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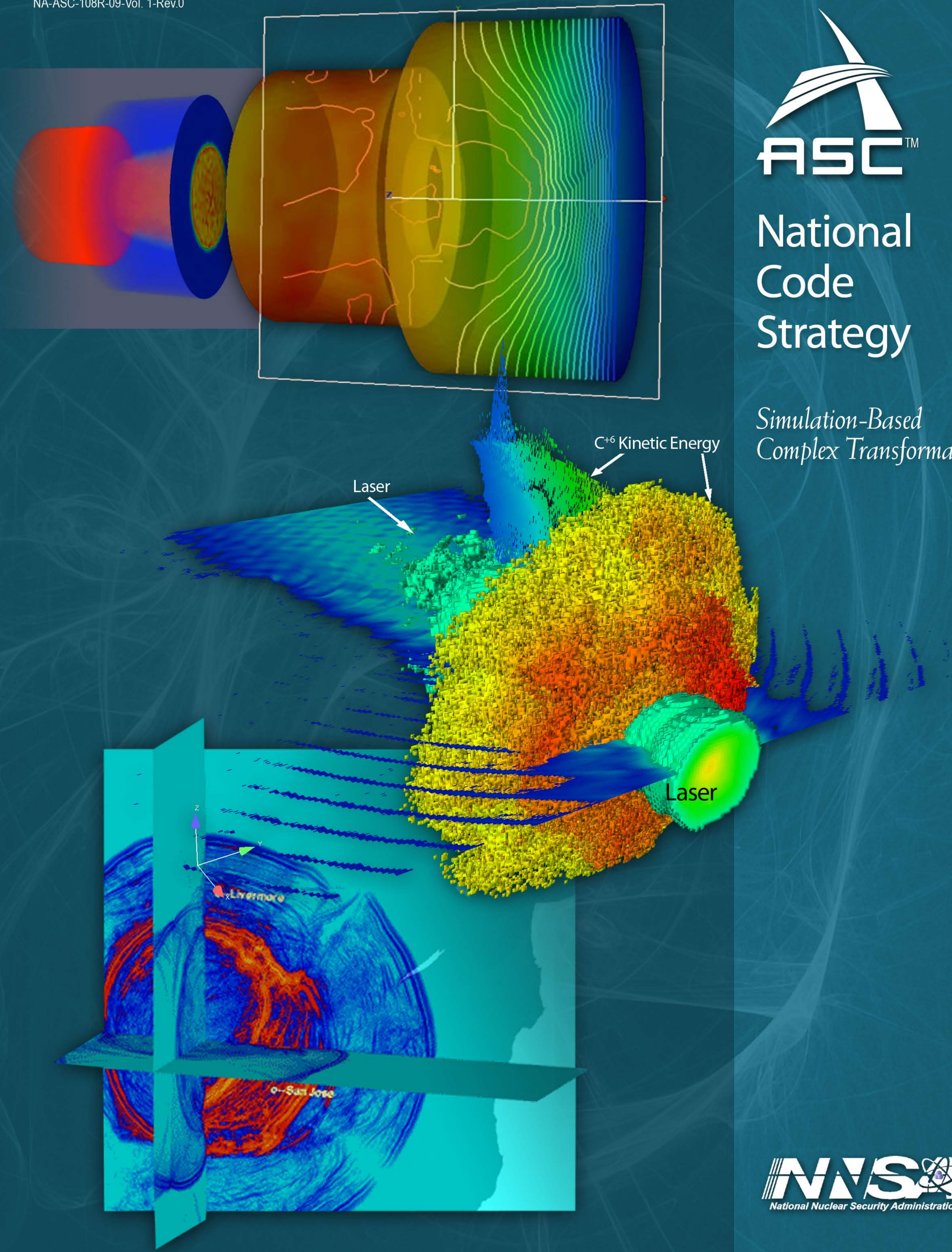

ASC™

National Code Strategy

Simulation-Based Complex Transformation

National Nuclear Security Administration

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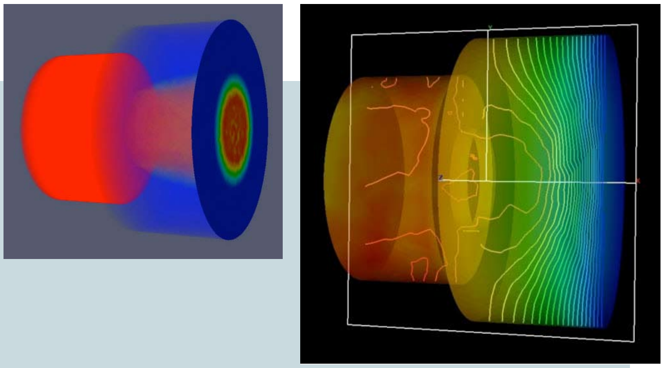

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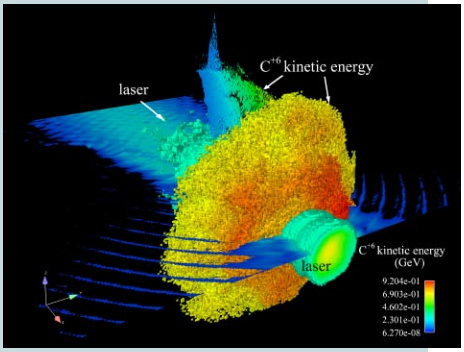

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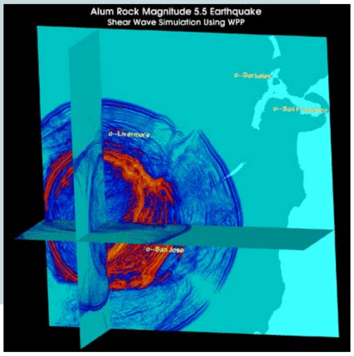

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

ON THE COVER:

Shown top-to-bottom:

1. (Left) Ion number density and current density. (Right) Potential field. *(Sandia National Laboratories)*

2. Large-scale 3D particle-in-cell simulations at realistic solid target density evince the generation of a beam of GeV carbon ions. Combined with a robust experimental effort, the kinetic simulations of ion acceleration by short-pulse laser are enabling the development of a new generation of ion beam sources and may enable the success of ion-based fast ignition inertial confinement fusion. *(Los Alamos National Laboratory)*

3. The image shows the damaging shear-wave motions from the Alum Rock earthquake simulated with the WPP code. The image shows shaking intensity (orange being the most intense) from a point of view below the surface with east and west reversed. Note that shaking is most intense in the Santa Clara Valley around San Jose and that the wave fronts spread at different speeds to seismic wave-speed variations. *(Lawrence Livermore National Laboratory)*

NNSA
National Nuclear Security Administration

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Advanced Simulation and Computing National Code Strategy

Simulation-Based Complex Transformation

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Advanced Simulation and
Computing Program, NA-121.2

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UNITED STATES OF AMERICA

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EXECUTIVE SUMMARY

The Integrated Codes (IC) program element plays a key role in the success of the Advanced Simulation and Computing (ASC) Campaign and the Science-Based Stockpile Stewardship Program (SSP). Stockpile stewardship encompasses a broad range of activities to ensure the safety, performance, and reliability of the nuclear weapons stockpile, from development and certification of the weapons design, through manufacturing, annual assessments, surveillance, and resolution of significant identified issues, to dismantlement. The IC provides software products that bridge nuclear weapons stockpile activities and the phenomenological and computational science underpinnings of stockpile stewardship. If the SSP is to be on the critical path for nuclear weapons certification, IC must deliver *predictive* ASC simulation capability by correctly representing the relevant physical phenomena in full three-dimensional detail for operational stockpile scenarios. Therefore, the role of IC is to ensure that accurate, robust, and usable codes are developed, deployed, and supported across the spectrum of ASC high-performance computing platforms to support the work of analysts and designers in performing credible, predictive ASC simulations for weapons certification. To accomplish this mission, IC must also perform research in algorithms to improve the current generation of simulation capabilities, lay the groundwork for the next generation of predictive simulation tools, and preserve the core competencies of computational sciences in physics, engineering, and mathematics that enable and steward advanced simulation sciences.

The direction from the Program's *ASC Strategy: The Next Ten Years*[1] is to emphasize a deeper understanding of the science issues underlying predictive accuracy of computational simulations, and the attendant uncertainties related to the limitations of modeling and simulation applied to the physical world. The complex, nonlinear, and multidisciplinary nature of weapons science problems requires that the ASC Program remain a leader in computational simulation science. It is only through such leadership that major sources of uncertainty in safety and reliability assessment of aging stockpile systems can be addressed as we move into the future, and the country can maintain its nuclear deterrence capabilities. These challenges have been examined in greater detail in the *ASC Roadmap*.[2] Goals have been set for addressing major sources of uncertainties in weapons phenomenology and simulation, with the associated advancements in enabling capabilities, such as computing platforms, to accomplish these goals.

As we look to the future of the ASC Program, and the larger mission of the National Nuclear Security Administration (NNSA), we see additional challenges to be faced, from infrastructure and capability lifecycle costs, to the broader needs of the stockpile systems and the national security challenges of the 21st century. In thinking at this scale, it is clear that computational simulation technologies will play an increasing role, not only in national security, but also throughout the technological landscape. Therefore, it is important that we understand the transformational phase of the current NNSA Complex, the larger transformations at work in the world driven by computing and information technologies, and the central role that IC plays in bridging computations to real-world scenarios. The overarching vision for the IC strategy is "simulation-enabled complex transformation," which signifies that computational simulation will play a critical enabling role not only in ensuring the continued stewardship of the stockpile without underground nuclear testing, but also in transforming the overall Nuclear Weapons Complex. This suggests that computational simulation will impact the full-system lifecycle, ranging from how we design, certify, and assess the performance, safety, survivability, and reliability of weapons systems, to how weapons assemblies and components are manufactured, transported, stored and safe-guarded, monitored, and finally dismantled. This vision is articulated through four major objectives, and the ASC National Code Strategy is designed to support these program objectives:

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[1] NA-ASC-100R-04-Vol. 1-Rev.0, August 2004

[2] NA-ASC-105R-06-Vol. 1-Rev.0, November 2006

1. Advance world-leading predictive science, providing the capability to sustain stockpile stewardship without returning to underground nuclear testing as weapons age and we move further from the test base.
2. Enable Quantification of Margins and Uncertainties (QMU)-based certification, transforming the broader certification process to allow more effective and selective use of aboveground experiment (AGEX), certification tests, flight tests, and other tests.
3. Catalyze a responsive infrastructure through pervasive simulation across all aspects of the stockpile lifecycle, such as design, certification, manufacturing, Significant Finding Investigation (SFI) resolution, transportation, security, safe dismantlement, outputs and environments, etc.
4. Enable a broadened national security mission, in which simulation tools extend beyond stockpile stewardship and enable the next-generation mission of the Complex.

This strategy maximizes the impact of the ASC Program on stockpile certification, addresses the four objectives given above, helps to manage the risks associated with upcoming programmatic and technical challenges, and ensures the continued relevance and effectiveness of the program into the future. The strategy is strongly aligned with the SSP strategic direction and the ASC strategic vision as defined in the 10-year *ASC Strategy* and the *ASC Roadmap*. The strategy clarifies the needed direction and approach for IC and defines a path towards its implementation.

The ASC National Code Strategy rests on three major strategic components to help it achieve its four objectives:

1. Establish the National Simulation Portfolio for Weapons Science and Engineering, and Stockpile Certification.

This strategic component defines a core simulation capability portfolio, consisting of seven modern application capabilities across six broad application areas, representing a consolidation of the current state of some 14 ASC and legacy codes. This component also includes ending development funding for legacy codes, a generalized capability to couple the various national code capabilities, and additional consolidation in the area of setup tools. The National Simulation Portfolio consists of the following:

Three Major Validated, National, Integrated, Full-System Capabilities
2 national nuclear performance systems, spanning primary and secondary performance, to provide peer-reviewed weapons performance assessment
1 national non-nuclear assessment system, spanning core simulation capabilities needed for stockpile lifecycle, including manufacturing and engineering certification
Four National Integrated Capabilities for Specific Applications
1 national nuclear explosives package (NEP) safety capability
1 national high energy density physics (HEDP)/ inertial confinement fusion (ICF) capability
1 national Radiation Effects capability for electrical systems
1 national diagnostics capability

2. Advance Computational Algorithms to Enable Predictive Simulation and QMU.

This component focuses on enhancing the scalability of underlying computational methods to peta and exa scale computing, collaborating on programming models for petaFLOP and exaFLOP scale computing, and delivering advanced capabilities for QMU and uncertainty quantification.

3. Broaden the Impact of ASC Simulation Capabilities on National Security.

This final component addresses the objective of broadening ASC impact through outreach, development, and support of interagency partnerships, and enhancing capabilities for expanded national security missions. These major strategic components will be explained in detail, with specific defined goals or activities for each of the three areas, and targets for implementing the strategies. The strategies represent a significant change in the operational culture of IC, moving from independent laboratory efforts designed primarily to meet the mission needs of their respective laboratory projects, to a coordinated and interdependent national program design to meet the mission needs of the overall SSP. The existing operational culture within the defense laboratories predates the current ASC Program and, as such, will require ongoing attention and perseverance in order to achieve its potential benefits. However, it is consistent with the larger trends towards consolidation and interdependence within the U.S. Nuclear Weapons Complex, and it should benefit from the broader increase in collaboration and teamwork among the national laboratories.

1.0 INTRODUCTION

From the Manhattan Project, through the Cold War, to the current Stockpile Stewardship Program, our capability to ensure the performance and safety of nuclear weapons has relied on the accuracy of scientific calculations. Now, as we work to sustain an aging stockpile—while maintaining a moratorium on full-scale nuclear testing—we are more dependent than ever on the predictive accuracy of our integrated codes for the annual assessment of our nation's nuclear stockpile.

The following code strategy introduces an essential evolution in the ASC Program that recognizes both its technical needs and the need to better utilize our resources. Since the inception of the Program, we have been exploring several approaches to weapons simulation simultaneously, supporting parallel efforts at the national laboratories to ensure robust peer review and to converge on the best numerical approaches and physical models to simulate the time evolution of a nuclear device. This multipronged approach has enabled us to deliver accurate and robust models of nuclear performance. In the process, we have learned a great deal about the most efficient ways to proceed and have developed technical approaches that will allow us to manage the enterprise in a sustainable manner.

To make optimal use of our resources, we have defined a national code portfolio focused on an essential set of simulation tools. This suite of tools will continue to ensure accurate representation of the data obtained from the days of nuclear testing and, at the same time, use modern representations of the most accurate models of essential physical processes, maximizing our ability to achieve the ultimate goal of a real predictive capability.

We have reached a point in the lifecycle of the ASC Program where transitioning to a modernized national code portfolio, as articulated in this strategy, is a necessary next step. This strategy positions the ASC integrated codes to take advantage of advanced computational algorithms for scaling to problem sizes that are orders of magnitude larger than current capabilities. Such advances are necessary to reach the weapons program's goals in predictive science and Quantification of Margins and Uncertainties (QMU). Furthermore, it builds the basis for the ASC Program to broaden the reach of the ASC simulation codes to application areas in national security that are outside of the realm of nuclear weapons and stockpile stewardship.

This is a crucial time for the Stockpile Stewardship Program, and I strongly believe that effective execution of this strategy will take the program to the next level.

— Robert Meisner
NA-121.2

2.0 OVERVIEW AND BACKGROUND

Role and Impact of the ASC's Integrated Codes Program

The ASC integrated codes provide the direct interface from ASC capabilities to the weapons designers and analysts who are users of those capabilities. These codes constitute a programming environment for virtual modeling and simulation of complex physical systems and phenomena. They are the frameworks for implementation of phenomenological science and numerical algorithms, and they are the target for ASC verification and validation studies, assessments, and metrics. In short, the integrated codes are arguably the key components that integrate the efforts of the entire ASC Program.

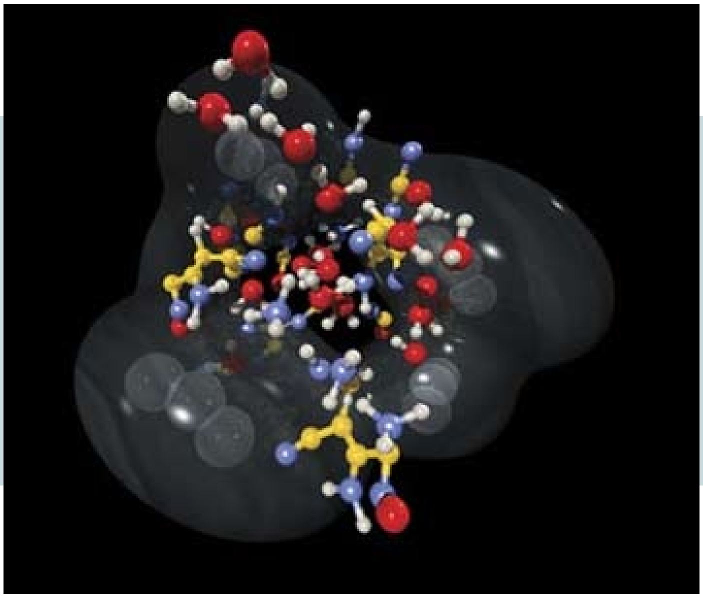
The Integrated Codes (IC) program element within ASC has the responsibility to develop and maintain these simulation code capabilities throughout their lifecycle, from planning and requirements management, though feature implementation and debugging, to user support and porting to future platforms. IC also has historically supported further enhancement and porting of pre-ASC "legacy" codes, research and development of computational algorithms to enhance codes and predictive capabilities, and ancillary setup tools to facilitate preparation of computational models for running advanced simulations.

As such, IC is critical to the SSP. The simulation capabilities embodied in the IC software products are used for analysis in a wide range of operational stockpile scenarios. For the SSP to be successful, the codes must be fast, robust, and capable of dealing with the wide range of phenomenology and the high degree of physical complexity inherent in these scenarios. The codes also must continue to improve in the content of their science, in the accuracy of their models and algorithms, and in their ability to model systems with the necessary level of spatial and temporal fidelity to resolve phenomenology in order to compensate for the increasing uncertainties posed by an aging stockpile and the cessation of underground testing. Finally, the IC program element must remain tightly integrated with the other program elements within ASC, as well as the other Defense Program elements, to ensure that phenomenological models and solution methodologies are continually improving and increasing the overall predictive accuracy of the simulation capabilities.

To provide further background and context, a description of the IC program subelements and the integration of IC with the other elements of the ASC Program, is provided in Appendix B.

Explosives at the Microscopic Scale Produce Shocking Results

Simulations show that molecules in detonating high explosives take on metallic properties. Metallic molecules are translucent, while insulating molecules are colored according to atom type: hydrogen is white, carbon is yellow, nitrogen is blue, and oxygen is red. *(Lawrence Livermore National Laboratory)*



ASC Program Strategy, Roadmap, and Predictive Capability Framework

The direction from the program's *ASC Strategy: The Next Ten Years* is to emphasize a deeper understanding of the science underlying predictive accuracy of computational simulations and the attendant uncertainties related to the limitations of modeling and simulation of the physical world. The complex, nonlinear, and multidisciplinary nature of weapons science and engineering problems require that the ASC Program remain a leader in computational simulation science. It is only through such leadership that major sources of uncertainty in safety and reliability assessment of aging stockpile systems can be addressed in the future and the country can maintain its nuclear deterrence capabilities. These challenges are examined in greater detail in the *ASC Roadmap*, wherein goals have been set for addressing major sources of uncertainties in weapons phenomenology and simulation, with associated advancements in enabling capabilities, such as computing platforms, to accomplish these goals.

The *ASC Roadmap* articulates goals for predictive science focus areas in the ASC Program. These focus areas are often referred to as "knobs," in that unresolved physics are often addressed by *ad hoc* parameters in the simulation models that are adjusted to provide a level of calibrated simulation capability. The planning activity around these predictive sciences issues has evolved into a broader integration activity across the major science, engineering, and technology development programs within stockpile stewardship. This integration activity has developed the Predictive Capability Framework (PCF), which defines major activities associated with the improvements in predictive capability for stockpile stewardship and coordinates those activities among the ASC, Defense Science, Engineering, and Inertial Confinement Fusion (ICF) campaigns. In this context, the present ASC National Code Strategy must serve to advance the *ASC Strategy*, support the *ASC Roadmap*, and help to accomplish the broad goals of the PCF over the next decade.

Role of Integrated Codes in Peer Review

Historically, the concept of rigorous peer review has played a key role in the development and maintenance of the nation's nuclear stockpile, to the extent of helping to define the structure, roles, and responsibilities of the Nuclear Weapons Complex. The physics and engineering assessments performed by the national laboratories for the stockpile are based on expert use of computer simulations and the results of focused and integral experiments. An assessment should be declared complete only if it can pass the test of a rigorous peer review. The peer review process for a given assessment could be as simple as reviewing a document or presentation of the work done or as complex as performing independent calculations and experiments for arbitration by external participants. The mission space of the ASC code portfolio discussed in this strategy covers nuclear performance, engineering assessment, nuclear explosives package (NEP) safety, high energy density physics, diagnostics, and radiation effects for electrical systems. In some application areas, new experiments are not possible, and peer review using multiple ASC-funded capabilities is necessary to reduce the risk of technological surprise. In others where experimental options are still available, peer review can be achieved through a combination of ASC capabilities, commercial tools, and small experiments.

Future Challenges for the ASC Program

For the ASC Program to integrate with stockpile certification methodologies, the ASC code capabilities must also be well aligned with the particular needs of the current and future stockpile. This means that the codes must have the capability to represent operational stockpile scenarios in a timely manner. Given numerous external pressures and constraints on the program, this implies that the IC program element must examine tradeoffs between strategic goals, manage its capability requirements, prioritize development activities to meet changing stockpile needs, and emphasize agility and responsiveness in capability development. Some of the particular challenges are detailed below.

Predictivity, QMU, and Achieving Sustainability

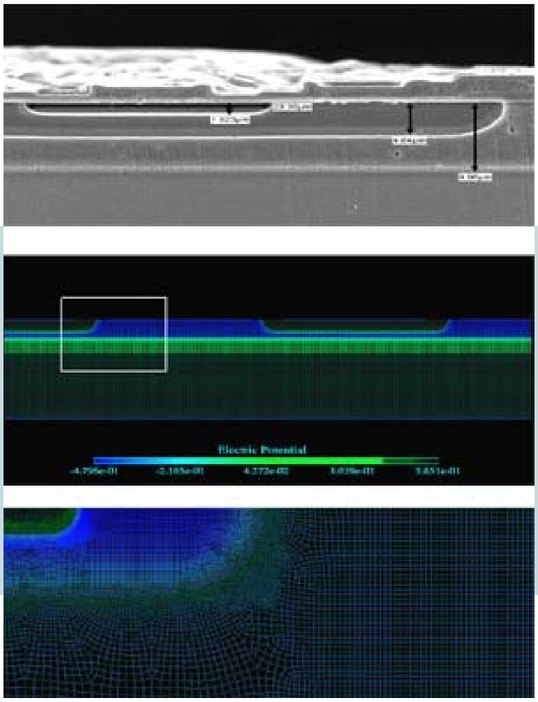
As detailed in the *ASC Roadmap*, the program is working closely with the other nuclear weapons science, technology and engineering (ST&E) campaigns, through the PCF. The program is thus advancing predictive science such that our ability to confidently predict the behavior of systems independent of underground nuclear test data is superior to our ability to extrapolate historical data to the current stockpile. To reach this "point of sustainability," we must make significant improvements in the predictive simulation of key phenomena. The current lack of predictive capability for these phenomena is managed by the adjustment of *ad hoc* parameters, using historical, integral test data. These so-called "knobs" must be resolved in favor of validated science-based phenomenological and age-aware models, with associated uncertainties. Achieving this scientific understanding, and integrating that understanding with advanced computational science, is a significant research activity.

We estimate that advanced models, with the requisite predictive capabilities to resolve key knobs, will require higher levels of spatial and temporal fidelity, large-scale platforms with up to 1 million teraFLOPS (1 exaFLOP) of computing capability, advanced scalable algorithms capable of executing accurately and effectively with over 1 million parallel processes or threads, and multiscale methods that can bridge from sub-nanometer to meter length scales. To apply these advancements to stockpile applications, these advanced algorithms and models must also be implemented into the integrated production codes to be used by stockpile designers and analysts, and the integrated codes must keep pace with advancements in computational platforms, enabled by the Program's platform strategy.

Finally, achieving "predictive science" and a "point of sustainability" cannot be fully understood without an overarching framework for certification and assessment of these complex systems. Within the context of stockpile stewardship, this framework is termed the Quantification of Margins and Uncertainties (QMU) approach. The practical impact of QMU on the goals and future challenges of the ASC Program is not only to clarify the focus and objectives of computational simulation for weapons applications, but also to emphasize the importance of uncertainty and error quantification in simulation science. Thus, increasingly the ASC integrated codes will be used in conjunction with stochastic methods, with the goal of quantifying output measures such as sensitivities, probability distributions, and uncertainty intervals. The increased computational demands posed by such output metrics will drive us to examine how algorithms can enable stochastic variables and solution gradients to be obtained more effectively from integrated codes.

Disruptive Changes in Computing Platforms

For the past 15 to 20 years, encompassing the history of the ASC Program, high-performance computing (HPC) technology has been coupled to high-end personal computing and workstation computing technology through its leveraging of commodity microprocessor designs. For much of that period, significant gains in overall computing capability have come from increasing gains in single processor chip speed. Recently, that trend has changed, in part because of an unsustainable increase in power requirements associated with increasing processor clock speeds. New trends in microprocessors include the use of multiple cores or processing elements per chip, as well as the use of co-processors or accelerators to increase overall system performance. These new microprocessors are designed to deliver improved performance at lower power-consumption rates, and are significantly replacing single core chips throughout all levels of personal and workplace computing.



Qualification Alternatives to the Sandia Pulsed Reactor's (QASPR's) Successful "Blind" Best Estimate Plus Uncertainty Predictions vs. Experimental Data for Radiation Effects Study

Electronic device micrograph (top), computational model of the device (center), and a detailed view of computational mesh used to model the device (bottom). *(Sandia National Laboratories)*

The ASC program is now faced with potentially disruptive software development challenges, if the full power of platforms based on these new processor trends is to be reached by our integrated production codes. The programming model that has been successfully used to support the wide spectrum of ASC capability and capacity clusters is the Message Passing Interface (MPI), implemented with a distributed memory architecture. However, this existing MPI programming paradigm may not translate effectively to new many-core and hybrid processor-based architectures. In particular, the communication bandwidths and memory limitations of such architectures are different than the current generation of homogenous processors clusters. This change in processor technology is akin to the change in the late 1990's when vector machines were replaced by clusters. That change was one of the driving factors for the establishment of the original Accelerated Strategic Computing Initiative (ASCI) program, and directly led to the development of the current generation of integrated weapons codes. We are at the beginning of another disruptive change in hardware technology that may require a corresponding effort to re-engineer the integrated weapons codes to take advantage of the hardware.

Future Budget Profile

The overall ASC Program budget has experienced gradual declines in the past two to three years, and these reductions are expected to continue and even accelerate in the next decade. The reasons for this are multifaceted, but given the increasing cost of resources to maintain code capabilities and address changes in computing hardware, the program will face difficult decisions to maintain current capabilities. The aforementioned need to advance predictive science while meeting stockpile demands cannot be addressed without reducing the amount of effort required to maintain current simulation capabilities. While the ASC Program will be actively managed to determine the best balance of investments across the program elements, it cannot be assumed that the program budget will be balanced without some level of reductions in budgets for the Integrated Codes element.

Robust and Usable Codes

The characteristics of code robustness, performance, and overall usability are critical to program success because the codes can have an impact on the stockpile only if they are used. Usability, in a general sense, depends on the code possessing the basic robustness, performance, and capabilities to be a viable tool for a particular application. The present portfolio of modern ASC simulation tools has reached a sufficient level of maturity and robustness to meet the requirements of the stockpile annual assessment and certification activities. However, the current codes must maintain this level of robustness while enhancing their levels of predictive accuracy. Furthermore, with the increasing use of uncertainty quantification algorithms, codes will need to continue to improve their robustness, in order to provide solutions over a broad space of variable parameters without extensive user intervention.

Broadening the Impact of ASC Capabilities

As the ASC Program matures, there is growing interest in its capabilities within the larger national security community. This represents both an opportunity and a challenge for the program. Having a widened footprint in the national security arena increases the realized benefit from ASC and stockpile stewardship investments and may help secure and stabilize the ASC investment with an increasingly constrained nuclear weapons program. As the attention of the national security issue shifts from the nuclear weapons "core mission," however, the ASC Program will need to extend its capabilities to meet the needs of national security partners whose main focus is not the assessment of the U.S. nuclear stockpile — these extensions present challenges to a program already struggling to maintain current capabilities. The conflict between deep-rooted sociology ("our mission is the nuclear stockpile and that's what we want to do") and financial reality (caused by gradual shift of the nation's priorities) will not be resolved without strong, decisive leadership and a clear, unified message from the NNSA. It is clear that the program has a responsibility to help the broader national security community find ways to leverage the government's considerable investment in ASC capabilities.

Risk Assessment for Integrated Codes

In this introduction, we have provided a context for the IC program element by examining its role in stockpile stewardship, the direction set for the overall ASC Program through the ASC Strategy and Roadmap, and the future challenges arising from the Program's direction and external constraints and pressures. Meeting the ASC Program's goals in the face of these challenges will be extremely difficult without changes in the IC program element. This risk assessment examines the IC program element in terms of anticipating future problems and developing mitigation plans to minimize mission, cost, and schedule losses. The ASC National Code Strategy, detailed in Section 3 of this document, can be understood as a mitigation plan to address high- and medium-risk exposures for the IC program element (Table 1).

The last column of Table 1 identifies the major components of the ASC National Code Strategy, which are designed to mitigate the Program's identified risks. In the next section, these major components of the strategy will be described in detail.

Table 1. Risk Assessment for IC Program Element

Risk Description	**Risk Assessment**			**Relevant Code Strategy Component for Mitigation**
	Consequence to Stockpile Stewardship	**Likelihood**	**Risk Exposure**	
Maintaining the status quo of developing and maintaining a broad range of application codes at each laboratory, with multiple approaches to mitigate risks associated with unquantifiable numerical simulation errors, will lead to less capable, robust, and effective codes, and unsustainable maintenance costs	Very High	High	High	1. (National Code Portfolio)
Without further advancements in computational algorithms, the ASC integrated production codes will fail to achieve sufficient levels of predictive capability to continue to certify and assess nuclear weapons systems without reverting to legacy testing Complex, including underground nuclear testing	Very High	Moderate	High	2. (Advanced Computational Algorithms)
Current ASC integrated production codes will not scale well on next-generation platforms, resulting in poor efficiency and an inability to achieve model and physics fidelity necessary for predictivity	High	Very High	High	2. (Advanced Computational Algorithms)
Codes will fail to have a broad impact on important elements of national security outside of nuclear weapons assessment and certification	Moderate	Moderate	Medium	3. (Broaden ASC Impact on National Security)

3.0 ASC NATIONAL CODE STRATEGY

As detailed in the introduction, the objectives of the IC program element are designed to realize the vision of "simulation-enabled complex transformation," and correspond, in a progressive fashion, to broader spheres of application, influence, and impact. These objectives are as follows:

- Advance world-leading predictive science, providing the capability to sustain stockpile stewardship without returning to underground nuclear testing as weapons age and we move further from the test base;
- Enable QMU-based certification, transforming the broader certification process to allow more effective and selective use of AGEX, certification tests, flight tests, and other tests;
- Catalyze a responsive infrastructure through pervasive simulation across all aspects of the stockpile lifecycle such as design, certification, manufacturing, SFI resolution, transportation, security, safe dismantlement, outputs and environments, etc.;
- Enable a broadened national security mission, in which simulation tools extend beyond stockpile stewardship and enable the next-generation mission of the Complex.

The ASC National Code Strategy itself rests on three major strategic components designed to help the national Program achieve its four objectives, while helping to mitigate the risks associated with future program challenges. These three major components are as follows:

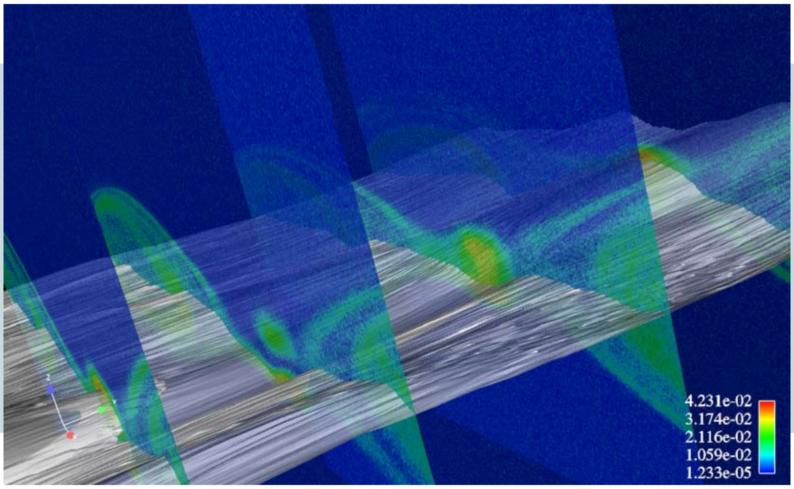
1. Establish the National Simulation Portfolio for Weapons Science and Engineering, and Stockpile Certification;
2. Advance Computational Algorithms to Enable Predictive Simulation and QMU;
3. Broaden the Impact of ASC Simulation Capabilities in National Security.

In the following sections, the three major components of the ASC code strategy are presented, with the major steps of each strategy detailed. In Appendix A, specific targets are laid out over the following six years to guide the program in the implementation of this strategy.

1. Establish the National Simulation Portfolio for Weapons Science and Engineering, and Stockpile Certification

This first strategic component focuses the Program's efforts on activities necessary to our mission, while increasing interdependence and collaboration, to establish a sustainable, predictive capability. Throughout the first 10 years of the ASC Program, the three laboratories have largely focused on developing simulation capabilities based on their

Magnetic islands and drift-kink instability observed in 3D large-scale fully kinetic VPIC simulations run on the Roadrunner base system of magnetic reconnection in electron-positron plasma. *(Los Alamos National Laboratory)*



own mission requirements. While these mission requirements are distinct in terms of the science and engineering work required for particular systems and subsystems, there are some significant overlaps among the laboratories in terms of the capabilities required to meet their respective missions. For example, multiple laboratories have requirements that drive the development of simulation capabilities for engineering assessment, high energy density physics, nuclear performance, safety, and diagnostics. Thus, in keeping with the concept of a national, three-laboratory (tri-lab) program, there are opportunities to consolidate the broad range of current simulation code efforts into a more integrated and streamlined program of production code projects. This will be termed the National Simulation Portfolio for Weapons Science and Engineering, and Stockpile Certification. The composition of the national portfolio is summarized in Table 2 and Figure 1. The steps required to establish the National Portfolio are detailed as follows.

1.1. Define the core simulation capabilities needed to achieve predictive capability and meet stockpile certification requirements

The first step of this strategy is to define the essential composition of the national portfolio, which is the core simulation capabilities needed to achieve predictive capability and meet stockpile certification requirements. This composition must provide for the necessary level of science inquiry and independent peer review needed to resolve outstanding weapons science uncertainties, while minimizing duplicative efforts across the complex. As explained in the background and introduction, ASC simulation capabilities play an important role in certification and annual stockpile assessments and affect how peer review is established for critical assessments. For example, when the computation algorithms used for simulation are central areas of concern or uncertainty in an overall assessment process, it can be necessary to perform calculations based on algorithms that have been developed, implemented, and verified independently to ensure that systemic errors have not been introduced in the assessment activity. For this reason, peer review requires that in particular application areas, multiple ASC-funded capabilities be developed and maintained, while in other areas peer review requirements can be achieved through alternate approaches.

In addition to understanding issues of peer review, it is also necessary to consider the integral, multiphysics nature of most stockpile assessment applications, the fundamental physics algorithms and the unique aspects of how those algorithms combine in each particular application, the need to manage the programmatic complexity of the national portfolio, and the need to provide the necessary transparency into the Program's activities for customers and stakeholders. For these reasons, we have chosen to describe the composition of the national portfolio in terms of integrated capabilities for a set of distinct application areas. While there are some overlaps between these application areas in terms of physics or algorithm components, each area has unique requirements in terms of how these components are built into an integral capability and in how simulation capabilities are used for assessment and certification.

Table 2. Composition of the ASC National Simulation Portfolio

Three Major Validated, National, Integrated, Full-System Capabilities	**Lead Laboratories**
2 national nuclear performance systems, spanning primary and secondary performance, to provide peer-reviewed weapons performance assessment	Los Alamos National Laboratory (LANL) & Lawrence Livermore National Laboratory (LLNL)
1 national non-nuclear assessment system, spanning core simulation capabilities needed for stockpile lifecycle, including manufacturing and engineering certification	Sandia National Laboratories (SNL)
Four National Integrated Capabilities for Specific Applications	**Lead Laboratories**
1 national NEP safety and surety capability	LLNL
1 national High Energy Density Physics/Inertial Confinement Fusion (HEDP/ICF) capability	LLNL
1 national Radiation Effects for electrical systems capability	SNL
1 national Diagnostics capability	LANL

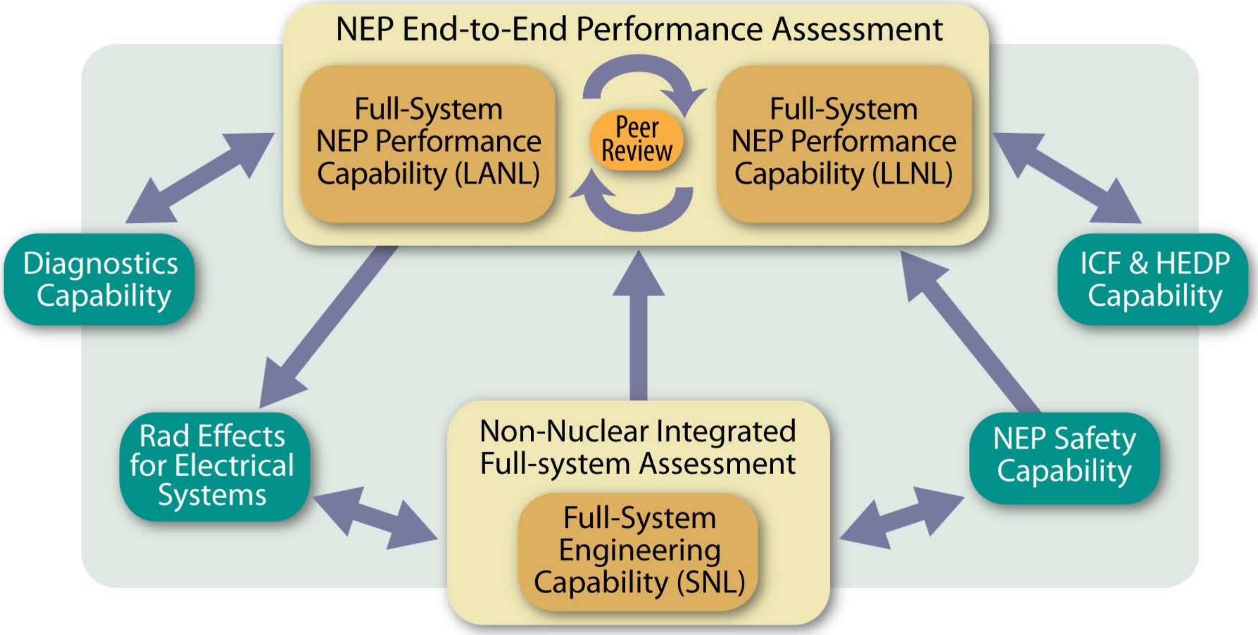


Figure 1. ASC National Simulation Portfolio for Stockpile Certification

Thus, to provide the core simulation capabilities for the national portfolio, we have identified six key application areas that require distinct simulation capabilities. The first two areas, weapons nuclear performance assessment and non-nuclear system assessment, are the broadest areas in terms of multiphysics complexity and scenario complexity. The other four application areas, NEP safety, HEDP, radiation effects for electrical systems, and diagnostics, are somewhat more focused than the first two areas in terms of the ranges of physics and scenarios considered, and thus are termed in the national portfolio as integrated capabilities for specific applications. Finally, in the area of nuclear performance assessment, to meet the need for peer review in assessments, we have identified the need to develop and maintain two independent national capabilities for nuclear performance assessment. In the following subsections, we provide a more detailed explanation of the simulation capabilities for each of the six application areas, and how those capabilities are to be used in a national tri-lab context.

One important aspect to note is that while each of these portfolio capabilities is being developed for the national program and for use at all three national defense laboratories, clear and focused responsibility is necessary within the program to manage requirements, work efforts, and expectations. Therefore, each capability has a lead laboratory that is responsible to the national program for the capability. This does not mean that the lead laboratory will necessarily be the only contributor to that capability, but rather that the laboratory is responsible for engaging with the federal managers and leads from the other laboratories to develop plans, execute the national effort towards the capability, and work to eliminate duplication of effort in the capability area. It is assumed that lab-to-lab agreements on issues such as co-development and user support would be negotiated in many cases to ensure that needs of the tri-lab stakeholders can be met. This issue is discussed later in this section.

The following subsections describe each of the capabilities in the national portfolio, including a high-level technical description of the capability, its role and importance to stockpile stewardship, and issues concerning the transition from the current state of national capabilities to the future, portfolio-based state for that application.

Nuclear Performance Systems

The role of the nuclear performance code systems is to predict the performance of the NEP of nuclear weapons. All that can be described of the physics modeled in nuclear weapons codes in an unclassified setting is that it may include hydrodynamics, radiation transport, fission, thermonuclear burn, high-explosives burn, and instabilities and mix. Modeling the interaction of these physics, with the fidelity to be predictive, places an enormous challenge on algorithm development, fundamental physics, computer science, and massively parallel computing platforms. Unlike some other components of nuclear weapons, the ultimate performance of the NEP, that is, detonation and production of nuclear yield, can no longer be determined experimentally. As an NEP changes from the exact configuration tested during the era of underground testing, the only recourse is simulation. These changes may occur unintentionally but naturally through the aging process, or intentionally through modifications made by design, for example, as part of a life-extension program. Nuclear performance code systems are central and indispensable to stockpile stewardship.

Non-nuclear Assessment System

The role of the non-nuclear assessment code system is to predict the condition and performance of both complete weapon systems and non-nuclear subsystems of nuclear weapons, including the integrity of structural and material components, in normal, abnormal, and hostile stockpile-to-target sequence (STS) environments in both their as-designed and aged conditions. This code system encompasses a broad range of physics and phenomenology, including structural and solid mechanics and dynamics, material failure and fracture, heat transfer and enclosure radiation, low-speed turbulent reacting flow and combustion, high-speed compressible fluid flow, thermal and fluid transport with chemistry, material melting, flowing, and solidification, and many diverse coupled multiphysics permutations of the phenomenological components listed above. While some STS environments can be simulated experimentally, thus providing evidence for stockpile non-nuclear certification and assessment, many cannot be approximated adequately. Others may present such a high degree of scenario uncertainty that experimental assessment is not a practical alternative. The uncertainties inherent in these scenarios are very broad and multifaceted, and the complexity of the weapon system and its failure modes makes it impossible to define a simple set of worst-case scenarios that can be assessed through physical testing. Therefore, fully assessing the safety and reliability of the weapon is possible only through validated computational simulation.

NEP Safety and Surety Capability

Surety simulations for the NEP involve a wide range of scenarios. The capabilities required for these assessments include some that overlap with those required for nuclear performance and engineering, as well as some that are specific to these applications. Because of the increasing importance on improved surety for the stockpile, and because of the unique physics associated with some of the assessments, it is necessary that there be a focused effort on these applications. The importance of surety assessments also raises the issue of peer review. For surety assessments, a sufficient peer review of the work can be done with the overlapping capabilities that exist in the nuclear performance codes, and potentially include some coupling of codes from the engineering suite that can be used to model the accident progression prior to the NEP response. There is a danger that a loose coupling of engineering capabilities will not be sufficiently accurate for some of the simulations, and this will need to be investigated. The next step required for this strategy to succeed is for the designated NEP Surety code activity to reach out to those who perform surety assessments across the Complex to identify a complete set of requirements for the physics and user support necessary.

High Energy Density Physics Capability

HEDP deals with the physics of matter and radiation under extreme conditions of temperature and pressure. The role of an HEDP capability is to design high-energy laser and Z-pinch experiments, including the design of experimental targets, simulation of the experimental HEDP conditions, and analysis of the measured data from those experiments. Such experiments are critical to stockpile stewardship by providing data on material response in x-ray and other extreme environments and validation data for phenomena relevant to performance. The HEDP capability is also relevant to many other high-energy physics research applications and provides a platform for research collaborations with the broader computational and experimental physics and astrophysics community.

Radiation Effects for Electrical Systems Capability

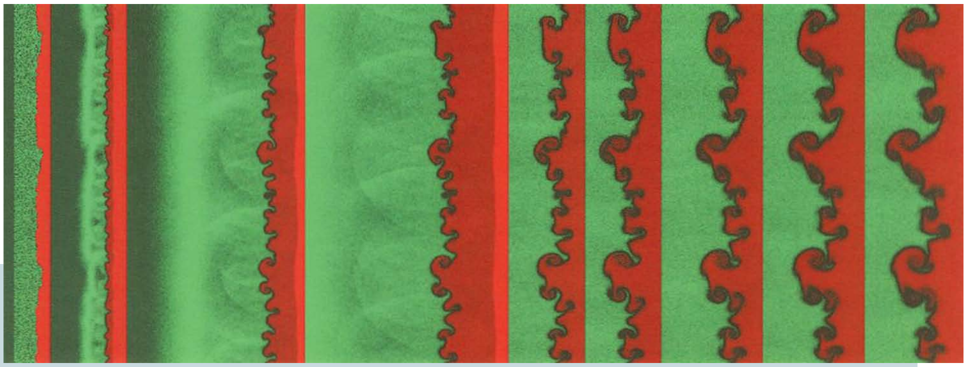
The role of the radiation effects for electrical systems capability is to predict the performance and reliability of electrical subsystems of nuclear weapons in radiation and other energetic environments. This system capability spans a range of physical phenomena, primarily involving radiation, electron and photon, and neutron-gamma particle transport, electromagnetic field behavior, semiconductor material and device response and damage, and overall circuit and integrated device electrical current response. Many of the hostile STS environments are no longer accessible to testing because of the cessation of underground nuclear testing and the consolidation and closure of nuclear reactor-based testing facilities. As a result, computational simulation has become the only viable method for understanding the response of weapon electrical systems to radiation environments. While the radiation environments of interest are primarily associated with hostile STS scenarios, additional normal and abnormal STS applications and scenarios require computational simulation. Given the many electrical subsystems that must function reliably for the weapon to act as an effective deterrent, certification and assessment of nuclear weapons systems require this simulation code capability.

Diagnostics Capability

Stockpile stewardship requires capabilities for the evaluation of nuclear diagnostic data, such as those collected on aboveground and underground nuclear tests, as well as radiographic data produced by current and proposed radiographic techniques. This in turn requires a diagnostics simulation capability for accurate transport of neutral and charged particles through detailed three-dimensional geometries using continuous energy cross-section sets and, particularly for radiographic applications, the implementation of accurate coupled neutral-charged particle transport physics. This diagnostics capability will also incorporate and perform transport calculations through hydrodynamic meshes from performance codes to allow a direct link from nuclear or hydrodynamic performance to observed nuclear or radiographic data. Finally, this capability extends beyond evaluation of nuclear diagnostics to such problems as criticality, vulnerability and lethality, and shielding assessment, as well as Special Nuclear Material (SNM) detection modeling and emergency response.

Ancillary Modular Capabilities and Setup Tools

In addition to defining the integrated capabilities of the national portfolio, there are opportunities to consolidate other efforts and increase collaboration across the IC program element. The first is in the area of physics models and software libraries that are integrated into end-user applications (see Appendix C for a description of common application architectures and terminology). These components range from application programming interfaces (APIs) for reading physical data, through modular physics packages such as particle transport or material constitutive models, to more general numerical libraries such as linear equation solvers and graph partitioning methods. Our goal in this area is to *enable cross-code sharing of physics modules and common material data APIs, and to drive the interoperability of solver libraries.* Sharing of physics modules should be done with caution to ensure that independence is maintained. Emphasizing common APIs for data and methods, and breaking down barriers to interoperability among components, will increase the leveraging of new capabilities across the laboratories, simplify applications by standardizing interfaces, and increase the diversity of physics and algorithms available to application developers and users.



A background gas (A < 1) inhibits jetting and leads to a more symmetric Richtmyer-Meshkov instability, as seen in the second simulation: Series of 9 snapshots, one every 50 ps, for Richtmyer-Meshkov instability development as a shock wave is transmitted from copper to a dense (0.5 g/cc) gas. In the third and fourth frames, one can clearly see the transmitted gas shock (still nonplanar), as well as a complex interaction of rarefaction fans from the roughened Cu/gas interface.
(Los Alamos National Laboratory)

The second area of focus is setup tools, or codes used by designers and analysts to set up models and input data to run physics simulations. Capabilities include geometry definition, generation of computational meshes, retrieval and insertion of material data into text input files, and workflow process assistants to help users organize and format model and case definitions for input to codes. Historically, meshing methods were related to the numerical schemes used in the simulation codes, and many setup tools and output file formats were developed exclusively for one, or a small number of codes. Over the years, our ability to reuse meshing technology for multiple applications and algorithms has greatly improved, and there are opportunities now to standardize around a smaller number of setup tools to support the national code portfolio. Our goal is *to standardize input and output data models for the national code portfolio and to consolidate efforts across the three labs related to setup tools.* Meeting this goal will require tri-lab planning and coordination, as well as cross-laboratory development and user support.

Implementing National Codes

As was discussed previously, the strategy of establishing code capabilities whose usage, and possibly development, extend across laboratory organizational boundaries is a significant cultural change for the weapons programs at the national laboratories. There are many potential pitfalls in terms of managing co-development work and user support, and, most importantly, expectations. While these challenges can also exist within a laboratory, they will need to be handled in more formal ways when the organizations in question are being governed under different contract arrangements with the federal government. There is precedent for such collaborations, and one approach that has worked is the establishment of a laboratory-to-laboratory Memorandum of Understanding (MOU), which clearly sets out roles, responsibilities, and expectations among the partners. The formalism of an MOU may not be required for all the national code interactions, but given the increased stake that each laboratory will have in the activities and products of the others, it will probably be needed in some instances. It is also expected that the federal program would play a role in the establishment of the MOU and that the negotiated arrangements would be reflected in the budgeting and implementation plans of the national program.

1.2. End development funding for legacy codes

Legacy codes, which are those whose development and usage predate the inception of ASCI, the precursor to the ASC Program, have played an extremely important role in stockpile stewardship and the development of the modern ASC modeling and simulation capability. During the first decade of the ASC Program, legacy codes helped to address major stockpile assessment and certification challenges both because of the familiarity and trust established in those codes among designers and analysts, and the relative lack of maturity in the newer ASC codes. However, because of the combined efforts of code developers and analysts committed to improving the capability and predictivity of ASC's modeling and simulation capabilities, the modern codes have now reached a sufficient level of maturity, robustness, and performance to become the default implementation framework for future simulation development activities. Therefore, to eliminate future duplication of effort, whereby improved physics capabilities would be implemented in multiple generations of simulation tools, the support for legacy codes should be limited to providing the continued capability to run benchmark calculations needed to assess modern code behavior. This means that legacy codes will continue to be ported and run on a subset of computing platforms, such as workstations and small capacity scale clusters, and that modifications to the codes will be limited to those necessary to ensure that the codes can be run in a correct and robust manner on hardware that is readily available to designers and analysts. The program will not support efforts to improve the parallel scalability or physics predictivity of the legacy tools, since investment in those efforts will be focused on the ASC modern codes.

While implementing this goal is not expected to result in an immediate significant reduction in overall development efforts, it will have long-term strategic benefits to the ASC Program. Completing the migration of users from legacy to modern ASC tools will produce long-term benefits by fostering a robust user community for the modern codes, and by helping to mature the modern tools through increased usage and testing. Experience has shown that an active user community is an important element of an overall user support network, and that support demands per user decrease as codes mature through usage and improve in their robustness, capability, and performance. Implementing this goal will also have broader ASC Program benefits, by focusing the efforts of the Physics and Engineering Models (PEM) and Verification and Validation (V&V) program elements on improving and evaluating the modern codes. It is envisioned that the legacy codes may continue to play a limited, but valuable, role for the program by, for example, supporting low-fidelity scoping studies and providing guidance for performance and robustness improvements in the modern codes. Finally, the costs and benefits of continuing to port legacy codes should be reconsidered as the implementation of the current strategy is being completed.

1.3. Establish the capability to couple between codes of national portfolio

The third step in establishing the national portfolio is establishing the capability to couple between codes in the portfolio. There are two primary reasons for establishing this coupling capability:

- Provide the capability to perform end-to-end, integral assessment of stockpile performance, safety, and survivability scenarios;
- Provide the capability to test multiple algorithms and alternate coupling strategies in order to better assess the predictive capabilities and uncertainties of the ASC modern codes.

In other words, the ability to couple the capabilities in the national portfolio will expand capability beyond those defined application areas to broader complex and multi-disciplinary assessment scenarios. It will also increase the algorithmic diversity of our portfolio, thereby mitigating the risks associated with the consolidation of code efforts.

Our purpose is to focus most resources towards developing well-integrated capabilities for each of the applications covered by the national code portfolio, rather than to develop a single sophisticated and deeply integrated framework to cover the full range of ASC application scenarios. Therefore, the ability to couple capabilities is envisioned to be flexible but nonintrusive for the code systems. For example, the establishment of common output file formats can accommodate the necessary internal variables to perform accurate transfers from one simulation domain to another, and common mapping and interpolation services can consistently link solution fields discretized on different meshes.

The coupling capability will be based on use cases that define common coupling scenarios of interest to designers and analysts. The following list is representative, though not exhaustive:

- Link nuclear performance systems to create combinations of different approaches to full system simulation (for discovery science, not certification);
- Link non-nuclear assessment and nuclear performance systems to perform integrated STS assessments;
- Link NEP safety and non-nuclear assessment capabilities to perform integrated safety assessment;
- Link non-nuclear assessment and electrical systems capability to perform integrated radiation effects assessment;
- Link nuclear performance systems to diagnostic simulations for simulation of nuclear or radiographic data;
- Incorporate sufficient HEDP/ICF physics into nuclear performance systems to support validation and design of experiments.

Implementation of the coupling capability will involve developing a prioritized list of these use cases in order to derive requirements, as well as the identification of current best practices for linking separately developed application codes to tackle both loosely and tightly coupled multiphysics phenomena.

National Simulation Portfolio Summary

The development of the ASC National Simulation Portfolio is the most extensive and significant component of the national code strategy. We have detailed the following steps:

- Defining a focused, minimal set of integrated, national application capabilities necessary to stockpile certification and weapons science;
- Accelerating the phase-out of legacy codes by ending development of new capabilities in those codes;
- Expanding the capability of the national portfolio through link-based coupling of the applications.

These three steps will allow the program to consolidate current efforts while continuing to meet stockpile certification needs, reduce long-term development and maintenance costs, and combine the best capabilities of the national laboratories for modeling physics and engineering processes and phenomena that occur under disparate, extreme conditions.

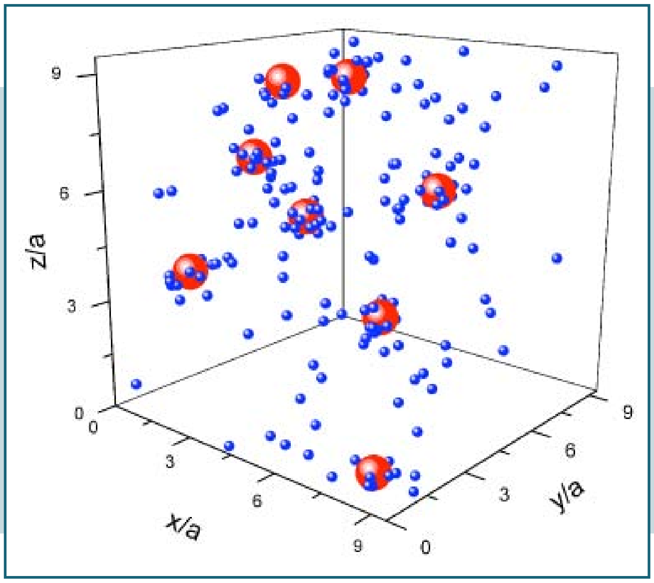
2. Advance Computational Algorithms to Enable Predictive Simulation and QMU

The second strategy addresses the predictive simulation and QMU goals of the ASC Program. Based on projections, this includes developing algorithms and implementations that will run effectively at petaFLOP and exaFLOP scales. There are major areas that must be addressed to achieve computational algorithms that can enable predictive simulation and QMU at these scales. The first is the design and properties of the algorithms themselves, which require focus on applied mathematics research. The second is on the software programming models that enable the coordination, scheduling, and memory management for millions of parallel, interdependent, execution threads across a computing platform. Current programming models are not expected to meet requirements at scales of 10 petaFLOPS and beyond.

2.1. Advance scalability of computational algorithms to petaFLOP and exaFLOP scales

A necessary condition for effective simulation at petaFLOP to exaFLOP scales is establishing a broad range of algorithms that are provably scalable, at least in a weak sense, to arbitrarily large numbers of variables and parallel tasks. Tremendous progress has been made in the past two decades on parallel, scalable numerical algorithms, but troubling bottlenecks still exist. These include not only increasing the generality and robustness of scalable linear solvers, but also scalable algorithms for coupling multiple nonlinear physics modules, algorithms for computing stability and eigenvalue characteristics of equations, discretization methods for addressing complex field equations, flexible dynamic load balancing capabilities for combinations of volumetic, surface, and particle mechanics kernels, and scalable methods for assessing errors in numerical methods.

Advancing algorithm scalability is a long-term research problem. The ASC Program has supported this research through the Focused Research, Innovation, and Collaboration (FRIC) element of the program, and has developed strong groups of applied mathematicians and algorithm architects at each laboratory to continue advancing work in scalable algorithms. Given constraints in future resources, as well as increasing demands to innovate new algorithms to meet petaFLOP and exaFLOP computing challenges, it is imperative that the program optimize its work and investments in this area. The best approach to improving the effectiveness of the program is to increase collaboration and coordination between the algorithm efforts across the labs and to leverage non-ASC investments in algorithms research. This can be achieved by coordinating tri-lab research efforts on scalable algorithms, engaging the newly initiated Predictive Science Academic Alliance Program (PSAAP) university centers on algorithms research and development, and expanding collaborations with other DOE national laboratories and universities.



Sandia ASC-funded researchers are developing novel kinetic algorithms to study the equilibration, stopping power, and fusion reactivity of dense, radiating, burning multi-component, multi-species plasmas.

Implicit electromagnetic LSP simulation of a moderately coupled, 50 eV iron plasma at charge state 25. The ions are shown in red, the electrons in blue.
(Sandia National Laboratories)

The next steps to achieving this overall strategy for scalable algorithms are as follows:

- Initiate annual planning at a national level of the FRIC component of the IC program element. This annual planning activity would assess the FRIC investments across the laboratories to look for synergies and disconnects in the tri-lab program, as well as discussing how to best engage the PSAAP centers and external communities to achieve the program's goals in scalable algorithms for predictive simulation.
- Within five years, employ peta scale (10+ petaFLOPS) computing, with improved fidelity and performance, on a mission-driven application.
- Define algorithm scalability requirements for exaFLOP scale simulation, including balanced increases in subgrid physics complexity, spatial and temporal grid fidelity, and other model enhancements needed to achieve predictive capability.

These actions are specific steps that will promote collaboration and demonstrate progress in the technology necessary to develop predictive capability for the ASC codes.

2.2. Collaborate on evolution of programming models for petaFLOP and exaFLOP scale computing

The Infrastructure Plan for ASC Peta Scale Environments articulates plans within the CS&SE and FOUS elements to address critical components necessary to the success and productive capability of peta scale computing platforms. One of the four technical areas in the infrastructure plan involves development environments and tools, which includes the issues associated with effective programming models for such platforms. This planning element naturally relates to the second area of focus in the current code strategy. It is worth noting the following summary from the section introduction:

> *Our challenge is to provide an environment that supports efficient use of emerging peta scale systems without requiring hundreds of person-years of new programming effort. We must provide new and innovative programming environments and tools to support code design, creation and modification, including building and debugging applications and tuning their performance. Each of these tasks involves significant complexity, particularly in the context of the multiphysics applications that characterize the ASC integrated codes.*

The infrastructure plan identifies 39 areas of concern and associated strategies for environments and tools, and all but three of these are identified as needing near-term activity. While the level of analysis in this plan is extremely valuable, it is difficult to see how the program will have the resources to pursue many of these tasks. Thus, it is critical for IC to engage deeply with CS&SE in the prioritization and execution of this work.

It is expected that FRIC will play a central role in the establishment of next-generation programming models and that research on these issues will be part of the national FRIC planning agenda. In addition, the following next actions have been identified:

- Coordinate research efforts on parallel programming with CS&SE and develop compact application suites for advanced programming model research;
- Establish a set of leading indicators that signal when the program should initiate development of next-generation integrated codes;
- Engage the broader HPC community to drive open standards towards the most effective solutions for ASC/NNSA.

Furthermore, to mitigate risks associated with next-generation platform technology, the IC program element must actively engage with CS&SE on new platform architecture design and development to ensure that specifications for operating systems, compilers, and libraries are consistent with proven programming models, and can be adopted by production code teams. While new platforms and programming models will still impact codes and drive redesign and refactoring efforts, this suggests that the program will balance the cost to achieve platforms at particular scales with the cost to effectively port integrated codes to those platforms, such that there is an overall benefit from these investments.

2.3. Deliver advanced capabilities for QMU and uncertainty quantification

To advance predictive simulation and QMU, future simulation studies must assess the variability of predicted quantities, given distributions of values for input parameters. The computational problem is to evaluate that variability, given a large number of input parameters, each with independent ranges of possible values. Possible approaches include random and structured sampling methods, reliability methods, and krieging methods. These methods are *nonembedded*, in that they interact only with simulation codes through changes in input parameters and otherwise use the normal forward simulation capabilities of codes. ASC supports development and implementation of these methods, through the FRIC and V&V program elements, to provide analysts with the capability to perform QMU studies.

Just as with scalable algorithms, the program must continue to invest in developing new scalable algorithms and methods for performing uncertainty quantification. Research directions with high potential for developing more scalable methods include embedded methods such as adjoints for error estimation and sensitivity analysis, automatic differentiation, and stochastic Galerkin methods. These methods are embedded because they require the calculation of new quantities of interest within the simulation codes and often involve new numerics or solution algorithms in addition to changes in the source code. The benefit of the additional software development is the ability to compute uncertainty measures with improved accuracy and at a reduced computational cost.

The IC program element will need to determine requirements to guide the development of advanced methods for QMU and uncertainty quantification. These requirements must reflect the dimensionality of the uncertainty problem itself, as well as the character of the physical processes being simulated, and the required fidelity of the calculated distributions. From these requirements, developers, analysts, and algorithm researchers can identify the needed capabilities of future tools, including the mixture of non-embedded and embedded algorithms, and plan the future algorithm research and capability development tasks for application codes and uncertainty quantification tools.

3. Broaden the Impact of ASC Simulation Capabilities in National Security

This final strategy is to increase the impact of the simulation capabilities of the ASC Program in national security, both within the nuclear security arena, as well as in the defense and energy security arenas. There is strong interest in ASC capabilities within the larger national security community, and this represents an opportunity and a challenge for the program. ASC capabilities are unique in their breadth of application to complex phenomena and in the degree to which they have been developed to employ advanced computing. As parallel, tera scale computing moves from being a unique, costly, and difficult-to-obtain resource to a commodity product, the interest in using that computational power to solve problems of interest to government and industry has grown substantially. And while ASC capabilities have potential application in many public and private applications, it is in the national security arena that ASC capabilities are truly differentiating and can have the greatest impact and value to the nation.

Having impact on other national security applications will not happen without focused effort. Experience shows that extending existing capabilities to new applications involves additional capability development such as new material models, source terms, and boundary conditions, as well as testing and optimization of solution algorithms. New problems beget new combinations of physical phenomena, and existing codes are usually robust and verified over only a small subspace of models and parameters. The challenge for ASC is how to manage additional requirements arising from new applications and the expectations of new stakeholders. The benefit to ASC is that broadening its "footprint" may help to stabilize the ASC investment in an increasingly constrained and uncertain budget future. There is also potential for bringing in new resources, and to leverage those resources to sustain our core competencies, attract the next generation of computational physicists, and maintain staff to support and improve codes for the complex in the future.

Executing this strategy entails leveraging our current capabilities, identifying new opportunities, building collaborations, and enhancing our capabilities for the broader security arena. Our path forward and next actions in this area are less specific because much depends on developing relationships with organizations outside NNSA and DOE, and ensuring that we understand, and can add value to, the missions of those organizations. In the following sections, we cover the key next actions that can foster and advance these relationships. These next steps are not exhaustive, and the ASC Program will need to identify further steps and plans as these relationships develop.

3.1. Develop a business "prospectus" for major IC Program capabilities

The broad range of ASC capabilities and how they might apply to problems outside the nuclear weapons program are not necessarily understood outside the ASC community. To educate the broader set of national organizations, each major ASC capability, from integrated codes, through frameworks and libraries, should outline its capabilities, known application areas within national security where it could have impact, and extended capabilities that could be developed to enhance its value in national security problems. These descriptions can be used by the labs, as well as federal managers, to engage potential partners in development of new applications of ASC capabilities.

3.2. Develop and support interagency partnerships in national security applications

Interactions between federal managers at ASC and federal agencies are important components of developing program partnerships. Without the support of managers on both sides, it is difficult to establish commitments to develop, deploy, and apply new capabilities. Therefore, it is necessary for the federal program to develop and support interagency partnerships, and increase the ASC Program presence in the broader national security modeling and simulation community. This can be through working groups with the Department of Defense, the intelligence community, and other agencies with responsibilities in science and engineering (e.g., NASA, National Science Foundation, etc.). Increasing the program's presence can also take the form of program participation in new ventures like the Capitol Hill Modeling and Simulation Exhibition. There is also benefit in increasing participation in technical conferences, where federal representatives attend to identify new research that is relevant to their mission. Laboratory personnel often participate in such conferences, but usually in the role of presenting research rather than developing high-level programmatic relationships.

3.3. Develop enhanced capabilities for expanded national security missions

This is the least developed strategic area, since enhancing capabilities requires a goal or application in mind. Given this ambiguity, however, there are specific actions and areas that should be explored, based on existing relationships outside the nuclear weapons community, and the potential impact of the capabilities. These actions are as follows:

- Defining requirements for a national outputs and environments capability. This capability would complement the ASC national portfolio, address applications in the nuclear security and nonproliferation arena, and strengthen capabilities of interest to organizations such as the Defense Threat Reduction Agency (DTRA).
- Developing information-based technologies. Leveraging ASC capabilities in HPC to tackle "big data" problems has applications within nuclear security, as well as considerable interest from other government agencies.
- Exploring ASC capabilities for decision support through, for example, integrating simulation with surveillance data, and developing capabilities to simulate networks of complex systems. These areas are transformational extensions of traditional physics-based modeling and simulation, but add considerable power through a broadened scope of applications and dynamics. Enhancing the ability of modeling and simulation to answer questions posed by decision makers in operational scenarios holds great value across a broad spectrum of applications.

Through such steps, and maintaining flexibility to adapt resources to new partnerships, the program should be positioned to have an impact in the broader national security arena.

4.0 RISK ASSESSMENT FOR THE NATIONAL CODE STRATEGY

The following risk assessment examines the current strategy by anticipating problems with its implementation and effectiveness, and developing approaches to mitigate those problems. As detailed in Section 3.0, the strategy itself is a mitigation plan to address high-risk exposures for the IC program element. However, the strategy poses risks in terms of both uncertainty in its future effectiveness and in the ability to implement components of the strategy. Table 3 summarizes these risks together with mitigation approaches for each. The highest identified risk exposure is the inability to sustain the full code portfolio because of pending funding cuts to the program. The preferred mitigation approach for this, given the need to sustain capabilities across the core stockpile application areas within the portfolio, is to further increase modularization and consolidation within each of the code systems. Another risk is an inability to fund implementation of the strategy, again because of limited resources. The mitigation plan to address this issue is to prioritize the implementation targets for the strategy. These prioritized implementation targets are detailed in Appendix B. Mitigation approaches for other identified risks have been integrated into the various detailed strategies in Section 3.0, but are listed here for clarity and completeness.

Table 3. Risk Assessment for the ASC National Code Strategy

Risk Description	**Risk Assessment**			**Mitigation Approach**
	Consequence to Stockpile Stewardship	**Likelihood**	**Risk Exposure**	
National code portfolio not sustainable; too many codes to support given funding cuts	High	High	High	Increase modularization and consolidation within code systems to further reduce maintenance costs
Code strategy is too ambitious; inadequate resources to implement complete strategy	Moderate	High	Medium	Define prioritized implementation targets, to adjust to available resources
Difficult to support national codes usage across lab boundaries	High	Moderate	Medium	Define expectations via lab-lab agreements
Lack of diversity in approach slows development of predictive capability	High	Moderate	Medium	Provide coupling capabilities to increase diversity of approaches
Disruptive changes in platform technology impacts code scalability faster than we can manage	High	Moderate	Medium	Work with CS&SE on platforms to incorporate proven next-generation programming models
Linkages in performance codes introduce large errors	High	Moderate	Medium	Develop improved coupling and error estimation algorithms; work with V&V to assess linkage errors

5.0 SUMMARY AND IMPACT

This document has detailed the background, goals, and new strategies for the Integrated Codes program within ASC. We have described the current objectives, the current program state, and the existing and future challenges. This is summarized through a risk assessment that identifies important issues for the program, and motivates the development of this strategy. We have described in detail the new strategy, including the establishment of a national simulation portfolio, efforts to advance algorithms and codes to enable predictive simulation and QMU, and efforts to broaden the program's impact in the national security arena. Finally, we have examined the risks associated with adopting these strategies and provided additional recommendations to mitigate those risks. A high-level description and impact of the current strategy on the program is given in Table 4.

Table 4. Impact of the Code Strategy on Future ASC Program

Focus Areas	Current State	Strategies	Future State
Integrated Simulation Capabilities (Application Codes)	• 14 modern + numerous legacy codes across 6 broad application areas • Core physics simulation competencies established	Establish the National Simulation Portfolio for Stockpile Certification	• 7 modern national capabilities • End legacy development • Core competencies sustained
Computational Science	• Tera scale computational science established (MPI programming model) • Basic capabilities for uncertainty quantification	Advance computational algorithms to enable predictive simulation and QMU	• Algorithms & programming models supporting predictive simulation at petaFLOP and exaFLOP scales • Advanced capabilities for uncertainty quantification and QMU studies
Scope of Applications	• ASC simulation capabilities focused on certification for tail numbers	Broaden the impact of ASC simulation capabilities in national security	• Capabilities for broader national security applications, including NNSA nuclear security and non-proliferation missions

The implementation targets related to the strategy are addressed in Appendix A. We have separated the strategy content and its implementation in order to keep the main document focused on the goals, strategies, and ideas, and to ensure that the ideas behind the strategy remain relevant in the event that the implementation plan is substantially revised in response to budget and schedule constraints in the coming years.

This strategy represents the ideas and efforts of the tri-lab integrated codes leads and managers, and the ASC program managers at NNSA. We believe the strategy developed herein will help the program to sustain its capabilities and meet future challenges, and to operate in a focused and interdependent manner for the benefit of the nuclear weapons complex. Adopting this strategy will mark a significant shift in the operational culture of the codes program, dating from before the inception of the ASCI Program. It is expected that such change will pose difficulties and require commitment from all organizations to succeed, but that the program and the laboratories see the necessity for change and will work together to make the program a continued success.

APPENDIX A.
Implementation of the National Code Strategy

The prioritized implementation plan presented in Table A.1 provides a set of targets over the coming six-year period from fiscal year 2009 through 2013. Given the nature of rapid change involved in the current program, it is not appropriate to plan at this level of detail beyond this time period. It is expected that additional efforts will be required to sustain this program direction and meet the program goals, and that additional implementation targets should be identified as the current six-year period concludes.

The targets in Figure A-1 and Table A-1 have also been prioritized into two levels to provide guidance to the program in how to manage the implementation given uncertainty in future budgets. The "theme" listed maps each target to one of the major strategies in the main document, and the relationship between the two should be clear to the reader. Rather than provide a more verbose explanation of each target here, the main document provides sufficient detail to understand the ideas and intent behind the targets and should be used in translating the target items to determine potential activities and deliverables in the program's annual implementation plan.

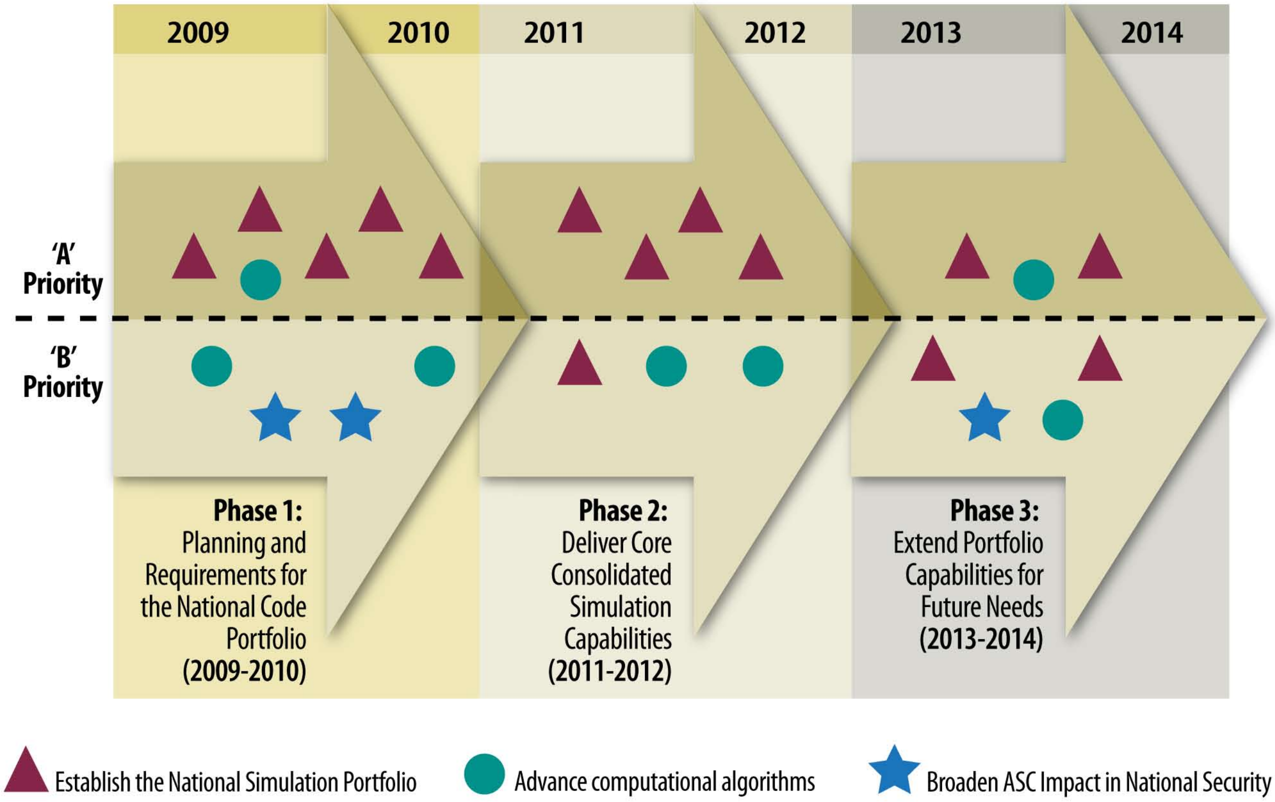


Figure A-1. Implementation Timeline and Major Phases for ASC Code Strategy

Table A-1. Prioritized Implementation Plan (FY09 to FY13) for the ASC National Code Strategy

Phase	Year	Priority	Theme	Target
Phase 1: Planning and Requirements for the National Code Portfolio	2009	A	I	End development funding for legacy codes
	2009	A	I	Negotiate capabilities and support expectations for national code portfolio with customers
	2009	A	I	Plan for setup tool consolidation
	2009	A	II	Initiate national FRIC planning
	2009	B	II	Develop national capability requirements for QMU and uncertainty quantification
	2009	B	III	Develop prospectus and support partnerships for national IC capabilities to impact national security
	2010	A	I	Establish requirements and priorities for coupling of national code capabilities
	2010	A	I	Define tri-lab physical data APIs
	2010	B	II	Develop compact application suite for programming model research
	2010	B	III	Define requirements for national outputs and environments capability
Phase 2: Deliver Core Consolidated Simulation Capabilities	2011	A	I	Complete evaluation of code capabilities for engineering assessment
	2011	A	I	Deliver two national nuclear performance capabilities that consolidate future development
	2011	B	I	Complete evaluation of code capability for casting/manufacturing applications
	2011	B	II	Deliver advanced capabilities for QMU and uncertainty quantification
	2012	A	I	Deliver an integrated national capability for non-nuclear assessment that consolidates future development
	2012	A	I	Complete setup tool consolidation*
	2012	B	II	Evaluate leading indicators for next-generation software implementations
Phase 3: Extend Portfolio Capabilities for Future Needs	2013	A	I	Complete implementation of tri-lab physical data APIs*
	2013	A	II	Employ peta scale (10+ petaFLOPS) computing with improved fidelity/performance on a mission-driven application
	2013	B	I	Achieve required coupling of national code capabilities
	2013	B	III	Enhance capabilities for expanded national security missions
	2014	A	I	Deliver national integrated capabilities for NEP Safety, HEDP, Diagnostics, and Radiation Effects for Electrical Systems, which consolidate future development in these areas
	2014	B	I	Consolidate transport capabilities for diagnostics, outputs, and radiation effects
	2014	B	II	Define algorithm scalability requirements for exa scale simulation

* This is the target date for completion. Planning will set a more definitive completion date.

APPENDIX B.
Taxonomy of Integrated Codes Program

Consistent with the *ASC Business Model* (July 2005), the IC program is organized into five Level 4 products as detailed below.

Modern Multiphysics Codes

This is a suite of large-scale, integrated multiphysics simulation codes and physics packages needed for the SSP, including the classified codes used by designers and analysts to simulate the nuclear safety, performance, and reliability of stockpile systems. The products are complex, integrated hydro, radiation-hydro, and transport codes for performance assessment; design and analysis of experiments; general-purpose hydro and radiation-hydro problems; and analysis of radiation and particle transport problems for a variety of applications. In addition, these codes are used to simulate other dynamic events, including high-explosive, laser, and pulsed-power driven systems; subcritical and above-ground experiments; ICF; and the response of energetic materials to thermal and mechanical insults. The codes are designed to run in parallel and make effective use of advanced ASC computing platforms.

Legacy Codes

This product is the maintenance and limited enhancement of the suite of legacy and support codes historically used for design of primaries and secondaries, and for engineering analyses. Legacy codes serve as established tools for nuclear weapons simulation, with well-understood capabilities and limitations for stockpile stewardship applications. They serve as reference points for the assessment of new codes, models, and algorithms. For designers, they represent a link to the era of active nuclear weapon design and testing, provide well-calibrated reference simulations, and serve as standards for evaluating the effectiveness of new simulation tools.

Engineering Codes

This product is a suite of engineering and manufacturing codes and supporting frameworks used for Stockpile Stewardship activities, life extension programs, and SFIs. Engineering codes support analyses such as thermal, structural, and electrical/electromagnetic modeling of weapon components and systems under normal, abnormal, and hostile environments. Manufacturing process codes support casting, welding, forging, and encapsulation operations.

Focused Research, Innovation, and Collaboration

This product is focused on research, innovation, and collaboration with other ASC elements, laboratories, and the scientific community to develop future technologies, algorithms, and computational methods. This research enables greater predictive capability by focusing on overcoming critical obstacles in integrated codes (e.g., the need for robust efficient solvers, optimization algorithms, and innovations to improve code effectiveness). Exploratory efforts include focused research projects, as well as basic research aimed at larger challenges. Activities include application-specific computational science research, such as development of software architectures that enable application of new and coupled physics, models, and verified algorithms to problems of interest. Research is conducted at the laboratories and with academic researchers.

Emerging and Specialized Codes

This product explores emerging technologies that are not mature enough for use in the modern codes, specialty codes that simulate complex processes in unique environments, and supporting codes for problem setup and analysis. This suite of codes will change as new methods and new application-specific requirements are identified. Specialty codes have detailed physics focused on applications (e.g., ICF laser-plasma interactions or direct numerical simulation of turbulence). The supporting codes are application-specific problem setup and physics-based post-processing codes.

Integration of Integrated Codes with ASC Program Elements

Physics and Engineering Models (PEM): The PEM program element is responsible for developing models of physics and material phenomena, as well as transport for particles, x-rays, and other phenomena. PEM includes the development, initial validation, and implementation of those models into the integrated codes. The implementation component of PEM must have requirements management, code testing, and version-control processes, and the planning of model development, implementation and deployment for future code releases must be coordinated with IC.

Verification and Validation (V&V): The V&V program element is responsible for predictive accuracy assessments, metrics, and methods that relate simulation capabilities to real world behavior. The IC program element develops the codes that V&V assesses for accuracy. The V&V program element is also responsible for the ASC program's Software Quality (SQ) process, including the SQ policy guidelines and assessments, and code and solution verification methods development. Finally, the V&V program element is responsible for developing methods for uncertainty quantification, which must be integrated with the IC tools in order to provide quantified uncertainties based on code predictions.

Computational Systems & Software Environment (CS&SE) and Facility Operations and User Support (FOUS): The CS&SE and FOUS program elements provide Integrated Codes users with computing environments for all ASC platforms, including capability, capacity, and advanced systems. For the ASC to have maximal impact, there must be close collaboration between IC developers and platform and operating system developers. IC developers are dependent on the CS&SE program element for system and development tools, including compilers, debuggers, optimized kernels, input/output services, run-time libraries, and message passing libraries.

APPENDIX C.

Code Project and Product Terminology

In the ASC Program, the term "codes" is synonymous with software, and "integrated codes" is generally understood as referring to the end-user software products that integrate and couple multiple numerical methods and phenomenological models of physical processes to simulate complex physical systems in operating scenarios. To understand the IC program element and strategy, it is helpful to have general definitions of software design and architectural components that are used in developing codes and that are often the product or deliverable of specific projects within the program. In particular, code suites, applications, frameworks, and libraries are defined below, and their relationships to one another and overall code architectures are depicted in Figure C-1.

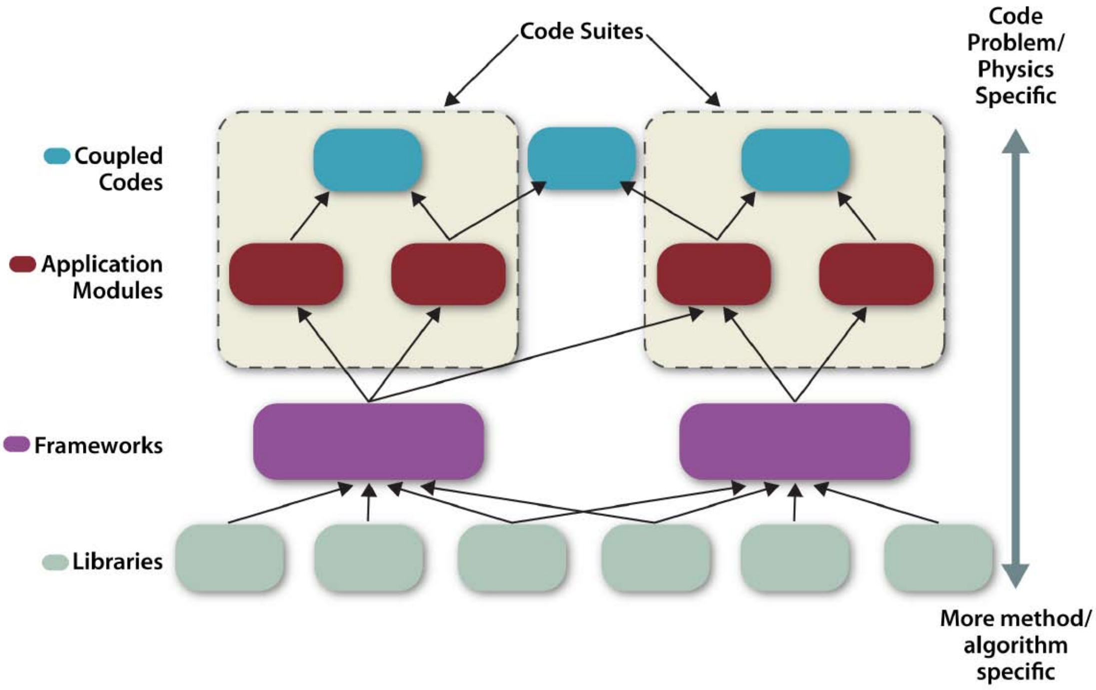


Figure C-1. Multiple Tiers of Software Products in Code Architecture Designs, Driven by Modularity and Code Re-use.

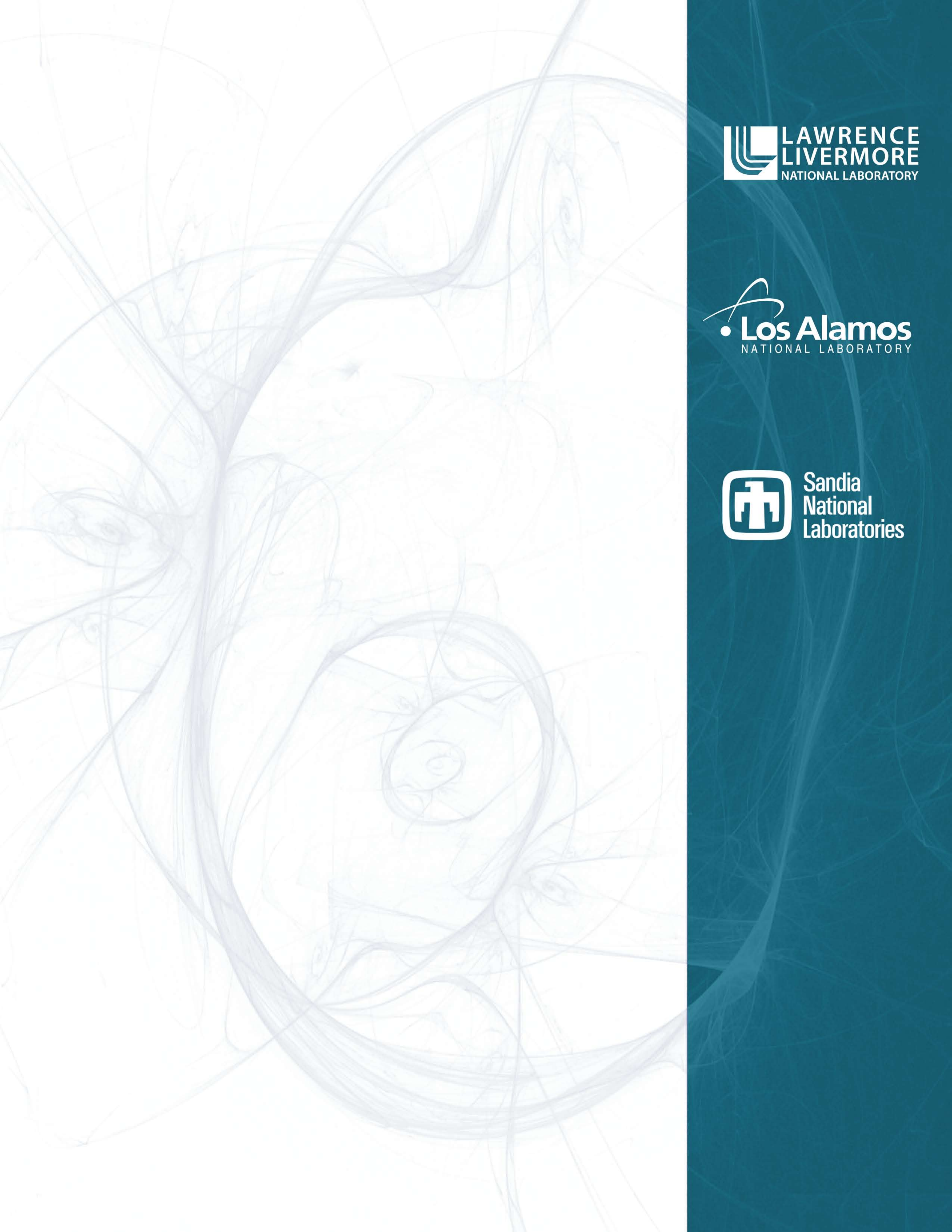
The complexity in software design results from maximizing the modularity of code components and re-using existing implementations of generic data methods and algorithms. The benefits of code re-use include leveraging development cost across a large base of applications, increased robustness, and lower maintenance costs. Modularity is synergistic with code re-use, in that reusable components are, by nature, modular. Modular designs also help manage complexity in a large integrated software product. However, modularity and code re-use comes at the price of architectural complexity (as exhibited in Figure C-1) and project management complexity. Managing software interfaces, requirements, and project interdependencies is an ongoing challenge to any major software development enterprise, including the ASC IC program element.

Code System or Suite: A code system or code suite is a grouping of modules used together to perform coupled physics or multidisciplinary analysis, and share underlying software architectures, libraries, and/or data models. Code suites are end-user software products that may be executables linking multiple applications with an in-core data model, or shell scripts, that run applications and manage couping data via external files.

Application Module: An application module is a code that performs a specific class of problems. A module is usually designed to solve a single dominant type of physics or mechanics, but may provide some tightly coupled multiphysics capability. Modules can be end-user executables, or libraries linked into a higher level executable, that are executed by analysts or designers to model and simulate physical systems and processes.

Library: A library is a set of software functions that can be linked into frameworks and applications to provide common re-usable methods and functions. Libraries are defined by an application programming interface, which defines data types and methods used to operate on the data. Libraries are products used by other developers and delivered in the form of statically or dynamically linkable object code (termed a library file).

Framework: A framework is a set of related software elements that provide common services used to implement algorithms in an application code. Frameworks are built around integrated in-core data models, where multiple capabilities are interdependent through the data model. Frameworks are software products used by other developers, are delivered as statically or dynamically linked libraries, and can range from monolithic to highly modular. A framework may be encapsulated into multiple libraries.



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