants, that there is a shared common understanding of the way the ASC Program works. It explains at a high level the components of the ASC Program and describes how those components operate together to form a national program. It articulates the managerial roles and responsibilities of HQ and the laboratories in service of the national program. It describes the elements necessary to succeed.

The *ASC Business Plan* helps people across the Department of Energy (DOE), NNSA, the Office of Management and Budget, and in Congress understand the ASC Program. It features the collection of tools, processes, and responsibilities of ASC Program elements and documents how the actions and activities funded by the ASC Program are strategically planned and compliant with NNSA direction and coordination. The *ASC Business Plan* demonstrates that the ASC Program is well planned and pursues its mission in a cost-effective manner while aligning ASC Program and laboratory priorities with national priorities.

Guiding principles

The ASC Program's guiding principles include:

- The ASC Program is a national program.
- The ASC Program is responsible for providing future stockpile-related simulation and computing capabilities.
- Requirements from Direct Stockpile Work, Life Extension Programs (LEPs), Science and Engineering programs, Nuclear Counterterrorism, and other related national programs drive the ASC Program and its associated budgets.

- The ASC Program is defined by a single work breakdown structure that is incorporated into the DOE Budget and Reporting Codes (B&R) system.
- The ASC Program is a Federally managed and coordinated program, with primary responsibility for execution assigned to the NNSA national security laboratories.
- Efficient management requires coordination and collaboration with other government agencies, particularly those with high performance computing (HPC) programs.
- Resource allocation in support of the ASC Program is informed by the right-sizing process, data collected on computer utilization, and other external requirements.
- Periodic reviews of the technical and administrative activities hold the participants accountable for their part of the ASC Program.

Business decisions

The ASC Program has evolved from its beginning in 1996 as the Accelerated Strategic Computing Initiative (ASCI) and the Stockpile Computing Program. The ASC Program reflects major business decisions made over the past years that now form the bedrock of the current ASC Program. These decisions include:

- A governance model based on a decision-making structure that involves the Federal program manager (director) making major decisions, in consultation with ASC Program executives at the three NNSA national security laboratories
- Resources for the three NNSA national security laboratories to ensure there are multiple approaches to solving the critical and difficult nuclear weapons design and engineering issues, which in turn ensures a peer review process that examines in detail the classified work and provides for disaster recovery and backup consistent with the classified nature of the work
- Development and application of separate integrated nuclear weapons design codes at each design laboratory as opposed to a single integrated nuclear weapons design code shared by both laboratories, to allow distinct physics models and numerical techniques and enable a form of risk reduction that avoids a single approach to complex simulations and greatly strengthens inter-laboratory reviews of results
- A portfolio of supercomputers at the NNSA national security laboratories:
  - Advanced technology (AT) systems, which represent the leading edge of HPC, are procured and sited at the two design laboratories on an alternating basis to ensure the nuclear weapons enterprise has the computing power needed to address the most demanding and complex problems associated with stockpile reliability. Use of these AT systems is managed through a formal proposal process run by the laboratories. The software engineers who are focused on developing techniques to take advantage of the advanced hardware in these machines and the porting of integrated codes to these machines are also given resources on the AT systems.
  - Commodity technology (CT) systems at all three laboratories are maintained and periodically refreshed to ensure a sufficient computing resource is available for everyday computing while also lessening risk in the event that one laboratory experiences a sustained outage. Time on CT systems is allocated by each laboratory according to local priorities, but there are no constraints on the size of the problems. Allocations permit both long runs of the integrated codes and short proof-of-principle calculations with codes that were developed specifically for research and enhanced understanding.
- ASC Program interaction and targeted investment in the vendor community to ensure future hardware platforms and software systems meet ASC Program needs
- Allocation of resources by HQ in conjunction with ASC Program executives at the laboratories to assure the ASC Program is appropriately balanced across all subprogram elements
- Academic community engagement through research programs at selected universities designed to advance the simulation sciences and engage scientific skills related to the NNSA mission

UNDERSTANDING THE ASC PROGRAM

WITHIN THE NATIONAL STOCKPILE STEWARDSHIP PROGRAM

NNSA's mission[1] is to enhance national security through the military application of nuclear weapons science, with responsibilities encompassing several areas:

- Maintaining the safety, security, and effectiveness of the nation's nuclear deterrent without nuclear testing
- Strengthening key science, technology, and engineering capabilities and modernizing the national security infrastructure
- Providing the critical simulation tools for national nuclear security interests in all security arenas
- Reducing global nuclear security threats
- Providing safe and effective integrated nuclear propulsion systems for the U.S. Navy

A key Stockpile Stewardship Program (SSP) strategy is to understand the various environments (normal, hostile, abnormal) and their potential impacts on weapons performance. These environments impose thermal, mechanical, and radiation loads that engineering models and experiments must address. Nuclear weapons are subject to aging during the decades between manufacture and retirement. This degree of aging was not originally expected nor factored into the initial design. These aging effects must be taken into consideration when assessing the reliability of safety systems and the ability of weapons to meet the requirements of the stockpile-to-target sequence. The SSP relies upon complementary approaches including theory, experiment, and simulation to understand how the nuclear weapons are impacted by these environments.

The experimental facilities that were built since 1992 in support of the SSP include the Dual-Axis Radiographic Hydrodynamic Test (DARHT) facility at LANL, the National Ignition Facility (NIF) at LLNL, the U1a Complex at the Nevada National Security Site (NNSS), and the Microsystems and Engineering Sciences Applications (MESA) facility at SNL. These and other capabilities have improved surveillance and maintenance of the existing stockpile and have provided methods and data to close significant finding investigations (SFIs). The quality and resolution of the data from these facilities and capabilities were and continue to be unprecedented; the data obtained are used to benchmark new physics models in the integrated codes and augment the archival test data used to develop the integrated codes. Facilities existing prior to 1992, such as the Z pulsed power facility, the Los Alamos Neutron Science Center, Saturn, the High Explosives Applications Facility, the Contained Firing Facility, and the High-Energy Radiation Megavolt Electron Source III, have been maintained and upgraded and continue to make essential contributions.

1 *Fiscal Year 2016 Stockpile Stewardship and Management Plan*, chapters 1 and 3, March 2015.

These experimental facilities are essential to validate the models that underlie the integrated codes upon which stockpile stewardship must rely. The simulation capability for the SSP is fully delivered by the ASC Program. ASC Program integrated codes serve as the computational surrogate for full-system testing to predict weapon environments, weapons effects, performance, and safety. Moreover, the ASC Program depends heavily on the understanding, experience, and data gained through Directed Stockpile Work (DSW) and Science Programs and benefits from collaboration with DOE's Office of Science (SC) for Advanced Scientific Computing Research (ASCR).

In coordination with other government agencies, the ASC Program supports nonproliferation, emergency response, nuclear forensics, and attribution activities. ASC Program resources are used to identify the special nuclear materials used to characterize devices via post-detonation analysis.

Contributions to stockpile stewardship

The *ASC Business Plan* describes the ASC Program's commitment to the design, analysis, and engineering communities to provide simulation tools and computing resources to assess the state of the nuclear stockpile and to assist in ensuring its continued safety and reliability. This is achieved by accomplishments in four major areas:

- Development of the integrated codes and models that simulate and analyze the behavior of a nuclear device through all stages, from manufacturing, storage, and delivery to detonation
- Acquisition and fielding of the computing infrastructure and attendant software systems
- Operation of laboratory computing centers
- Partnership with the broader scientific community in areas of importance to the ASC Program

The ASC Program has repeatedly demonstrated its ability to provide necessary tools to the SSP's overall nuclear security mission, including:

- Simulation and computing capability usable by designers and analysts and relevant to their stockpile work scope
- Improved physics fundamentals for the integrated codes based upon insights derived from NNSA national security laboratories' research (at times, this improved physics understanding comes from work performed outside of the national security laboratories, such as the other DOE national laboratories and universities)
- Industry-provided HPC systems adapted to meet stockpile stewardship needs

Computing facilities enable new levels of detail in modeling and, thus, deeper scientific insight through the computing power they provide.

Customers

Just as in business, it is critical in a capability- or tool-producing organization to know who the customers are for its products and services. There are three classes of customers who use or consume products and/or services provided by the ASC Program: customers internal to NNSA, external customers related to stockpile stewardship work scope, and external customers related to national security beyond the stockpile.

The internal-to-NNSA customer includes those within the SSP who maintain the stockpile and other components of the SSP. Designers and analysts rely on the capabilities and tools of simulation and computing to assess the performance of nuclear weapons as they conduct SFIs, develop LEPs, and consider advanced safety and surety features. Continued analysis of the archived data from over one thousand full-system tests takes advantage of the modern integrated codes to provide new insights into these tests. Scientists are achieving new understanding of test results that was not possible at the time of the tests, allowing for the resolution of historically unresolved anomalies.

Experimentalists rely on the ASC Program tools and capabilities to plan, design, and evaluate experiments. A major example of this is the Inertial Confinement Fusion (ICF) effort to achieve ignition with laser-driven imploding capsules.

The external stockpile stewardship customer includes the Department of Defense (DOD), who relies upon the assurances from simulations of system performance coupled with expert judgment that the systems in the stockpile are safe, secure, and reliable.

The powerful and flexible integrated codes and the capabilities of the supercomputers on which they run have expanded the customer base for the ASC Program to include broader aspects of national

"The ASC Program is commited to providing simulation tools and computing resources to assess the state of the nuclear stockpile and to assist in ensuring its continued safety and reliability."

security. The intelligence community and those with responsibilities for counterterrorism have turned to the NNSA national security laboratories to develop and apply ASC Program tools to support their efforts in addressing external threats, including:

- In forensics, ASC Program integrated codes are used to simulate the explosion and resulting debris of the theoretical detonation of an adversary's nuclear weapon. Data produced by such simulations are valuable to the nation's nuclear forensics effort to identify the origin of the weapon in such a situation. These simulations are very complex and demanding in order to capture the specific signatures that would be produced by a device in a particular emplacement.

- Regarding potential nuclear threats and foreign weapons assessment, ASC Program tools are routinely used for simulating foreign threats (for example, the Redbook effort funded by the Defense Threat Reduction Agency). Integrated codes can perform detailed simulations of possible foreign weapons systems, exploring the impact of the assumptions made by intelligence analysts working with only a partial knowledge of foreign designs.

- For improvised devices, the study of such systems requires detailed three-dimensional simulations to explore the boundary between yield-producing and non-yield-producing designs, for example, to model dispersal in urban street canyons or to evaluate and quantify the effectiveness of several render-safe techniques.

Identifying customers and knowing the ASC Program products on which they rely is critical for the ability of the ASC Program to understand and meet expectations. For the three classes of ASC Program customers, their expectations include:

- Integrated codes and supercomputers that are available and reliable

- Integrated codes that reflect current and evolving physics and engineering understanding while moving these codes towards predictability and, therefore, capable of addressing existing and known future issues

- Integrated codes that have extensive, documented verification and validation, including baselines against existing underground test (UGT) data and detailed simulations of current (non-nuclear) experiments (for example, NIF capsules and hydrodynamic shock tube experiments)

The scope of application of ASC Program-supported technologies has grown as other Federal agencies turn to large-scale simulations to meet their missions. The NNSA national security laboratories play an important role as both proponents of simulation and providers of expertise in the general field of scientific computation. This positions them to become resources for other Federal agencies that seek science, technology, and engineering solutions for problems associated with the nation's security.

Rigorous peer review

DOE's Nuclear Security Enterprise is comprised of two design laboratories, one engineering laboratory (which, taken together, make up what is referred to in this document as the NNSA national security laboratories), the NNSS, and the weapons production facilities.

Since the early days of the nuclear weapons program, the three NNSA national security laboratories have successfully provided the simulation capability that has enabled the nation's nuclear deterrence. SNL was charged to develop the non-nuclear components in support of LANL's early designs, while LLNL was created in 1952 to work with LANL on what was then called the "Super," a two-stage thermonuclear device.

From those early days, much has changed and much has remained the same. LLNL and LANL have continued their focus on the physics design, no longer with new designs but rather with the goal of maintaining the reliability of the devices in the stockpile without the benefit of full-systems tests, which were halted over two decades ago. SNL has continued to focus on the engineering aspects of the entire delivery system, including its safety, surety, and ability to withstand attacks during the stockpile-to-target sequence. The integrated engineering codes are also used to develop design requirements based on environmental specifications.

A most important responsibility of the ASC Program's expert staff is to focus a critical eye on the results of companion and often duplicative efforts within the ASC Program. From the early days of the nuclear weapons program, it was well recognized that DP must follow the lead of the scientific community at large and insist upon rigorous internal examination of results. Today, the two physics laboratories in conjunction with the engineering laboratory support one another (although often in competition) by withering analysis of each other's work. This greatly reduces the likelihood of error, reduces the uncertainty that naturally attends lack of full-system testing, and gives assurance to the Secretaries of Energy and Defense and, through them, to the President that he or she can rely on the assessments the designers provide.

Following the moratorium of September 1992 and at the direction of President William J. Clinton in 1995, an annual reporting and certification process was established. In Section 3141 of the National Defense Authorization Act for Fiscal Year 2003, the three defense laboratory directors were mandated to deliver an annual assessment of the condition of the devices in the stockpile and to either affirm that the stockpile continues to be reliable, that each weapon in the active stockpile could be counted upon to work as expected, or to recommend that full-system tests be reinitiated.

This successful approach has resolved key stockpile lifetime questions and has led to proposed stockpile modifications to address conditions created by the complex and aging systems. Robust peer review enables the final customers of the nuclear weapons program within the DOD to have confidence in the national security laboratories' annual weapons assessments.

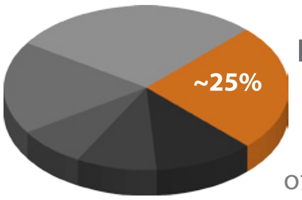
Organization, deliverables, and investment

For the ASC Program to develop the tools and technical competence necessary to meet the mission requirements set by the NNSA, significant technical accomplishment and financial investment are necessary.

To deliver its products, the ASC Program has been structured into interacting technical thrusts or subprograms that together form a coherent simulation and computing program. The subprograms are:

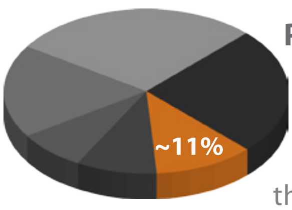
- Integrated Codes (IC)
- Physics and Engineering Models (PEM)
- Verification and Validation (V&V)
- Advanced Technology Development and Mitigation (ATDM)

- Computational Systems and Software Environment (CSSE)
- Facility Operations and User Support (FOUS)



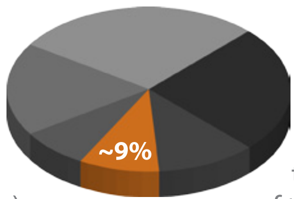
Integrated Codes

Development of the integrated codes, which are the culmination of the software development efforts of the ASC Program, embodies the simulation capability upon which a believable nuclear deterrence must rely. The integrated codes are the surrogates for full-system tests, and without them, there could be no credible SSP. The “real world” applications related to nuclear security to which the integrated codes are applied include annual assessments, design and qualification of LEPs, resolution (and in some cases generation) of SFIs, and the development of future stockpile technologies. Furthermore, national efforts to foster non-proliferation depend critically on the capacity to simulate systems known or believed-to-be possessed by potentially militant states.



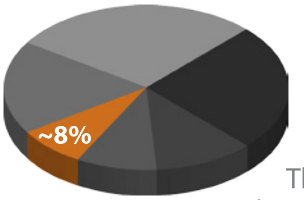
Physics and Engineering Models

The PEM subprogram is the physics and engineering research and development (R&D) arm of the ASC Program and provides the models and databases implemented into the integrated codes. The PEM subprogram is also the connection of the ASC Program to the Science Programs, which carry out the experimental portion of the SSP. As a result of an expanded knowledge of the physical processes and materials that must be modeled to characterize the time evolution of a nuclear device and the increase of computing power that makes it possible for the calculation of finer structures at shorter time scales, the designers are able to explain behaviors that were previously ill-understood and approximated. This is critical as the ASC Program expands on the demands to further develop understanding of relevant physical processes, to respond to LEPs, and to move into territory not explored in the full-system experiments of the testing era. These new realms result in large measure from device aging and the critical need to use new materials as replacements for the legacy materials.



Verification and Validation

Once the models are implemented into the codes, they must be tested to ensure a correct implementation of the equation, or other representation, into the code. This is verification that the models are correctly translated into the language of the codes. The codes then undergo a rigorous series of tests—generally by comparisons with experiments, small-scale test, and UGTs—to ensure the models are an accurate representation of physical reality. This is the validation of the model. These tests are often run on focused physics codes first, but, ultimately, the verification and validation process is applied to the full suite of integrated codes. The V&V subprogram is also responsible for developing uncertainty quantification methods for use in stockpile assessments. Additionally, under the V&V subprogram is the preservation of archived test data. There were over one thousand full-system tests fired between 1945 and 1993, which have yielded large amounts of data, albeit with gaps and sometimes anomalous behaviors. These data provide ground truth for simulations and inform the modern codes as well as provide a training ground for future designers.



Advanced Technology Development and Mitigation

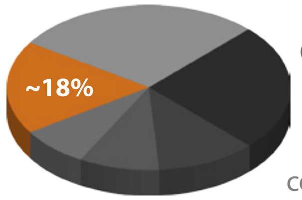
The ATDM subprogram addresses the technological disruptions resulting from the evolution of HPC to radically different and more complex architectures. The ATDM subprogram tackles the most critical subset of issues occurring during this period of disruptive change in HPC architectures to continue the current level of support to the Nuclear Security Enterprise mission. As part of this subprogram's work scope, the ASC Program has engaged with DOE's ASCR to address the barriers to exascale and evolving architectures.

The ATDM subprogram includes three focus areas:

- Next Generation Code Development and Application is focused on developing new simulation tools that address emerging HPC challenges of massive, heterogeneous parallelism using novel programming models and data management. Modern codes will be developed through co-design of applications by laboratory scientists and engineers and co-design of computer systems by computer vendors. The end product of this work is a next-generation set of simulation tools that may complement and/or replace the current set of production tools for the Nuclear Security Enterprise.

- Next Generation Architecture and Software Development is focused on long-term computing technology research of advanced architectures in areas such as extreme in-node parallelism. This includes efforts to mitigate disruptive effects and to allow ASC Program simulation tools to take advantage of more powerful computing resources while advancing capabilities.

- Future High Performance Computing Technologies is focused on evaluating alternative HPC technologies after limits of current semiconductor technologies are reached (post Moore's law era).



Computational Systems and Software Environment

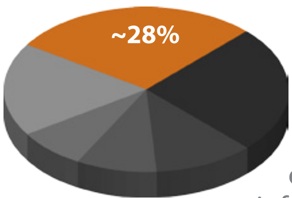
The ASC Program provides the computational infrastructure to the NNSA national security laboratories. The computing infrastructure is a complex environment that integrates many types of hardware and software products. HPC platforms are integrated into an ecosystem of workflow processes, support tools, storage systems, and communication devices. ASC Program management seeks to understand the unmet demand for computing resources and to make appropriate investments in hardware acquisitions; however, quantifying demand requires capturing a moving target.

In an attempt to inform decisions for future acquisitions, Federal managers for the ASC Program receive regular usage reports for machine utilization. Federal managers track trends, evaluate whether those trends are important, and then make decisions about future investments to ensure sufficient computing resources will continue to be available.

Whenever possible, the ASC Program utilizes products from commercial vendors and the open source software community. However, when the required technology is not available from these sources, the

ASC Program invests in internal R&D and one-time, vendor-conducted engineering activities to close the gaps. The ASC Program and the laboratories maintain close collaborations with computer vendors to ensure features essential to the ASC Program's needs are regularly identified, integrated, and supported in future products.

To leverage investments and reduce the total cost of ownership of to-be-deployed systems, collaborative procurements of ASC Program AT systems with ASCR leadership-class systems will form the basis of future deployments. A Memorandum of Understanding between the DOE SC and the DOE NNSA coordinates exascale activities within DOE.



Facility Operations and User Support

Facilities are the support skeleton of the ASC Program's computing infrastructure, providing space, power, cooling, and systems monitoring to increasingly complex and densely packaged computing and storage systems. As the ASC Program looks to the challenges of the next generation of computing technologies and architectures, the demands on facilities will increase and resources must be invested to meet these demands. The ASC Program collaborates with institutional facility strategic planning and construction working groups to ensure the facility requirements are planned in the ten-year site plans published annually.

The ASC Program seeks to align laboratory-specific activities into a common tri-laboratory computing environment to maximize investment value and provide backup resources should a disaster befall one of the NNSA national security laboratories. One example of how this plays out in the computing area is the use of the Advanced Technology System Scheduling Governance Model (discussed later in this document).

FY2010–FY2015 budgets at the subprogram levels

Table 1 describes the ASC Program budget and gives a sense of scale for the major elements in the ASC Program, highlighting the balance and priorities within the ASC Program.

Table 1: FY2010–FY2015 ($Ms)

	FY2010	FY2011	FY2012	FY2013	FY2014	FY2015
Integrated Codes	140.882	166.994	161.011	145.702	143.153	149.189
Physics and Engineering Models	61.189	68.989	70.431	68.932	61.469	68.469
Verification and Validation	50.882	57.243	57.241	56.232	48.878	52.878
Advanced Technology Development and Mitigation					35.000	50.000
Computational Systems and Software Environment	157.466	148.506	163.446	151.121	118.628	109.181
Facility Operations and User Support	155.650	169.112	167.866	173.031	162.201	168.283
	556.069	**610.844**	**619.995**	**595.000**	**569.329**	**598.000**

ESSENTIAL ELEMENTS FOR SUCCESS

SCIENTISTS, SKILLS, FACILITIES, INNOVATION, AND PARTNERSHIPS

Weapons scientists training, mentoring, and development

The codes the ASC Program develops, both integrated codes and focused physics, are tools in the hands of staff who possess the expert judgment to apply them. In approximately five years, there will be no designers at the laboratories who possess direct, full-system testing experience. It is essential that those few with previous hands-on experience mentor future generations of designers and guide them in the next few years. NNSA through the national security laboratories must provide opportunities for those upon whom the credibility of the nuclear deterrence will depend in future years to be trained in weapons-relevant science, to increase their understanding of weapons physics and engineering and the appropriate utilization of the archival test data, and to test that understanding by studying, for example, results from UGTs that have never been satisfactorily explained by the older models and older codes. They must also be given assignments in design and development of steps to be taken as part of the LEPs; and with their mentors, they must participate in designing, modeling, and predicting weapons-relevant experiments, including small-scale, focused, and integral experiments (for example, ignition capsules). It is a major priority for the ASC Program to make mentoring and training possible to ensure that a critical element of the capability—namely, expert judgment tempered by applicable practices—will continue to be available.

Skills mix and adequate staffing

In a mid-2008 study, ASC Program management commissioned the laboratories to estimate the size and balance of scientific staff needed to sustain advanced simulations as a core component of the SSP. In October 2010, the ASC Program published the *Right Size*[2] document, with the sub-title *Determining the Staff Necessary to Sustain Simulation and Computing Capabilities for Nuclear Security*.

The "right size" analysis focuses on the level and mix of staff with expertise who now and into the future make it possible for the ASC Program to meet its commitments to the SSP. This analysis of technical staffing is an important tool for understanding the necessary level of staffing, as well as for supporting the critical skill base in the face of continuing attrition. The study uses industry-accepted methods and is an important element of the budgeting process that formally connects technical staffing requirements with ASC Program functional and budget categories. The right-size information provides the basis for an annual reporting process of staffing versus costs.

In 2015, the ASC Program directed that an update to the 2008 study take place. The outcome of this review will likely result in a re-baselining of staffing requirements.

2 Advanced Simulation and Computing, *Right Size, Determining the Staff Necessary to Sustain Simulation and Computing Capabilities for Nuclear Security*, NA-ASC-121R-10-Rev.0, SAND-2010-8541P, October 2010.

Robust facilities

HPC allows the physicists and engineers of the weapons program to perform simulations at a proper scale and accuracy to enable them to draw conclusions about the performance of a weapon system. A driver behind the growth of computing power available to the weapons design community is the need for scientific staff to extend their capabilities for simulating weapons performance to greater precision, enabling them to develop models that better represent the physical processes that take place within a nuclear device and to improve the algorithms for efficient and accurate implementation of those models.

Power and space considerations are primary concerns of facilities. The infrastructure required for high-end systems is significant. For example, the Trinity computer system at LANL, built by Cray Computer and running at about 40 petaflops, requires 5,200 square feet of space and approximately 10 megawatts of power. Anticipated exascale computer systems are expected to require 20 megawatts. The ASC Program must plan far in advance and incorporate sufficient flexibility to facility designs to account for demands well into the future.

Both local area networks (LANs) and wide area networks (WANs) must support the two system classes, AT and CT systems. Latency requirements will be driven by response time for visualizations. File transfers dictate the bandwidth needs. Both the AT and CT systems will place demands on each site's LANs. As system capabilities increase, so will the load on the networks. Each AT system is unique and is a shared ASC Program tri-laboratory resource, which will in turn stress the WAN. Of particular concern is maintaining and upgrading the encryption devices used for the ASC Program's classified computing services.

To measure progress and areas for improvement in operations, metrics must be collected that accurately quantify efficiencies and areas for improvement. Whereas DOE computing facilities were once the largest in the world, data centers run by industry now eclipse the ASC Program centers in terms of floor space and power consumption and, in some cases, efficiency metrics. While the usage of the ASC Program systems compared to industry data centers is quite different, the facility issues are much the same. Close collaboration with other HPC data centers to identify best practices and attainable standards is necessary and desirable.

Importance of innovation

Maintaining the operational capabilities of nuclear devices without full-system testing, but relying primarily on computing simulations and small-scale experiments, is an enormous scientific challenge. The ASC Program has learned through the years that it cannot succeed by mere application of ready-made models and computing solutions; instead, its credibility and understanding of the limits of simulations depend heavily on innovation.

Examples of innovation at the NNSA national security laboratories include:

- Development of algorithms for the simulation of hydrodynamics and transport that can run efficiently on millions of processors
- Development of sub-grid models to capture the behavior of turbulence
- Development of new, multiscale models to simulate material fracture and failure
- Extension of open source operating systems to massively parallel machines

Innovation does not just happen. It must be encouraged and rewarded, even if the directions pursued, which may have looked promising at the beginning, turn out unpromising.

Partnerships

The ASC Program engages in many partnerships to influence, remain current in scientific progress, and engage other Federal agencies.

With industry

The ASC Program has sought to develop and sustain vendor partnerships with the goal of influencing

"The ASC Program has learned through the years that it cannot succeed by mere application of ready-made models and computing solutions."

what are, after all, commercial enterprises, and of continuing to provide the ASC Program with capabilities that allow the ASC Program to meet its responsibilities for national security.

Close vendor relationships have resulted in several computer systems that would not have existed otherwise. Notable examples include the SNL/Cray-developed XT3 line, the LLNL/IBM collaborative Blue Gene series of computers, and the LANL/IBM-collaborative Roadrunner machine that explored coprocessor technologies.

Despite these successes, major challenges remain for the ASC Program in the high-end computing arena:

- Develop computing systems that are 100–1000 times faster than current ASC Program systems.
- Achieve power consumption that is a factor of 10 below 2010 industry projections.
- Address high failure rates and application portability issues.
- Advance state-of-the-art hardware and software information security.

Looking to the future is an important responsibility that the ASC Program shares with the DOE ASCR program to ensure computer systems will exist to meet programmatic needs.

With universities

Staff in the Nuclear Security Enterprise must be encouraged to remain current with scientific progress in the world outside and within their non-nuclear studies, not only for the knowledge gained but also because a reputation in the wider community is part of the perceived credibility of the SSP's confidence in the stockpile and, hence, contributes to the deterrence capability. NNSA benefits from university collaborations through creation of new ideas and methods as well as the development of next-generation technical staff. These same collaborations provide the NNSA a means to engage academia in technical areas or processes, that is, uses of HPC and scientific computing that are important and relevant to the national security laboratories.

The goal of the Predictive Science Academic Alliance Program (PSAAP II) is to establish validated, large-scale, multidisciplinary, simulation-based "predictive science" as a major academic and applied research program. This aspect of the ASC Program has the potential to expand the pipeline of staff for the NNSA national security laboratories. Although the work is non-nuclear, it still provides students relevant experience for the weapons code development and design communities.

With the Department of Energy's Office of Science Advanced Scientific Computing Research

ASCR is largely focused on scientific problems of current interest to the broad scientific community. The ASC Program directs mission-critical science, and although much of the scientific work is classified, it still has important overlaps with the interests of the open scientific community. Examples include material science, behaviors of hot plasmas, combustion, and HPC.

In the areas where the ASC Program and ASCR overlap, the two programs are complementary and work in close collaboration. Joint planning to leverage computing technologies, support, and systems software is common and has proven to be fruitful. For instance, the essential software that enables the use of the massively parallel ASC Program computers by the weapons community is the Message Passing Interface (MPI), which is a product of SC's Argonne National Laboratory. The unique computer architectures developed within the ASC Program for the application suites—Cielo (LANL) and Sequoia (LLNL)—were adopted for the leadership systems portfolio at SC sites. Sharing reduces the development costs and results in cost-effective solutions for the DOE at large. Other areas of collaboration include joint acquisition reviews and procurements, data management, visualization, and algorithm development. Research in linear solvers is a prime example of an area in which both the ASC Program and ASCR have a vested interest for myriad scientific applications from combustion to weapons physics. The plan is for future ASC Program AT system procurements to follow a joint ASC Program-ASCR procurement model.

ASC PROGRAM DYNAMICS

PROCESS FLOW DIAGRAMS

To ensure the many elements of the ASC Program work together smoothly, support one another, and maximize the potential synergy, ASC Program management has recognized the essential nature of both the flow of work and information and also the connections between the elements. The process flow diagrams in this section are diagrammatic representations of the connections between major elements of the ASC Program. They are visual realizations of information and workflow and include both the drivers of requirements and feedback loops. Each diagram exhibits the cycle of interactions and interfaces, and each displays the customer-supplier relationships. The goal of these diagrams is to clarify the relationships between the essential activities by depicting the information and process flows between them.

These diagrams do not include specifics as to which organization is performing the work nor when or how the work is getting done; neither do they address the effectiveness or efficiency of the processes for getting the work done. These aspects are discussed in the program plan and annual implementation plan documents for the ASC Program.

Diagram 1 describes the path of development and deployment of the integrated codes. It depicts the steps and linkages between the requirements and the final products, moving from theory and model development to the implementation of the models

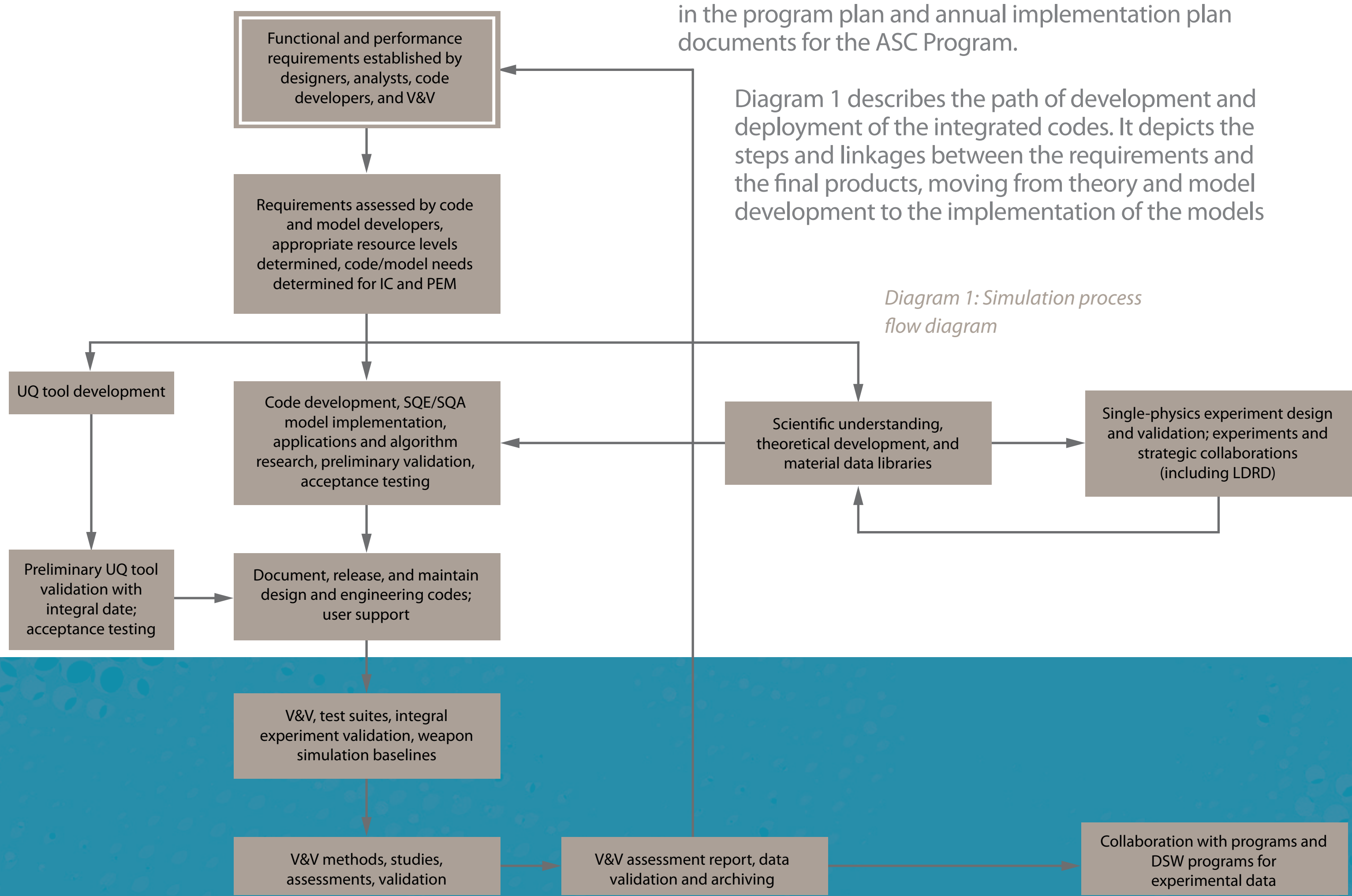


Diagram 1: Simulation process flow diagram

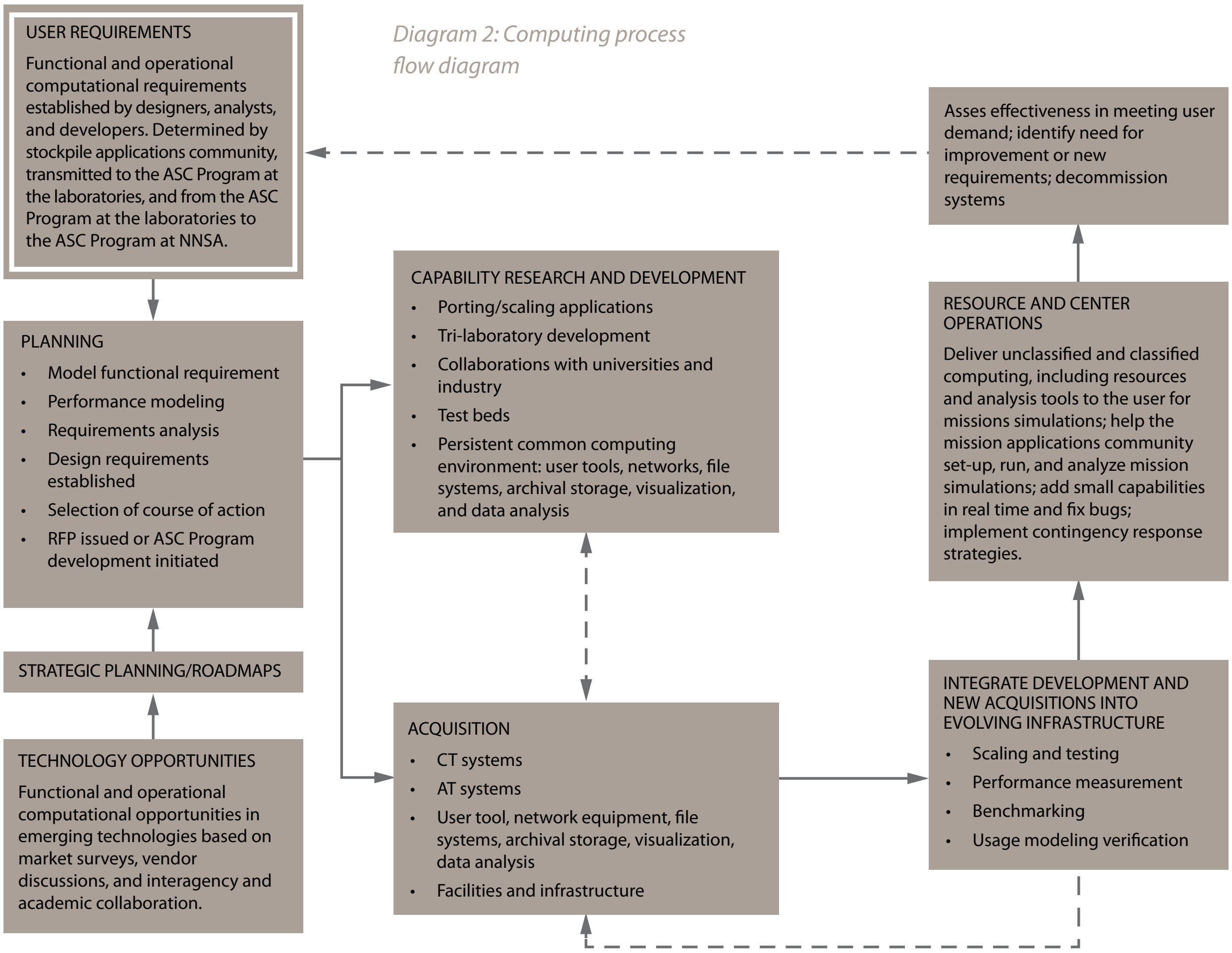


Diagram 2: Computing process flow diagram

into the codes and their verification and validation through the application of rigorous numerical analysis techniques and small-scale experiments. Furthermore, in the last decade, great strides have been made in the ASC Program's ability to quantify the uncertainties in calculations and to include error bars with the results; this is specifically called out in this flow diagram.

Diagram 2 describes the components involved in the acquisition and operation of the ASC Program's HPC centers. The ASC Program allocates resources for the acquisition and deployment of two classes of computing platforms, CT systems and AT systems, along with their associated operating environments. The CT systems are based on predominantly commodity hardware and software and make computing cycles readily available to the user community. The AT systems incorporate novel hardware and software features that, if successful, will lead to a significant increase in the capability of high-end computing and may well become future commodity technologies. These first-of-a-kind systems may require major modifications in the simulation tools for the user community to take full advantage of the exceptional capabilities offered by the new technologies. The national laboratory centers that house both these types of systems include the high-end systems themselves and the essential networking, storage, and support services.

PLANNING, TRACKING, AND OVERSIGHT

THE RELATIONSHIP BETWEEN HEADQUARTERS AND THE NATIONAL SECURITY LABORATORIES

The national security laboratories are government-owned, contractor-operated (GOCO) entities that are Federally Funded Research and Development Centers (FFRDC) established to meet the special long-term R&D needs of the Federal government.

FFRDCs must :

- Meet a special long-term government R&D need that cannot be met as effectively by the government or the private sector.
- Work in the public interest with objectivity and independence, and with full disclosure to the sponsoring agency.
- Operate as an autonomous organization or identifiable operating unit of a parent organization.
- Preserve familiarity with the needs of its sponsor(s) and retain a long-term relationship that attracts high-quality personnel.
- Maintain currency in field(s) of expertise and provide a quick response capability.

The management and operating (M&O) contract concept, used by the Atomic Energy Commission, predecessor to the DOE, and supported by the Joint Committee on Atomic Energy, provides a framework for the relationship between government and the national security laboratories :

- The basic substantive relationship between NNSA and the laboratories is an FFRDC partnership.
- The management relationship is a GOCO.
- The FFRDC relationship is based on a partnership between the government and the laboratory in which the government decides what problems need to be addressed, and the contractor determines how best to address those problems.

It is vital that a clear understanding of roles and responsibilities exists for both Federal program managers and the national security laboratories. The governance model, collaborative meeting venues, and roles and responsibilities that ease this understanding follow.

Governance

The governance model was put in place with the nature of the Federal/laboratory relationship in mind. Federal managers are expected to articulate the requirements as expressed by the military services; and the national security laboratories provide the technical approaches to meet those requirements. This is fundamental to the GOCO concept, and the ASC Program has been mindful of this division of responsibilities and has responded accordingly with a structured governance model consistent with the GOCO concept.

To ensure successful execution of the ASC Program strategy, an organizational structure, program management processes, and a performance measurement mechanism have been instituted within the ASC Program tri-laboratory framework. The ASC Program's organizational structure is designed to foster a focused, collaborative effort to achieve ASC Program objectives. The following elements make up this structure:

- An executive committee consists of a high-level representative from each NNSA laboratory and the Federal program manager (director), with HQ setting the overall policy, developing programmatic budgets, and overseeing the ASC Program execution.
- Subprogram management teams work through the executive committee and are responsible for the planning and execution of the implementation plans for each of the ASC Program subprograms. These management teams are made up of primary and alternate representatives from each laboratory and the corresponding subprogram manager from HQ. Tasking originates with the Federal manager and is communicated through the executive committee.
- HQ oversees interactions with other government agencies, the computer industry, and universities. HQ staff set programmatic requirements for the laboratories and review management and operating contractor performance.

ASC Program management planning

ASC Program management planning documents include the following:

- The program plan provides the strategy and targets for the ASC Program based on the Future Years Nuclear Security Plan (FYNSP) planning horizon. It includes the top risks and key issues, the goals, the WBS, and strategies and their associated performance indicators. The plan is reviewed every other year to ensure that the ASC Program supports SSP needs.
- The annual implementation plan describes the work planned for one-year intervals at each laboratory in support of the ASC Program objectives. It is prepared using the President's budget request as the initial basis and is updated to reflect the signed appropriation bill for the fiscal year.

- Other ASC Program strategy and planning documents are published periodically, including the *ASC Strategy* (NA-ASC-100R-04-Vol.1-Rev.0), the *Business Model* (NA-ASC-104R-05-Vol.1-Rev.1), the *ASC Roadmap* (NA-ASC-105R-06-Vol. 1), *Total Cost of Ownership* (NA-ASC-108R-06-vol.1-Rev.0), the *ASC Platform Strategy* (NA-ASC-113R-07-Vol. 1), *ASC Computing Strategy* (SAND-2013-3951P), and the *ASC Code Strategy* (NA-ASC-108R-09-Vol. 1-Rev.0). The *Defense Programs Program Execution Guide* (DP PEG), NA-10 *Program Management Tools and Processes*, provides DP program execution policy and guidelines to programs within DOE, NNSA, and DP, including implementation plan and program plan content.

Meetings and conferences

Collaboration among the three national security laboratories, industry, universities, and international partners is facilitated, encouraged, and leveraged through meetings and conferences such as these examples:

- Annual principal investigator meetings provide a forum for the ASC Program principal investigators at each laboratory to present and discuss progress in their research areas with their laboratory peers. The meetings include participants from outside the weapons laboratories to provide broader ASC Program peer insights and comments. The meetings also serve as an annual technical review for the HQ team.
- Executive committee meetings are held twice a month via teleconference. These meetings ensure relevant issues are identified, discussed, and resolved in a timely manner. The teleconferences are supplemented with face-to-face meetings on an as-needed basis.
- The Supercomputing Conference is the premier international conference on HPC and related technologies. It brings together the leading minds in supercomputing from industry, academia, and research facilities around the world. It is the largest computational science conference, and major computer, storage, and networking vendors participate and bring the latest commercial thinking and technology for exhibit. Participation at this conference is an essential component of advancing DOE/NNSA's research in HPC, computer science, and computational science and engineering.

Roles and responsibilities of Headquarters

The Federal managers are responsible for setting requirements and prioritizing the elements of the national ASC Program, allocating resources at the subprogram level, and monitoring and evaluating both the technical execution and the stewardship of allocated resources. Federal managers are expected to ensure an integrated organization and to advocate for the ASC Program with the sponsors who appropriate the resources. Advocating for a program of such complexity with so many interleaving components has to be framed clearly to affirm the importance of the ASC Program and make the case for sufficient resources to enable success. Major areas of Federal oversight include:

- Technical oversight to ensure mission needs are met and simulation tools are applied to the appropriate challenges, both those of the standing stockpile and those associated with the

administration's commitment to non-proliferation; and to measure delivery of products with the mutually agreed upon commitments in the Level-2 and Level-3 milestones

- Financial oversight to review spending annually to ensure costing is consistent with allocations, to review uncosted balances and request explanation where anomalies exist, and to respond to requests for shifts of resources in Level-4 elements of the WBS and require cognizance of reallocations by the sites at Level-5

- Oversight of staffing levels to participate in and review results of annual right-sizing efforts, to support efforts to ensure the availability of critical skills for the national ASC Program, and to allocate resources to enable hiring and retention of staff with essential skills

- Oversight of computing infrastructure to review results of supercomputer workload characterization and take appropriate measures to enable best use of these critical resources, to analyze the usage data to inform ongoing and future acquisitions, and to continue work to improve operations of the computing centers

- Oversight of ASC Program integration to work with the national security laboratories to integrate the simulation and computing program, and to support healthy competition and a robust system of peer review to ensure maximally credible products and application of those products to issues associated with the continued safety and reliability of the nuclear stockpile

Oversight of the ASC Program is provided by HQ with particular individuals charged with specific elements of the oversight functions.

The Federal program manager (director) for the ASC Program provides the following specific oversight:

- Provide strategic guidance to set high-level policy to provide guidance to the national security laboratories, obtain input from customers and set requirements for the national ASC Program, develop a program strategy and a roadmap with timelines specified, and ensure coordination with the Predictive Capability Framework, which outlines both near- and long-term programmatic goals for the development of a predictive capability.

- Obtain and distribute resources to allocate funding to the WBS Level-4 subprograms and resource load the WBS Level-5 products, put into place a procurement critical decision process, and articulate the value of the ASC Program to the stockpile and nuclear security complex as well as to congressional appropriators and authorizers who set the budget parameters.

- Evaluate progress to provide input to the annual performance evaluation of the contracting sites, to conduct program reviews and principal investigator meetings, and to approve initiation and closing of milestones.

The Federal managers for a subprogram provide the following specific oversight:

- Provide technical input and oversight, as appropriate.

- Monitor milestone progress.

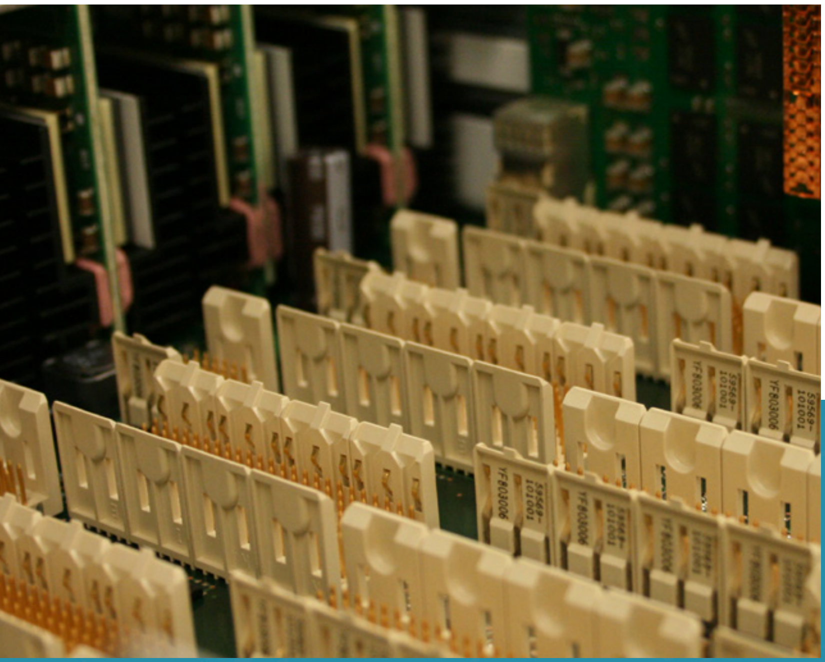
- Assess computing center performance.

- Effect comparisons between planned and actual, for example, milestone accomplishment and costs.

Roles and responsibilities of the national security laboratories

The national security laboratories are charged with the development of the simulation tools that make it possible to maintain the nuclear stockpile in the absence of nuclear testing. This includes developing the theoretical models, implementing these models in the integrated codes, and designing and analyzing the results of small-scale experiments used to validate the integrated codes. The laboratories also play a key role in the acquisition of the large computers, fielding the infrastructure to operate them, and supporting the system software that underlies their operation. In addition, the laboratories are relied upon to apply the tools (the products of their labors) to identify risks to the stockpile and to propose possible remedial actions and alternatives. The labs also provide each other with critical peer review, as previously described. This work must be done within the resources appropriated by the Congress and allocated by the Federal managers.

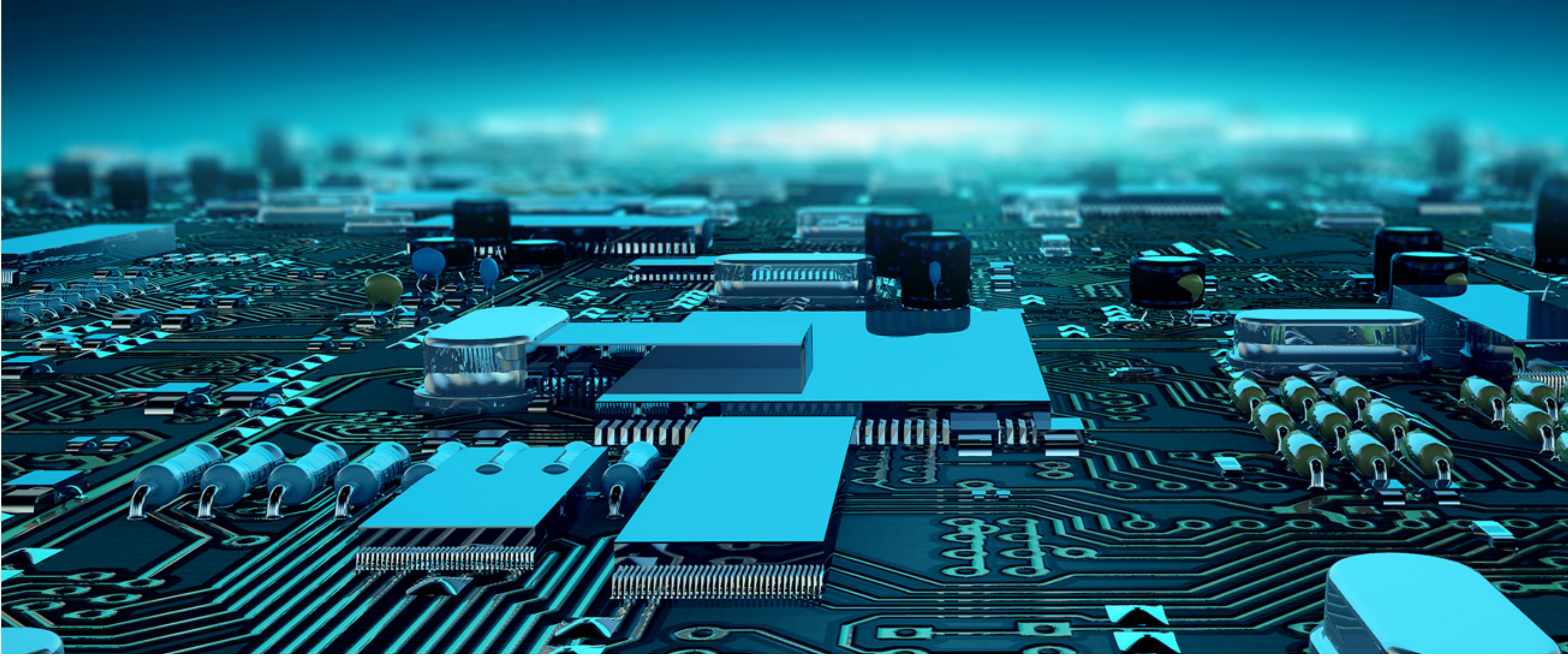
The responsibilities of the ASC Program managers at the laboratories are to provide oversight at their individual sites. They plan the local ASC Program, allocate resources at the project level, monitor and evaluate the technical execution of the ASC Program, and report progress to the Federal managers on a regular basis. The managers at the laboratories are expected to work closely with their colleagues at the other national security laboratories to create an integrated national ASC Program with close cooperation and critical mutual reviews.



Specific roles for assuring continued progress in the ASC Program are distributed among site managers and staff.

The ASC Program laboratory executive, the ASC Program laboratory deputy executive, and the subprogram executives provide the following specific oversight:

- Develop long-term local simulation and computing strategic plans.
- Inform the ASC Program strategic plan developed and written by HQ.
- Evaluate computing center performance and propose improvements to enhance user support and maximize value of investment.
- Maintain WBS Level-4 subprogram budgets according to HQ allocations and finalize resource loading of WBS Level-5 products; work with Federal managers to achieve a balanced and integrated program; and move funding within a single WBS Level-4 subprogram after notifying Federal managers and budget staff.
- Execute implementation plans according to scope, schedule, and budget.
- Interact with HQ and with other laboratories to improve collaboration and manage redundancy in the ASC Program that is not required for peer review.



- Provide oversight of the quality of products delivered.
- Furnish progress reports, as appropriate (weekly, monthly, quarterly, annually).
- Operate computing centers and submit workload characterization reports to HQ.
- Draft white papers and presentation materials at HQ request, for example, on issues and technologies.
- Provide technical workforce management, recruiting, and retention.
- Integrate planning with the activities and schedule of the Predictive Capability Framework.
- Report accomplishments.

ASC Program laboratory technical staff provide the following specific oversight:

- Interface with and collect requirements from the design and engineering communities that apply the simulation tools.
- Implement responses to requirements by developing new modeling and computational capabilities.
- Identify work scope from which Level-2 milestones are developed and against which laboratories are evaluated.
- Provide technical input into high-level strategic ASC Program planning.
- Provide technical input to program plan and annual implementation plan documents.
- Develop project plans in the form of site work packages that directly map to the Level-6 projects identified in the implementation plans.
- Perform risk analyses as required by the national ASC Program.

PROGRAM, SUBPROGRAMS, AND PRODUCTS

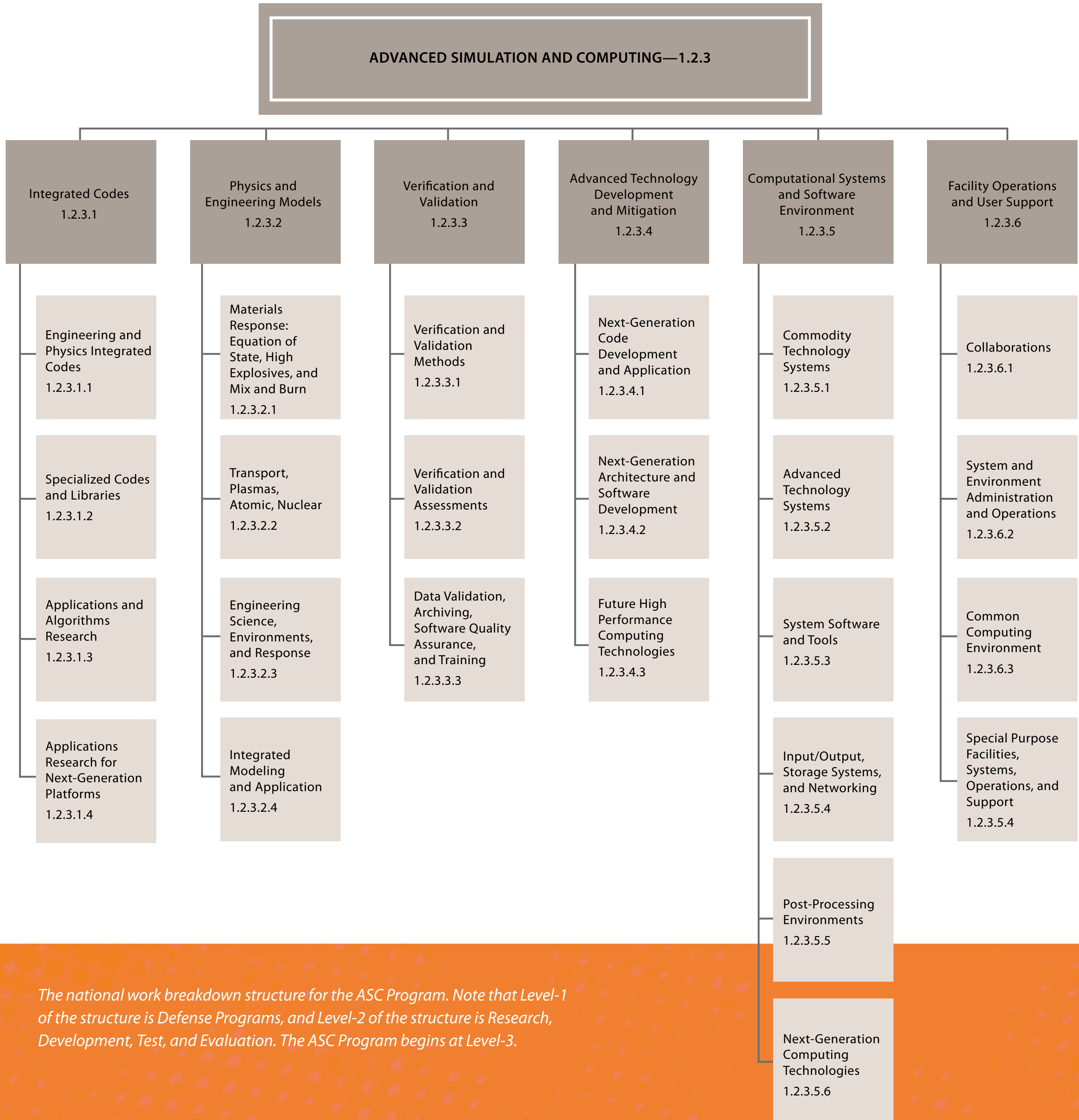
THE STRUCTURE OF A SUCCESSFUL PROGRAM

The ASC Program national work breakdown structure (nWBS) is a compendium of the ASC Program components that form the entire program. It is "national" because all sites participating within the ASC Program accept and use the same work breakdown structure. Each subprogram and product is given a clear title that reflects its content, and as a result, there is a generally accepted understanding across the ASC Program of the focus of each element.

The ASC Program nWBS is made up of subprograms (six) and their elemental products (twenty-three). The ASC Program itself is at Level-3 of the DP WBS. The difference between the ASC Program nWBS and a classic WBS is that the ASC Program nWBS is built around its "products" while the classic approach focuses on processes and steps. In the ASC Program nWBS, subprograms identify the major and relatively self-contained (although interdependent) areas in which accomplishment is necessary for the overall ASC Program to meet its commitments and provide deliverables successfully. The ASC Program subprograms are at Level-4 of the DP WBS, which is B&R Level 6 (B&R6) of the DOE Accounting System. The ASC Program products exist at Level-5 of the DP WBS and Level-9 (B&R9) of the DOE Accounting System. The ASC Program is managed (that is, Federal managers make budget decisions) at the B&R6 level (subprograms), but the B&R9 level (products) is included for Federal managers to track product delivery.

By definition, an integrated nWBS assumes that at times some activities are performed by a single laboratory and at other times shared or even duplicated. As has been noted elsewhere in this document, such replication or redundancy greatly enhances the ability to meet mission needs credibly through intensive internal debate and peer review. To preserve this function, some capabilities must be independently developed and applied at more than one laboratory. Some activities are more effective as multilaboratory collaborations in providing the ASC Program with a standard tool or capability. A good example of the latter is the visualization of three-dimensional features that are the output of complex simulations.

The projects, tasks, activities, and milestones associated with the twenty-three products are documented through a combination of the annually drafted ASC Program implementation plan and laboratory-specific work plans and packages.



The national work breakdown structure for the ASC Program. Note that Level-1 of the structure is Defense Programs, and Level-2 of the structure is Research, Development, Test, and Evaluation. The ASC Program begins at Level-3.

A VISION OF PREDICTIVE CAPABILITY

ADVANCING SCIENTIFIC UNDERSTANDING

The nuclear weapons design codes used in the days of full-system testing contained the best physics models and most accurate numerics available at the time. Designers predicted the behavior of the to-be-detonated device and then, after the experiment, compared their pre-shot calculations with the test data. Post shot analyses often revealed discrepancies, which could then lead to the insertion of ad hoc factors into the nuclear weapons design codes to compensate for shortcomings in models and numerical approximations. These factors were needed to calibrate the nuclear weapons design codes with the diagnostic results and became part of the integrated codes, which were then used for future design work. This calibration, often referred to as baselining, was the *modus operandi* before the superior simulations, made possible by both enhanced physics understanding and, most particularly, by far more powerful computers, led to a nearly "predictive" approach to numerical representations of device behavior.

The environment has changed. Consistent with U.S. policy since 1995, the U.S. continues to uphold its moratorium on the use of full-scale nuclear weapons testing; however, physics understanding and computing capabilities have increased significantly over the past decade. The weapons complex has spent the past decade in transition to production HPC, including significantly more accurate representations of the physics and subcritical tests to make predictions. Changing material availability over the years has necessitated that certain components or parts be supplemented or replaced, which requires a deeper understanding of fundamental material properties for the prediction of device performance. Moreover, given the introduction of modern materials that meet present day health, environmental, and safety requirements, LEPs also shift the nuclear weapons stockpile from the as-tested configurations. Designers and analysts must understand these perturbations and their effects on performance through highly resolved calculations in three dimensions with precise models based on basic physics and engineering principles.

The ASC Program is committed to developing the capabilities and integrated codes based on more accurate models and increasingly powerful computers, to move scientific understanding toward ever more precise representations of physical reality. Evidence of this advancement is the basic and applied research activities that have made significant progress since the formation of the ASC Program. To successfully address these significant challenges, the ASC Program combines technical and business planning. The technical component is addressed within the program plan and implementation plan documents. The business component is addressed within the business plan document, with attention to customers, products, and clearly defined roles and responsibilities of HQ and the national security laboratories. Through the business plan document, the ASC Program is structured and focused on the essential elements of success to remain a major player in reaching the stockpile stewardship goal of predictive capability.

APPENDIX 1

DEFINING THE NATIONAL WORK BREAKDOWN STRUCTURE

Appendix 1, Defining the National Work Breakdown Structure, connects the Defense Programs work breakdown structure with the actual DOE accounting system B&R classification codes. The B&R codes, titles, and definitions—as shown in the following table—are found in the DOE's Budget and Reporting Code System (BARC). They correlate with DOE activities that are used within the DOE accounting system for the reporting of obligations, costs, and revenues by DOE field offices; the formulation of budgets; and for the controlling and measuring of actual (versus budgeted) performance.

WBS	B&R	Title	Definition
1.2.3.1	DP.15.15.00.0	Integrated Codes	This Subprogram constitutes laboratory code projects that develop and improve the weapons simulation tools, the physics, the engineering, and the specialized codes.
1.2.3.1.1	DP.15.15.06.0	Engineering and Physics Integrated Codes	Engineering and Physics Integrated Codes delivers a suite of large-scale, integrated codes needed to support Stockpile Stewardship Program activities such as annual certification, life extension programs, and significant finding investigations. These codes include both classified and unclassified codes, codes used to simulate the safety, performance, and reliability of stockpile systems, codes used for the design and analysis of experiments, and codes to support analyses of weapons components and systems under normal, abnormal, and hostile environments. The codes are designed to run in parallel and make effective use of advanced ASC computing platforms.
1.2.3.1.2	DP.15.15.07.0	Specialized Codes and Libraries	Specialized Codes and Libraries deliver both codes that have specialized function and libraries that are incorporated into integrated codes. Specialized codes have detailed physics focused on unique applications (e.g., radiation transport or ICF laser-plasma interactions) or are specific applications such as problem setup, meshing tools, and physics-based post-processing codes such as diagnostics tools. Libraries include mathematical solvers or physical database access routines.
1.2.3.1.3	DP.15.15.08.0	Applications and Algorithms Research	Applications and Algorithms Research is focused on research to investigate and develop algorithms, computational methods, and future physics, engineering, and numerical simulation technologies. This research enables advances toward greater predictive capability by focusing on overcoming critical obstacles in integrated codes (e.g., the need for robust and efficient solvers, design and optimization algorithms, and innovations that improve code effectiveness). Exploratory efforts include short-term focused research projects, as well as longer-term, more innovative efforts aimed at the large challenges.
1.2.3.1.4	DP.15.15.09.0	Applications Research for Next-generation Platforms	Applications Research for Next-Generation Platforms is focused on research to investigate how the other areas within integrated codes will be able to exploit the next generation of platforms, including new technologies for massive parallelism both on-node (e.g., GPUs and large number of threads) and off-node (e.g., many nodes operating in parallel and new I/O technologies), as well as new programming models and resilient application codes.

WBS	B&R	Title	Definition
1.2.3.2	DP.15.16.00.0	Physics and Engineering Models	This Subprogram develops microscopic and macroscopic models of physics and material properties, as well as improved numerical approximations to the simulation of transport for particles and x-rays and other critical phenomena. This Subprogram is responsible for the development, the initial validation, and the incorporation of new models into the integrated codes.
1.2.3.2.1	DP.15.16.16.0	Materials Response: Equation of State, High Explosives, and Mix and Burn	Responsible for the development and implementation of science-based predictive models, including physics discovery at different length and time scales, for the dynamic response of materials used in ASC codes for performance and safety simulation. It includes models at normal and extreme conditions for describing the thermodynamic response of materials; the dynamic strength, damage, and failure response of materials; the dynamics of high explosives and polymers; and the evolution of complex hydrodynamic and burning flows. It also provides capabilities to predict the change of property, geometry and function of material due to aging. This sub-element requires the integration of advanced theory, specialized computer codes and experimental data, and provides cross-program support for new model implementation and verification in ASC codes for improved predictive capability.
1.2.3.2.2	DP.15.16.17.0	Transport, Plasmas, Atomic, Nuclear	Responsible for the delivery of accurate nuclear cross-section evaluations and databases; for the delivery of science-based models and databases that represent the interactions of radiation with matter; and for the behavior of plasmas and transport phenomena (thermal, radiation, electrical etc.) at extreme temperatures, pressures, and densities. The nuclear properties and opacity databases are produced in forms sharable between the laboratories. Specialized nuclear physics codes integrate experiments and advanced theory. For opacity calculations both equilibrium and non-equilibrium models calculate data in an ab initio manner. This sub-element supports the implementation of models and databases into ASC integrated safety, design, and diagnostics codes for improved predictive capability.
1.2.3.2.3	DP.15.16.18.0	Engineering Science, Environments, and Response	Responsible for the delivery of predictive science-based models that describe complex thermal, mechanical, electrical, chemical and fluid transport in materials for component manufacturing and performance; complex aerodynamic and aerothermal flows and response for gravity and reentry systems; and material and electrical system effects produced by exposure to electromagnetic pulses both external and internal, x-ray, gamma and/or neutron radiation. Models are developed through integration of theory, computational simulation and analyses of experimental data. The resulting models are implemented into ASC integrated engineering and physics codes for improved predictive capability.
1.2.3.2.4	DP.15.16.19.0	Integrated Modeling and Application	Responsible for supporting efficient use of models in ASC codes, including the need to address technology mitigation issues for all PEM models in new hardware architectures and implementation of models in next generation codes, along with ensuring the robustness of PEM models when integrated in multi-physics simulations.

WBS	B&R	Title	Definition
1.2.3.3	DP.15.17.00.0	Verification and Validation	Based on the functional and operational requirements established by designers, analysts and code developers for greater fidelity of codes and models, this Subprogram establishes a technically rigorous foundation for the credibility of code results.
1.2.3.3.1	DP.15.17.07.0	Verification and Validation Methods	Verification and Validation Methods provides methods and measures necessary to assess the credibility of the ASC codes and models, quantify uncertainties in ASC calculation results, and measure the progress in the ASC predictive capabilities. In this role, V&V will be aware of leading research, perform its own research, and be an advocate for advanced research and methods development in the areas of code verification, solution verification, validation metrics and methodology, and uncertainty quantification (UQ) as enabling technologies for validation and quantification of margins and uncertainties (QMU) in a risk-informed decision context.
1.2.3.3.2	DP.15.17.08.0	Verification and Validation Assessments	Verification and Validation Assessments delivers science-based assessments of the predictive capability and uncertainties in ASC integrated performance, engineering, and specialized codes' phenomenological models, numerical methods, and related models, to support the needs of the Stockpile Stewardship Program. This area focuses on establishing credibility in integrated simulation capabilities by collecting evidence that the numerical methods and simulation models are being solved correctly, and whether the simulation results from the mathematical and computational models implemented into the codes agree with real-world observations. This requires extensive collaboration with the various ASC elements, DSW, and the Science and Engineering Campaigns.
1.2.3.3.3	DP.15.17.09.0	Data Validation, Archiving, SQA, and Training	Data Validation, Archiving, SQA, and Training provides traceable and reproducible work products and processes for stockpile certification (short and long term), as well as foundational elements for establishing software quality standards and training weapons scientists in the application of verification, validation, and UQ methods. The scope of this product includes integral validation of physical property data that that are used as inputs for various weapon relevant simulations. Additionally, this product includes work product and data archiving and simulation pedigree tracking. It also includes establishing high-level software quality requirements, assessment techniques and methods, and development of Software Quality Engineering (SQE) tools. Finally, it supports the adoption of stockpile QMU assessment methodologies through computational simulation by providing training for use of V&V and UQ tools to establish credible simulation-based performance margin and uncertainty estimates.
1.2.3.4	DP.15.20.00.0	Advanced Technology Development and Mitigation	This Subprogram includes laboratory code and computer engineering and science projects that pursue long-term simulation and computing goals relevant to the broad national security missions of the National Nuclear Security Administration.
1.2.3.4.1	DP.15.20.01.0	Next-generation Code Development and Application	This product is focused on long-term research that investigates how future code development must address new HPC challenges of massive, heterogeneous parallelism, (both on-node and off-node) that require adoption of new programming models and data management techniques including co-design of applications and systems.
1.2.3.4.2	DP.15.20.02.0	Next-generation Architecture and Software Development	This product is focused on long-term computing technology research to influence the shift in computing technology to extreme, heterogeneous architectures and to mitigate its impact and advance its capabilities for ASC simulation codes.
1.2.3.4.3	DP.15.20.03.0	Future High Performance Computing Technologies	Evaluating alternative HPC technologies after limits of current semiconductor technologies are reached (post Moore's law era).
1.2.3.5	DP.15.18.00.0	Computational Systems and Software Environment	This Subprogram provides ASC users a stable, seamless computing environment for all ASC deployed platforms, including capability, capacity, and advanced systems.
1.2.3.5.1	DP.15.18.08.0	Commodity Technology Systems	Includes costs for production platforms and the associated planning and deployment necessary to integrate the overall system architecture with projected user workloads.

WBS	B&R	Title	Definition
1.2.3.5.2	DP.15.18.03.0	Advanced Technology Systems	Includes costs for advanced architectures and problem-optimized systems in response to program need.
1.2.3.5.3	DP.15.18.04.0	System Software and Tools	Includes costs for the system software infrastructure, including the supporting operating system environments and the integrated tools to enable the development, optimization, and efficient execution of application codes.
1.2.3.5.4	DP.15.18.05.0	I/O, Storage Systems and Networking	Includes costs to provide I/O (or data transfer), networking technologies, and storage infra-structure in balance with all platforms and consistent with integrated system architecture plans.
1.2.3.5.5	DP.15.18.06.0	Post-processing Environments	Includes costs to provide integrated environments to support end-user post-processing visualization, data analysis, and data management.
1.2.3.5.6	DP.15.18.09.0	Next-generation Computing Technologies	Includes costs for planning, coordinating and executing next-generation computing technology R&D activities to prepare the ASC applications and computing environment for the paradigm shift in computing technology to extreme, heterogeneous, multi-core on-node parallelism.
1.2.3.6	DP.15.19.00.0	Facility Operations and User Support	This Subprogram provides both necessary physical facility and operational support for reliable production computing and storage environments as well as a suite of user services for effective use of ASC tri-lab computing resources.
1.2.3.6.1	DP.15.19.03.0	Collaborations	Includes costs to provide collaboration with external agencies on specific high-performance computing projects.
1.2.3.6.2	DP.15.19.04.0	System and Environment Administration and Operations	This product provides requirements planning, initial deployment, configuration management and on-going operational support for reliable production computing and storage environments, necessary physical facility, and other utility infrastructure. Activities include: system and network administration and operations, user support, hardware maintenance, licenses, and common tri-lab computing environment integration and support.
1.2.3.6.3	DP.15.19.06.0	Common Computing Environment	Includes costs associated with the development and maintenance of a common tri-lab computing environment through R&D projects that focus on a common software stack to include, but are not limited to, operating system software; application development tools; resource management; HPC monitoring and metrics; and common tri-lab environment issues of configuration management, licenses, wide area network access, and multi-realm security.
1.2.3.6.4	DP.15.19.07.0	Special Purpose Facilities, Systems, Operations, & Support	This product provides special purpose high-performance computing resources to the DOE community, and the necessary support and maintenance of these systems and facilities. This includes special security controls and special purpose facilities in addition to the standard high-performance computing operations and support activities necessary to support these resources.
1.2.3.6.2	DP.15.19.04.0	System and Environment Administration and Operations	This product provides requirements planning, initial deployment, configuration management, and ongoing operational support for reliable production computing and storage environments, necessary physical facilities, and other utility infrastructure. Activities include system and network administration and operations, user support, hardware maintenance, licenses, and common tri-laboratory computing environment integration and support.
1.2.3.6.3	DP.15.19.06.0	Common Computing Environment	This product includes costs associated with the development and maintenance of a common tri-laboratory computing environment through R&D projects that focus on a common software stack, including (but not limited to) operating system software, application development tools, resource management, HPC monitoring and metrics, and common tri-laboratory environment issues of configuration management, licenses, WAN access, and multirealm security.
1.2.3.6.4	DP.15.19.07.0	Special Purpose Facilities, Systems, Operations, and Support	This product provides special-purpose HPC resources to the DOE community and the necessary support and maintenance of these systems and facilities. This includes special security controls and special-purpose facilities in addition to the standard HPC operations and support activities necessary to support these resources.

APPENDIX 2

IMPLEMENTATION OF DOE ORDER 413.3B

On March 31, 2003, a memorandum was issued by former Deputy Secretary of Energy Kyle McSlarrow on "Project Management and the Project Management Manual," directing programs to implement DOE Order 413.3, *Program and Project Management for the Acquisition of Capital Assets*. This order was revised and is now 413.3B.

The ASC Program AT system acquisitions follow the Enhanced Management B program management category in the *Defense Programs Program Execution Guide*.

The ASC Program completes a critical decision process, adapted from DOE Order 413.3B, for capital asset projects that have a total project cost greater than or equal to $10M. Per DOE Order 413.3B, acquisition executive authority may be delegated from the under secretary to a deputy administrator for projects between $100M and $750M. In the case of the ASC Program, this means the NNSA administrator delegates to the deputy administrator for DP. For AT systems acquisitions under $400M within the ASC Program, the acquisition executive authority is regularly delegated to the deputy administrator for DP per the HQ #516973-v1 memo.

APPENDIX 3

CRITICAL DECISION PROCESS

Month Counter	Advanced Technology System Acquisition Activity
Month 0	Project start/request for information released to industry to gather information
Month 6	Draft technical requirements posted for vendor review
Month 7	Mission needs statement CD-0 signed by HQ
Month 8	Formal design review
Month 9	Request for proposal independent review
Month 13	Field office and NNSA Acquisitions and Project Management approval for request for proposal release
Month 13	Conceptual Design Document CD-1/3a signed by HQ; includes alternative and risk analysis
Month 13	Request for proposal released
Month 16	Evaluation and selection complete
Month 21	Independent cost review
Month 22	Build contract negotiation complete
Month 23	Performance Baseline/Construction Readiness CD-2/3b signed by HQ
Month 23	Field Office and NNSA Acquisitions and Project Management approval of contract award
Month 24	NNSA awards contract to selected vendor

APPENDIX 4

ADVANCED TECHNOLOGY SYSTEM SCHEDULING GOVERNANCE MODEL

In the fall of 2005, the ASC Program appointed a team to formulate a governance model for allocating resources and scheduling the stockpile stewardship workload on ASC Program systems (formerly termed "capability" systems). A revision of this document was completed on June 11, 2015. The *Advanced Technology System Scheduling Governance Model* takes into account the new technical challenges and roles for AT systems and the new ASC Program workload categories that must be supported.

The objectives of this governance model are to:

- Ensure that AT system resources are allocated on a priority-driven basis according to SSP requirements.
- Utilize ASC Program AT systems for the most demanding workload categories, for which they were designed and procured.
- Support the role of AT systems to prepare ASC Program resources (including people, applications, and computing environments) for significant changes in future computer system architectures.

APPENDIX 5
DISASTER RECOVERY PLANNING

As part of the ASC Program's contingency planning, aligned with the NNSA's *Enterprise Contingency and Disaster Recovery Plan*, the national security laboratories maintain an information security contingency plan and multiple cooperative disaster recovery and operations agreements. Each laboratory's data backup and retrieval plan details the procedures that will be used to maintain continuity of critical operations in the event that an HPC system suffers from partial or complete loss of availability. The data backup and retrieval plan addresses various loss scenarios, including power loss and other facility problems, as well as individual component losses due to equipment failure. These plans also address full-scale disaster situations such as threat by wildfire or other natural calamities, including the complete evacuation of the site for any reason. They focus on those components that if lost or compromised for more than the maximum allowable downtime of sixty days would seriously impact the laboratory's performance of its mission.

Cooperative disaster recovery and operations agreements between laboratories provide a means to protect mission-essential data from corruption or destruction in the event of a widespread disaster. These agreements make it possible for mission essential operations to be resumed by the affected laboratory on the other laboratory's computing resources either remotely or onsite as circumstances dictate. These agreements are documents signed by cooperating laboratory ASC Program directors. Specifically, LLNL and LANL maintain an agreement. SNL New Mexico and SNL California maintain an agreement. These agreements are exercised annually.

APPENDIX 6
THE ASC PROGRAM AS LANDLORD

The facilities for which the ASC Program is considered landlord are comprised of the computing centers at the three NNSA national security laboratories. As the landlord, the ASC Program is:

- Primary user of the facility
- Chief programmatic advocate for the facility and the operations within
- Primary source of justification during strategic planning and priority setting for construction and major renovations/upgrades to the facility

Each laboratory computing center (facility) integrates the following, sometimes physically located in more than one building:

- Facilities and services required to run nuclear weapons simulations and operate CT and/or AT systems
- Physical space, power, and other utility infrastructure, including storage, file systems, and LAN/WAN for local and remote access, as well as system administration, cyber-security, and operations services for ongoing support of HPC systems and support equipment
- Computer center hotline and help-desk services, account management, Web-based system documentation, system status information tools, user training, trouble-ticketing systems, common computing environment, and application analyst support

As landlord, the ASC Program budgets for the modification of the computing centers and looks ahead toward the delivery of future systems; this requires allowing sufficient lead time and long-range budget planning. Budget and costs are captured in the FOUS subprogram B&R codes. FOUS provides both necessary physical facility and operational support for reliable, cross-lab production computing and storage environments as well as a suite of user services for effective use of ASC Program tri-laboratory computing resources.

The funding necessary to operate and modify the computing centers comes from a combination of direct programmatic funding out of the FOUS (DP1519) B&R code and credits from other non-weapons programs that may utilize the same buildings. In addition, indirect overhead charges on dollars that come into the laboratories can be used for some aspects of facilities operations.Within weapons activities, the Readiness in Technical Base and Facilities program provides program capabilities and special nuclear materials infrastructure for the Nuclear Security Enterprise. However, it does not fund maintenance and operations of the ASC Program computing centers.

APPENDIX 7
GLOSSARY

Annual Assessment and Certification
This is the formal assessment of the systems in the existing stockpile to alert the Secretaries of Energy and Defense to any potential problems and to inform the decision whether or not to continue the moratorium on full-system tests. The annual assessment also provides a formal certification of the safety, reliability, and performance of modified or rebuilt devices.

ASC
The Advanced Simulation and Computing Program
The ASC Program provides the simulation tools essential for the annual weapons assessment and certification. The elements of this capability include EPICs, specialized codes, weapons science codes, advanced computer platforms, and the facilities to house them.

ASCI
Accelerated Strategic Computing Initiative

ASC Program Executive Committee
This committee consists of two high-level representatives from each national security laboratory and HQ. The committee sets overall policy for the ASC Program, provides oversight for the execution of the ASC Program, and develops programmatic budgets.

ASCR
Advanced Scientific Computing Research
The mission of the ASCR program is to discover, develop, and deploy computational and networking capabilities to analyze, model, simulate, and predict complex phenomena important to the DOE.

AT
Advanced Technology
AT systems are advanced computing platforms fielded in the NNSA nuclear security laboratories. They incorporate features that have the potential to become future commodity technologies. These large, first-of-a-kind systems require software modifications to the integrated codes to take full advantage of their exceptional capabilities.

ATDM
The Advanced Technology Development and Mitigation Subprogram

B&R
Budget and Reporting Code

Campaigns
Campaigns develop and maintain specific critical capabilities directed at making the scientific and technological advances necessary to assess and certify weapon performance now and over the long term.

CD
Critical Decision

CSSE
The Computational Systems and Software Environment Subprogram

CT
Commodity Technology
CT systems are based on predominantly commodity hardware and, thus, require minimal changes to simulation tools when porting to these machines and making the machines available to end-users.

DARHT
Dual-Axis Radiographic Hydrodynamic Test

Design and Production Agencies
These agencies are the NNSA national weapon laboratories, the NNSS, and the plants that make up the Nuclear Weapons Complex.

DOD
Department of Defense

DOE
Department of Energy

DP
Defense Programs (NA-10)

DSW
Directed Stockpile Work
This includes all activities that directly support the nuclear weapons stockpile, including maintenance and surveillance, planned refurbishment, reliability assessment, weapon dismantlement and disposal, and R&D and certification technology efforts to meet stockpile requirements.

EPIC
The Design, Engineering, and Physics Integrated Codes
The term EPIC refers to the B&R classification code within the DOE accounting system. These codes contain multiple physics capabilities for solving integrated design, engineering, and safety/surety problems.

Exascale Computing
Exascale computing systems are capable of at least one exaflops (a billion billion calculations per second). Such capacity represents a thousand-fold increase over the first petascale computer put into operation in 2008. Exascale systems are needed to support areas of research critical to national security objectives as well as applied research advances in areas such as climate models, combustion systems, and nuclear reactor design not within the capacities of today's systems. The computational power of exascale systems is needed for increasing capable data-analytic and data-intense applications across the Federal complex. Exascale is a component of long-term collaboration between the ASCR program and the ASC Program.

FFRDC
Federally Funded Research and Development Centers

flops
Floating Point Operations per Second

FOUS
The Facilities Operations and User Support Subprogram

FYNSP
Future Years Nuclear Security Plan

GOCO
Government-Owned, Contractor-Operated

HPC
High Performance Computing

HQ
Headquarters

I/O
Input/Output (data transfer)

IC
The Integrated Codes Subprogram

ICF
Inertial Confinement Fusion

LAN
Local Area Network

LDRD
Laboratory Directed Research and Development

LEP
Life Extension Program
A list of activities designed to extend the operational service life of an existing nuclear weapon by providing new subsystems and components. Note: sometimes referred to as service life extension program (SLEP).

Level-1
This is the top level of the budget categories in the nWBS of DP.

Level-2
Different from a Level-2 milestone, this is the second level for the nWBS and refers to the Office of Research, Development, Test, and Evaluation (NA-11).

Level-3
Level-3 for the nWBS refers to the Office of Advanced Simulation and Computing (NA-114).

Level-4
Level-4 for the nWBS refers to the subprograms within the ASC Program. Federal managers allocate funds to this level unless the Federal program manager (director) elects to allocate resources to a specific activity.

Level-5
Level-5 for the nWBS refers to the products that the ASC Program develops and delivers. Federal managers collaborate with laboratory managers to plan product strategies. Federal management and oversight are focused on the integration of the products. Level-5 products are the culminated results of Level-6 projects. Level-5 products may be the result of single or multiple laboratory efforts. Sites can shift funds among Level-5 products within the same Level-4 subprogram.

Level-6
Level-6 for the nWBS refers to the projects that make up the technical work necessary to develop and deliver the Level-5 products. The Federal managers are cognizant of the specific projects; however, the individual laboratories manage and execute them.

M&O
Management and Operating

MPI
Message Passing Interface

This term refers to bulk synchronous coarse grain parallelism.

National Security Laboratories
This term encompasses three NNSA laboratories: Lawrence Livermore National Laboratory (LLNL), operated by Lawrence Livermore National Security, LLC; Los Alamos National Laboratory (LANL), operated by Los Alamos National Security, LLC; and Sandia National Laboratories (SNL), managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation.

nWBS
National Work Breakdown Structure

PEM
The Physics and Engineering Models Subprogram

Petascale
A computer system capable of reaching performance in excess of one petaflops (one quadrillion floating point operations per second). Examples of ASC Program petascale platforms include Sequoia (LLNL), Cielo (LANL), and Roadrunner (LANL).

Predictive Capability
This is a summary phrase used to describe the ASC Program’s strategy of emphasizing a deeper understanding of the underlying science, with the goal of replacing the phenomenology in the integrated codes by better theoretical models and a quantification of their limitations.

PSAAP
Predictive Science Academic Alliance Program

QMU
Quantification of Margins and Uncertainty

R&D
Research and Development

SC
Office of Science

SFI
Significant Finding Investigation

SQA
Software Quality Assurance

SQE
Software Quality Engineering

SSP
Stockpile Stewardship Program

Stockpile
Warhead types that equip strategic land, air, and sea-based forces with nuclear capability.

Stockpile Requirements Addressed by the ASC Program
Workload of the ASC Program in support of the lifecycle management of nuclear weapons, which includes, but is not necessarily limited to, annual certification, LEPs, and SFIs.

STRATCOM
U.S. Strategic Command (USSTRATCOM) controls operational commitment of strategic nuclear forces. STRATCOM provides the primary voice for strategic nuclear force structure, modernization, and arms control. It assures the integration of strategic nuclear policies and prepares for use if deterrence should fail.

UGT
Underground Test

UQ
Uncertainty Quantification

V&V
The Verification and Validation Subprogram

WBS
Work Breakdown Structure
For the ASC Program, it is the hierarchical representation of the total work of the program based on products and projects.

Weapons Science Code
These computer programs, or "codes," are used for single-physics modeling at a fundamental level, often involving molecular dynamics codes, nuclear physics, or atomic physics.