ASC™

Advanced Simulation and Computing
SIMULATION STRATEGY

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Front cover: Two high-resolution simulations, with and without plasma transport, of the classical Rayleigh-Taylor instability-driven mixing of carbon and deuterium under ICF conditions, are performed. In the top figure, plasma transport is not included, and a great deal of turbulent mixing—indicated by the fine-scale structures—persists. The bottom figure is the same simulation with plasma transport included where all of the fine-resolution turbulent structure is washed away in favor of greater atomic mix shown by the blurred larger-scale structures. This mechanism to suppress turbulent mix and enhance atomic mix, leaving larger-scale residual structures, points to the feasibility of capturing these physics outcomes in coarse-resolution simulations with suitable models. (LANL)

Advanced Simulation and Computing

Simulation Strategy

NNSA
David Etim
Anthony Lewis
James Peltz

LLNL
Tom Arsenlis
Teresa Bailey
Chris Clouse
Richard Klein

LANL
Marianne Francois
Rob Lowrie

SNL
Joe Castro
Mike Glass

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Foreword

The mission of the National Nuclear Security Administration (NNSA) Office of Defense Programs (DP) is to maintain a safe, secure, and effective nuclear weapons stockpile for the United States. Essential to this mission is the Advanced Simulation and Computing (ASC) program's high-performance simulation and computing capabilities that inform critical DP stockpile stewardship decisions. The ASC program's success relies on its ability to provide simulation tools, which enable broad and deep knowledge of the complicated, coupled physical processes involved in the full stockpile-to-target sequence for a nuclear weapon. By continually developing and deploying for NNSA the credible, science-based simulation tools to certify the current and future stockpile, ASC provides the required confidence in the Nation's nuclear deterrent.

To ensure a reliable nuclear deterrent in the face of a changing geopolitical climate, NNSA must imbue in its stockpile stewardship management and modernization programs, the responsiveness and agility to stay ahead of emerging threats. The ASC program will be called upon to contribute to the development of new weapons options, which could be very different from those in the current stockpile. To enable the nuclear security enterprise (NSE) to field these options with agility, the ASC program also will be required to extend the application of its tools to improve the efficiency of the NNSA production complex. In the near future, the modeling of weapons systems beyond the stockpile's lifetime and new simulation of the production processes, enabling the production complex to become more efficient, will be an expanded program scope beyond current programmatic commitments.

As the ASC program's scope increases to meet the expanding DP mission requirements, the program must also contend with major disruptive computing architecture changes. The challenges associated with potential application performance and facility equipment—in addition to management practices that could result from these changes—continue to be formidable obstacles for the program and must be dealt with proactively to address NNSA's current and future requirements.

This 2022 *ASC Simulation Strategy* outlines how the program will endeavor to stay responsive and agile—in the midst of fast-paced technological changes and priority shifts—to ensure that current and future generations of ASC simulation capabilities and resources will continue to underwrite our Nation's nuclear deterrent. It identifies the high-level strategic objectives and necessary research, development, and deployment investments to ensure ASC is ready to meet the challenges of the future deterrent. The exact, tactical execution details of the simulation activities outlined in this document are developed by and maintained at each of the NNSA laboratories.

Looking ahead, we will earnestly execute to the new NNSA slogan of "Innovate. Collaborate. Deliver." as it aligns perfectly with ASC's core principles that have served us well for the last 26 years and will continue to do so in the future.

Thuc T. Hoang
Director, Office of Advanced Simulation and Computing
& Institutional Research and Development Programs
NNSA Office of Defense Programs

Executive Summary

This Advanced Simulation and Computing (ASC) program's Simulation Strategy will guide future ASC investments in simulation technologies to ensure timely and cost-effective availability of the capabilities needed for NNSA to maintain a safe, secure, and effective stockpile. Additionally, the NSE will also depend on ASC simulation tools to meet production and manufacturing requirements to support both the existing and future deterrent.

This document presents three technical objectives that will guide investments in the ASC Simulation portfolio to address critical DP mission requirements:
- assess the performance and safety of an evolving stockpile,
- optimize design options and address threats, and
- enable an efficient production enterprise.

A common theme in this ASC Simulation Strategy in response to many future technical challenges is "innovating through efficiency." This concept is about innovation achieved by laboratory computational scientists who should be freed from time-consuming workloads, such as code porting or optimization work on advanced architecture systems, so that they can direct their attention and time toward solving problems via new methodologies, essentially "doing more with less." It's a reinforcing cycle, i.e., results should be easier to achieve, leading to faster insight, which in turn drives new results that will enable new insights.

Along with pursuing code development efforts for improved understanding of aging and production issues, ASC will augment the exploitation of legacy data and the quantification of associated uncertainties. This effort translates to prioritizing capabilities that serve multiple missions: those that broaden the user base for the evolving ASC simulation tool suite and those that extract maximum knowledge from information that already exists. This prioritization will improve the tri-lab ability to manage resources needed to advance emerging simulation capabilities in mission areas such as production and manufacturing.

As the Nation's nuclear stockpile evolves to support a responsive and resilient nuclear deterrent, so must ASC simulation capabilities that underpin the Stockpile Stewardship Program. The shift from stewarding the nuclear weapons to fielding a responsive nuclear deterrent demands that ASC simulation capabilities become more predictive in addressing rapidly evolving threats. ASC application codes will need to be trusted by the end users for application beyond annual certifications and assessments, particularly for use in design beyond the underground test basis. For proper investment prioritization, it is important to recognize that computational capabilities often provide the best value when augmented with physical experiments; the former are not meant to and cannot fully replace the latter.

Introduction

The ASC program provides science-based simulation and computing capabilities that, when combined with historical nuclear tests and non-nuclear tests (with new non-nuclear experiments), are used to assess and certify the Nation's nuclear stockpile in the absence of underground nuclear testing. ASC provides the simulation and computing tools to generate the data that lead to insights to enable experts to assess the stockpile's safety, security, and effectiveness. High-performance simulation and computing are the two major functional elements of the program, and this document covers the strategy for the simulation activities. The strategy details for the ASC computing elements can found in the 2022 *ASC Computing Strategy*.

The ASC simulation activities are part of the Defense Applications and Modeling (DAM) portfolio, currently funded by four program elements:
- Integrated Codes (IC)
- Physics and Engineering Models (PEM)
- Verification and Validation (V&V)
- Advanced Technology Development and Mitigation (ATDM)'s Next-Generation Code Development and Application (CDA) product group (until end of FY 2022)

The IC program element provides the multiphysics simulation codes that allow analysts to perform certification and qualification studies. The PEM program element sponsors research to create, curate, and improve models of the different materials and phenomena that are represented in the ASC integrated design codes. The V&V program element verifies the soundness of the simulation codes, supports studies to validate the physics models and algorithms, and develops universal standards of practice for simulations. Lastly, the ATDM CDA product group deploys a new generation of simulation codes developed to target exascale platforms and address the need for increased developer productivity and user responsiveness. Development of new algorithms, novel programming models, data management techniques, and software architecture researched under ATDM CDA has culminated in a next generation of simulation capabilities that are actively being enhanced and validated for production use.

Requirements and gaps to address with new capabilities flow down to the ASC program through official NNSA documents such as the *2018 Nuclear Posture Review*, the *NNSA Strategic Vision*, and other strategies within the NA-11 Office of Research, Development, Test, and Evaluation (RDT&E). These documents are updated regularly; however, the following objectives remain valid for the RDT&E mission:
   (1) to provide innovative technological solutions for the nuclear deterrent,
   (2) to support an evolving nuclear security enterprise, and
   (3) to develop and retain a highly skilled workforce.

The ASC program's history has shown that developing and delivering a production-ready code base to weapon scientists and engineers is costly and time-consuming and warrants physical experiments needed for code validation. However, as ASC codes become the tools of choice for design and analysis, the program in the near future will prioritize investments that lead to improved efficiencies and user

productivity while ensuring that more physics capabilities continue to be added to the code base. This task requires a special focus on efforts that

- systematically model physical behaviors at sufficient fidelity to expand the predictive envelope of the codes,
- develop computational technologies that enable enhanced usability and ease-of-use in ASC simulation capabilities, and
- allow test data to be fully exploited regardless of particular mission applications.

This prioritization will allow future development of capabilities to serve multiple missions, broaden the user base for the ASC tools, and extract maximal knowledge from existing data. As an exemplar, the Los Alamos National Laboratory (LANL) xRAGE code is supporting multiple missions to solve various application problems (see Figure 1).
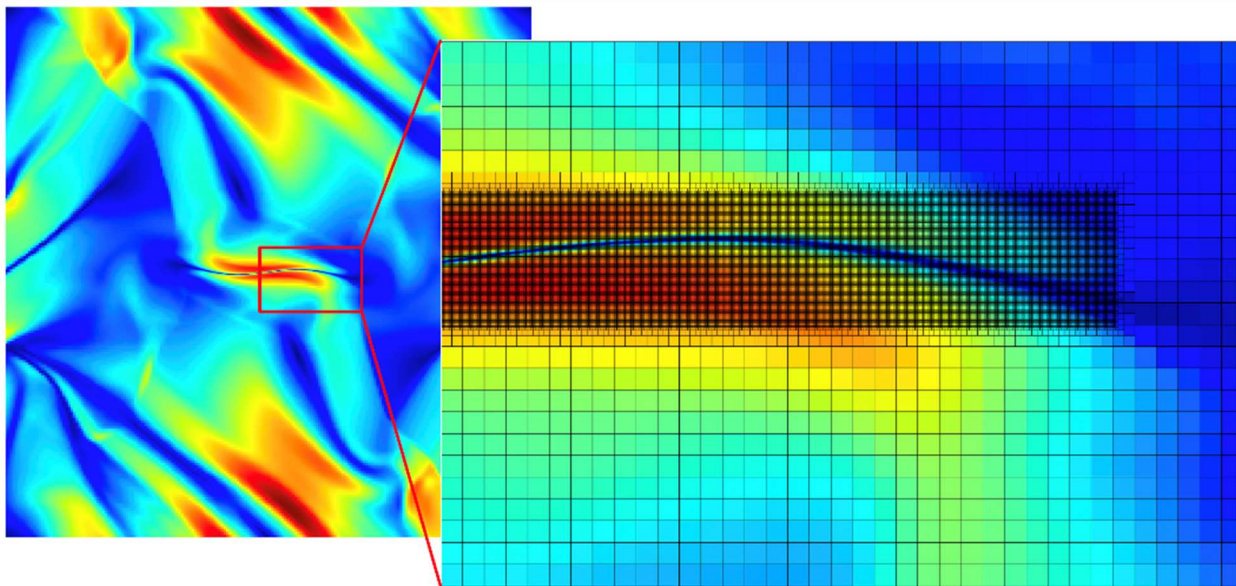
Figure 1. Magnetohydrodynamic (MHD) simulation with LANL xRAGE multiphysics code under the ASC IC Eulerian Applications Project. MHD simulations are important to many inertial confinement fusion (ICF)/high-energy-density (HED) and stockpile applications and continue to be improved to support modeling experiments using laser-driven hohlraums. Based on physics improvements and inline laser cross-beam energy transfer developed in collaboration with the University of Rochester's Laboratory for Laser Energetics, xRAGE can now be used to design and analyze all experiments performed on the National Ignition Facility.

The ASC program's priority of building a highly specialized workforce is primarily within the purview of the NNSA laboratories because they are mainly responsible for attracting, hiring, developing, and retaining the talent needed to work on their cognizant NNSA missions. The unique challenge of the NNSA missions and ASC's long-time leadership in high-performance computing (HPC) are major factors for drawing top talent and young staff to the NNSA laboratories. ASC supports the laboratories' workforce development efforts by its continued funding of the ASC Predictive Science Academic Alliance

Program[1] (PSAAP; see Figure 2) and the U.S. Department of Energy (DOE) Computational Science Graduate Fellowship[2] (CSGF), a jointly funded effort with the DOE Office of Science. Forging stronger partnerships between NNSA Headquarters and the NNSA laboratories is key to enabling the RDT&E programs to increase return on investment from various DP RDT&E academic programs, including the NNSA Stewardship Science Graduate Fellowship, the Laboratory Residency Graduate Fellowships, the Joint Program in High Energy Density Laboratory Plasmas, the Minority Serving Institution Partnership Program, and the Tribal Education Partnership Program.

Figure 2. Students from the recently established PSAAP III Center at the University at Buffalo.

Objective 1: Modeling and simulation for assessing the performance, safety, and security of an evolving stockpile

As an engineered system, the weapon systems in the stockpile require routine maintenance and continuous verification, validation, and improvement. Mundane but potentially impactful physical effects such as aging, repairs from maintenance, and design changes require assessments to understand their effect on weapon performance and safety. The assessments are informed by physical tests (when possible), computational experiments that are accepted, and qualified surrogates to confirmatory physical measurements via rigorously verified and validated codes. ASC continues to support the NSE by delivering trusted modeling and simulation capabilities, via modernized and validated integrated codes,

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[1] https://psaap.llnl.gov/

[2] https://www.krellinst.org/csgf/

used to assess the performance and safety of an engineering system that experiences change over its lifecycle.

Objective 1 requires the following three response pathways for delivering credible modeling and simulation capabilities needed to rapidly and accurately assess an evolving stockpile:
- Support the readiness of an aging stockpile,
- Quantify uncertainties routinely for the current stockpile, and
- Augment the exploitation of legacy data.

Pathway I: Support the readiness of an aging stockpile

The aging of materials in the stockpile is a natural occurrence but a very complex process to model. It is not a single phenomenon but rather a collection of observed phenomena with no integrated measurable characteristics. Because of this complexity, for the larger-spatial scales at which aging is observed, new methods and new modeling approaches need to be developed as truly multiphysics, multiscale simulations. In the context of ensuring that these tools contribute to NSE readiness posture, which can be viewed as allowing scientific and engineering insights to be gained faster, the ASC program must invest in methods that generate simulation data quickly and a computational infrastructure that produces rapid and meaningful results. This effort also means that ASC tools and their ancillary analysis suites for quantifying uncertainties must be easy to use and readily available as soon as possible.

ASC will prioritize resources to improve (1) workflows that reduce turnaround times for model setup, initiation, and analysis; and (2) methods such as in situ data analysis to support rapid exploration of trade spaces with reliable documentation of the results. Improved workflows present a promise to eliminate inefficiencies in current life extension programs and to free up the subject matter experts (SMEs) to focus on research that addresses capability gaps. Making the tools easier to use will also allow for more rapid modeling assessments and broader utilization. Standardizing workflows can improve access and allow code developers and SMEs to spend more time performing scientific investigations rather than performing more mundane or routine tasks.

Collectively, concentrated efforts on improving the infrastructure to model materials and optimizing workflows will position the ASC program well in delivering simulation capabilities that will model more rapidly the physical effects, while allowing more targeted work to guide technical progress for modeling aging effects. Investments in this challenge area will improve collaboration among multi-domain experts and enable great gains in developing ab initio and coupled ab initio/phenomenological models of aging. Advances from emerging technologies such as machine learning (ML) are promising methods because ML-based surrogate models can capture the relevant phenomena and are computationally cheaper than molecular dynamics (MD) simulations and related high-fidelity simulations. A multiscale approach that considers first-principle simulations—coupled with in situ or first-principle, machine-learned methods with models trained off-line—should greatly expand the predictive capabilities of the ASC simulation tools.

Performing research and development (R&D) to understand aging requires large-scale, expensive computations. Efforts are ongoing to develop such a simulation capability, but the real issue is the value proposition or trade-off between what the data represent and the long time it takes to acquire them. Accuracy of the data represented by integrated, large-scale, and multiphysics simulations depends on

fundamental data from first-principle models or science codes. Improving accuracy for modeling complex, in situ conditions (e.g., aging effects) will require multiscale modeling approaches, such as using sub-grid models, to capture microstructure-aware and more advanced models that employ localized molecular dynamics (MD) and density functional theory (DFT) simulations. This effort would represent a significant step forward for modeling more complex conditions that are currently limited by having to use look-up data tables.

> **Strategy**: To support the readiness of an aging stockpile, ASC will develop new methods and modeling approaches for multiphysics, multiscale application codes that can model the physical mechanisms and effects of aging, thereby improving SME workflows to deliver agile simulation capabilities for stockpile sustainment.

Pathway II: Quantify uncertainties routinely for the current stockpile

Errors in problem formulations, models, measured data, and software implementations are quantified in the form of uncertainties. Uncertainty quantification (UQ) activities in the ASC program are focused on understanding and reducing these uncertainties through rigorous verification and validation practices, which can take decades and require enormous SME resources. The future requires designers to have a working knowledge of statistical methods and be trained in the use of UQ methodologies. The ASC program addresses the demand of UQ efforts being performed routinely and more quickly by making them more user friendly and more easily integrated into daily practice. Making these UQ methods more efficient requires them to be more widely known and adopted via education, training, and practice; readily available as production tools; and easy to use on all ASC computational platforms.

Improvement should enable the automation and easy execution of UQ assessments by the design community and other end users. Additionally, common formats and interfaces improve access and data sharing and build the infrastructure needed for better archiving of data. Conducting these activities together, along with investing in designer training and knowledge systems, will result in a consistent execution of methods that more broadly support qualification and certification and enable understanding the consequences of aging much more rapidly. In addition, a potential exists to advance UQ methods by taking advantage of efficiencies offered by novel programming models (e.g., runtimes that break codes down into data, tasks, and dependencies rather than into a single monolithic executable), enabling integration of information from a hierarchy of models (e.g., multi-fidelity UQ), and seamlessly incorporating reduced-order models and surrogates in the characterization of errors.

Continuing development of the necessary tools and infrastructure to support verification, validation, and uncertainty quantification (VVUQ) activities—while also considering an integrated workflow that is systematic, reproducible, and user friendly—is a key strategy to achieving efficiency. The ASC program continues to support mature tools currently in use at the NNSA laboratories, even though these tools remain computationally expensive and require their own dedicated subject matter expertise. Although these "older" tools contribute to a slower pace of adoption, they are essential to several missions so they must continue to be ported to new architectures with their code base updated to be performant on new HPC systems. The program will pursue various paths to mature its credibility assessment processes and support their routine use by incorporating newer methods. Non-Bayesian methods and techniques developed as part of the ASC Advanced Machine Learning Initiative (AMLI) will be integrated with in situ,

inline UQ capabilities to further enhance next-generation methods and techniques. The development of new workflow tools is needed to ensure consistency across ASC application codes and to capture a simulation pedigree in a manner that will be useful to customers and future analysts who have relevant experience at all levels.

Improvement of the tri-lab Common Model Frameworks (CMFs), henceforth used to convey both physics and engineering CMF activities at NNSA labs, and their porting to new HPC platforms are needed for all modeling activities supported by ASC. CMFs are suites of similar simulations produced for various design, engineering, and production mission applications and allow systematic UQ to be performed while minimizing bias from relying solely on single experiments. They encompass system and software engineering design principles, codes, data management, and simulation workflows, with the goal of increasing confidence in simulation results. CMFs are becoming a staple across the laboratories for providing a means of validation and gauging progress in predictive capabilities. They ensure repeatability of simulations and enable peer review of each step in an analysis; however, their use has been somewhat limited by suite-specific learning curves and tools opaque to new users. Additionally, many users and projects maintain their own separate parallel frameworks that can diverge from the common repository. A special focus on sharing an infrastructure across these suites can provide clarity in parallel with sustained efforts to integrate UQ assessments. Sharing also necessitates automation of these workflows—making them more easily executed by the application users—and provides flexibility to discourage inconsistent or fragmented use of V&V tools by some users. Archiving data provenance for all data used throughout the workflow is another aspect of improving the utility of the CMFs and should be captured automatically (yet still be human auditable). Common formats and interfaces need to be more broadly adopted by all ASC-funded programs at the NNSA laboratories, which should improve access and sharing of experimental data that include both initial conditions and results of the test diagnostics used to collect measurements.

Successfully quantifying uncertainties requires routine investments in technologies that make UQ methods easier to implement, more computationally tractable, and reproducible. Users of these methods will be included in the development efforts to properly manage expectations and set value judgment of these future UQ tools. Resources will be invested in training programs and knowledge systems to train users and to advertise new UQ capabilities. Foundational efforts such as the CMF also have a role in user training and adoption; experience shows much of the same challenges when this construct was first implemented by ASC more than a decade ago. Addressing the user adoption issue demands the continued execution of ASC's "One-Program/Three-Laboratories" principle because of the need to share across the three NNSA laboratories methods and priceless historical underground tests (UGTs), and more recent experimental data for efforts more specific to current technical problems such as aging.

> **Strategy**: To better quantify uncertainties for the stockpile, ASC will continuously evolve our UQ and AI/ML tools to take advantage of immense computational power, in addition to maturing credibility assessment processes, promoting common formats and interfaces, and investing in user training and knowledge systems.

Pathway III: Augment the exploitation of legacy data

Together, the archives of legacy and evolving data constitute an essential and valuable NSE-wide resource. CMFs represent a key enabling initiative for long-term management of both legacy and new data archives. The development of CMFs enables management of legacy data as an institutional resource and creates the potential for establishing enterprise-wide standards for seamless data sharing. Although several challenges that stem from data accessibility, institutional policies, and governance associated with data security and ownership are beyond the scope of the ASC program, it can pursue priorities, in collaboration with other DP programs, to enable efficient data collection for future experiments and to establish a trusted process that improves accessibility and use of legacy data.

Legacy data present a hurdle to programmatic planning because of the variability in their value for code development and model validation. Although some legacy data are directly usable as input parameters for ASC simulation tools or for output validation, other data may require additional analysis and interpretation or may only indirectly influence the determination of simulation inputs or output parameters. Nevertheless, untapped value in the legacy data exists in terms of supporting constitutive relationship development, V&V of simulation tools, and UQ of results. All are worth pursuing because legacy data from nuclear tests, weapon qualification tests, stockpile surveillance, component production, and phenomenology-discovery experiments together represent an irreplaceable resource. Understanding legacy data often leads to better quantified margins and uncertainties of a variety of systems and potentially enables new interpretations of manufacturing requirements. State-of-the-art data analysis methods including ML tools offer an opportunity to reexamine and extract more information from legacy data and leverage them in new ways.

Metadata, provenance, and other curation and quality standards will be developed and sustained within the ASC program. The program will coordinate with other DP R&D activities that are responsible for archiving nuclear and non-nuclear test data to guarantee that the data are not merely preserved but also are available in forms that allow for easier and secure electronic access, analysis, and exploitation. Once available, these data can provide opportunities for new techniques such as those developed in the ASC AMLI portfolio to inform future stockpile studies. The program will incorporate legacy data resources into simulation workflows that will be managed through CMF efforts across the enterprise. Addressing technical needs of data sharing with NNSA laboratory and plant stakeholders can be accomplished through improved curation of the legacy data. Broader acceptance and adoption of this approach means addressing a variety of technical and policy issues regarding network access and a resourced plan that incentivizes sharing.

Increasing our understanding of existing data, or determining their usefulness, requires investments in the infrastructure that make it easier to share information and ways to automate laborious and time-consuming methods. Pursuing these tasks and continuing to deliver reliable modeling and simulation for assessing performance and safety of an evolving stockpile means gaining efficiencies rather than merely seeking additional resources.

> **Strategy:** To better utilize legacy data, ASC will incorporate the rich set of legacy data into a new set of data-driven workflows that seamlessly combine simulation and experiment with complete provenance and reproducible workflows.

Objective 2: Modeling and simulation for optimizing design options and addressing threats

The ASC program is responsible for developing code capabilities to support new designs because NNSA must be prepared to respond to new threats quickly to safeguard the U.S. nuclear deterrent in the global security arena. Requirements for future weapons systems imply new configurations and materials for operation and weapons performance in new environments, as well as some possible effects not known in the current stockpile. The challenges articulated for this objective build on the same underlying concepts in Objective 1; therefore, using the same approaches should extend the previous efforts to increase efficiencies and make tools easier to use in assessing and responding to new threats. In addition to stewarding the nuclear stockpile, the expansion of the NNSA mission to field a responsive nuclear deterrent demands new code capabilities that can simulate nascent threats and new environments. The simulations must be trusted for use beyond annual certifications and assessments, particularly for use in designs that have limited data beyond the historical UGT basis. As the Nation's nuclear stockpile evolves to support a responsive and resilient nuclear deterrent, so must the ASC simulation capabilities that fulfill the program's commitments to the NSE.

Achieving this objective relies on replacing a time-consuming physical build/test learning cycle with a virtual, embedded testing capability through the development of next-generation codes. Ensuring the evolution from a clean-sheet design to a prototype system in under 5 years (as planned for the Fiscal Year 2032 Stewardship Capability Delivery Schedule's "First Production Unit in 5 Years" pegpost) demands enhanced physics models for related mission areas and technological advances that enable capabilities more productive for the nuclear security enterprise. These advances expand the broader use of modeling and simulation capabilities and allow code pedigree and simulations to be reproducible in support of the peer review process, as routinely exercised in all aspects of mission-relevant work.

Objective 2 requires three prominent response pathways to drive activities toward delivering responsive and reliable modeling and simulation capabilities in support of the future deterrent:
- Improve codes and code development processes to bolster design activities,
- Deliver trusted simulations within and beyond the test basis, and
- Decrease the time-to-solution window for design and qualification.

Pathway I: Improve codes and code development processes to bolster design activities

Threats to our national security, as well as technological surprises, can outpace the development of processes that produce validated models used in an informed decision-making process. Successful development and delivery of new code capabilities, such as the Lawrence Livermore National Laboratory (LLNL) MARBL code depicted in Figure 3, often arise from balancing the persistent trade-offs between code responsiveness and the demands for solution accuracy and precision. Although these can be perceived as conflicting characteristics of the physics and engineering code development process, the ASC program views them as opportunities for risk management and support for activities that determine the necessary or best steps, processes, and tools that result in responsiveness. Assessing best practices for technologies that support ASC workflows—such as containers, data labeling, provenance capture, reproducibility, trustworthiness, composability, data curation, and archiving—makes the technologies more robust and prevents unintended duplication of efforts. Executing this pathway means that

developed tools are deployed regularly to a wider range of users, at all levels of training and experience, and provided as part of a documented, credibility-based workflow.
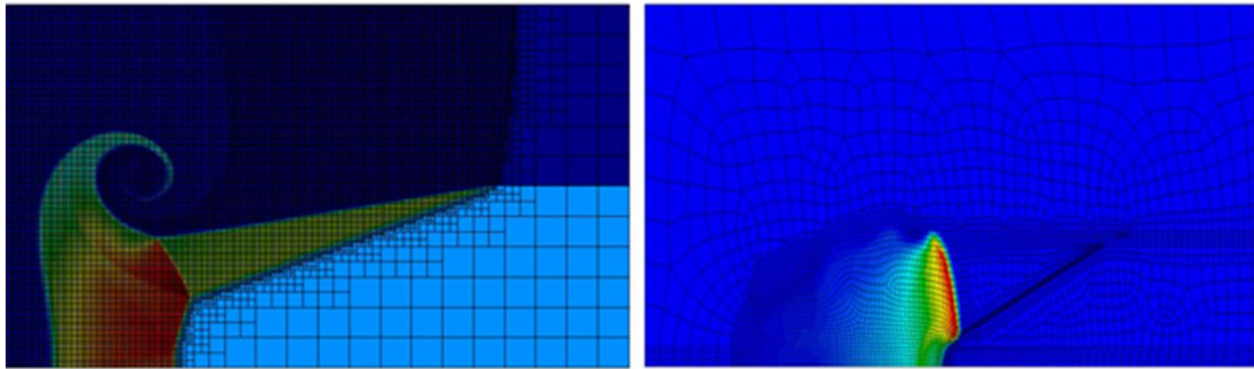

Figure 3. LLNL's MARBL code has improved its dynamic adaptive mesh refinement, providing a highly efficient capability for capturing finer details in 2D/3D multiphysics calculations with high accuracy. In the left figure, mesh refinement is being used exclusively to capture fine details in the physics of a shock interacting with a material interface in the "triple point" test problem run in a fully Eulerian mode. In the right figure, a shaped-charge simulation uses high-order, fully unstructured, arbitrary Lagrangian-Eulerian mesh motion—with new target-matrix optimization, paradigm-based mesh motion methods, and mesh refinement to capture detonation fronts and material interfaces efficiently and robustly.

ASC will support the future nuclear deterrent mission with full-system lifecycle models and predictive assessment of lifetime performance in all environments. Developing full-system lifecycle models requires integration of agile physics and data-centric model development processes. Physicists and engineers need to evaluate the impact of manufacturing defects, as-built geometries, modeling approximations, surveillance data, and more over the course of the life of a weapon system; they also need to understand the resultant effects that these attributes have on safety and performance. Such a hierarchical modeling approach requires sophisticated databases, interrogated by models of varying fidelity, scale, and associated uncertainties. To emulate key combined environments, enhanced physics development and modular coupling across multiphysics applications are also needed. During the design phase, the impact of this data-centric ecosystem—from concept to surveillance—will demand matured design tools and a real-time modeling capability. Moreover, in later lifecycle phases with digital twins that are virtual replicas of physical items, data must be assimilated from surveillance measurements and margins understood for each individual system, along with a constant exploration of system health, all of which are challenging goals.

Establishing some key software practices used by the commercial industry can lead to faster cycles of learning but requires a shift in culture for widespread adoption within the NNSA laboratories. Practices such as continuous integration and continuous delivery are well proven for introducing capabilities to analysts faster while addressing issues of code use expansion. Maximizing impact to the nuclear deterrent community prompts an early engagement of computational analysis in the weapons development lifecycle and a rapid delivery of models that are optimized for accuracy. Efficiency concerns mandate improvements to workflows, with advancements in and hardening of computational tools and analyses that are easier to execute, repeatable, and amenable to rigorous peer review.

Problem setup, such as geometry manipulation and mesh generation within a CMF, are targeted improvements for saving analyst time and are efforts to make the ASC environment persistent and consistent across all platforms. These processes also should incorporate methods for quantifying uncertainties in parallel with model development such that the inherent physics are characterized and UQ is both integrated within code development and production activities. This integration promises insight and faster cycles of learning and enhances legitimacy to the UQ process.

AI and ML are emerging technologies that have the potential to improve both the development of ASC capabilities to meet future requirements and the critical decision-making ability throughout the weapons lifecycle. AI/ML for data-centric and full-system models could enable an automated refinement of workflows and analyses of multimodal experimental data and enhance the quality of analysts and engineers' training. The use of AI/ML can positively impact computational efficiency and scientific advances and enable end users to intelligently explore the design space for a variety of applications faster by avoiding computation of nonphysical responses, or quantities of interest, and with less repetition of the same problem set and parameter spaces from multiple analysts (see Figure 4). To assist the designers and users, the ASC program must build a centralized repository of existing methods/capabilities and document technology gaps and projected needs, with the goal of optimizing the search for new methods. In this regard, an AI-powered knowledge management system enables continuous update and real-time interrogations of existing capabilities, projects, milestones, users, etc., while capturing a real-time and accurate gap analysis. AI could also assist in validation experiments to produce suites of experiments that are optimized for both cost and measurements that lead to better physics models.

Bolstering design activities with code improvements and leveraging efficiencies demands embracing methods and simulation technologies that provide insight through faster cycles of learning. Success in meeting this challenge means developing capabilities that document exploration of design options, expand the user base, and result in codes that are more auditable to support peer review.
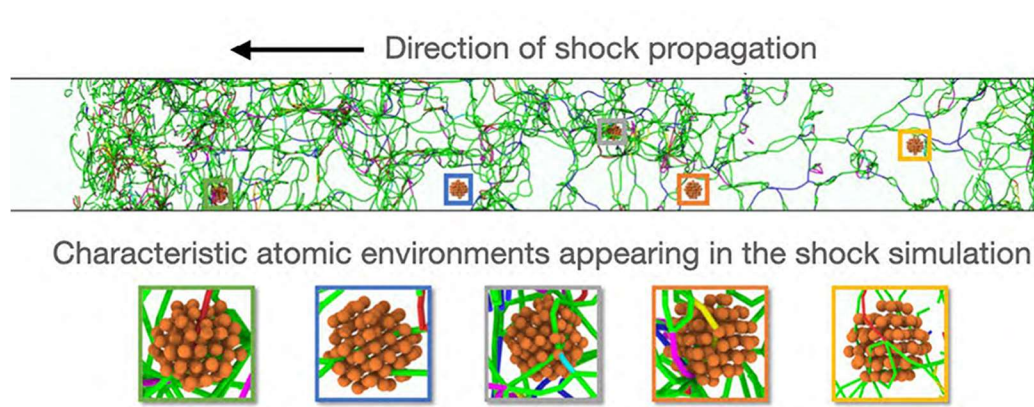

Figure 4. Snapshots from an ML-driven shock simulation with 1.3 million aluminum atoms. The shock creates crystal imperfections such as dislocations (green lines). ML-predicted forces agree with reference DFT calculations to within 3% error, as tested on randomly sampled atomic environments (orange clusters). (LANL)

Strategy: To improve software for design activities, ASC will pursue development of full-system lifecycle models, more effective user workflows, AI/ML methods, and improved ability to address demands for solution accuracy and code responsiveness.

Pathway II: Deliver trusted simulations within and beyond the test basis

VVUQ capabilities form the basis of the quantification of margin and uncertainty (QMU) framework, which in turn establishes confidence in the existing stockpile. Future QMU process efforts will require more efficient and more rapid VVUQ methods to fully utilize the computing power provided by new architectures. Existing UQ foundational theories are inherent to maintaining confidence in the future nuclear deterrent. Furthermore, an enhanced conceptual framework is required to treat new uncertainty dimensions that result from insufficient diagnostics facilities or resource shortage for generating the data that fully trusted analyses would require. The new VVUQ framework must be equipped with mechanisms that identify all sources of uncertainties and quantify them in a transparent and trusted manner that is easier to use and does not require intensive labor cost. Simulation capabilities that support responsive weapons options will likely need to involve a different paradigm for assessing maturity and for quantifying and establishing confidence intervals that reveal risks associated with code limitations.

In an ongoing ATDM project, Sandia National Laboratories (SNL) researchers obtained a 4500x speedup for the SPARC (SNL Parallel Aerodynamics Reentry Code) full-order model simulation—while keeping the approximation error below about 1%—by automatically constructing a reduced order model (ROM; see Figure 5). The ability to construct a ROM expeditiously, without sacrificing physical fidelity, will help accelerate the analyses of delivery environments and the construction of computational evidence for environmental specifications and qualification for nuclear weapon systems.
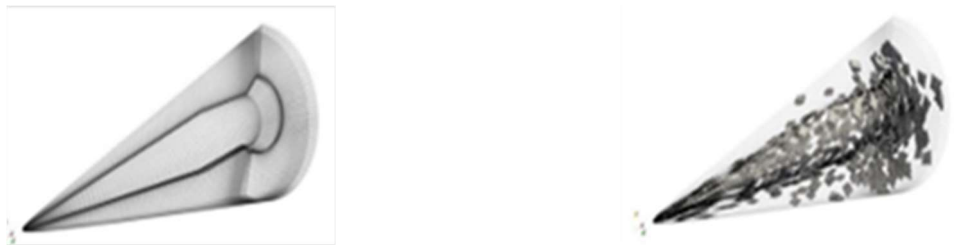
Figure 5. Left: Vehicle geometry with conventional finite volume mesh. Right: Hyper-reduced mesh for a ROM, which resulted in significant speedup of the simulation runtime (analysis results using the ASC ROM capability are courtesy of SNL's Laboratory-Directed Research and Development program).

Certain VVUQ processes require laborious research and analyses that may span decades. It is imperative to speed up the process of implementing and running codes while exploiting in parallel the experimental and simulated data. AI frameworks of knowledge management systems can alleviate some of these challenges and provide knowledge bases that capture—to a sufficient extent—the expertise of experienced researchers and experimentalists. AI also can help drive the decision-making process and lead to a disciplined, auditable methodology for conducting validation experiments, as well as reasoning

on their feasibility and practicality in an automated manner, because of how these methods drive standardization of processes and data to employ them properly. Ultimately, the UQ for the new deterrent must address comprehensively epistemic, aleatory, and ontological uncertainties. Establishing high-level confidence will require much more benchmarking data beyond existing integral test data. Likewise, a significant effort must be dedicated to understanding and reducing model-form errors.

The ASC program will invest in emerging technologies and tailored mathematical and computational frameworks so that a user-friendly system can be realized for VVUQ tasks while still prioritizing UQ method development. Meeting this challenge shifts the current laboratory culture away from sequential validation activities to those that create "born-credible" VVUQ software. The new tools must have transparent levels of accuracy that show the linkages to integrated tests, single-effect experiments, and first-principles simulations. Consequently, operational requirements demand these improvements be timely and trusted by program sponsors and customers.

> **Strategy**: To deliver trusted simulations within and beyond the nuclear underground test basis, ASC will advance computational frameworks, accelerated by AI tools, that identify sources of uncertainties and quantify them in a transparent and trusted manner.

Pathway III: Decrease the time-to-solution window for design and qualification

The demand for a safe, secure, and reliable nuclear stockpile, together with the need for a responsive deterrent, calls for DP programs that can rapidly develop and deliver advanced capabilities. The ASC program must ensure that NNSA national laboratories continue to deliver on current and future mission needs while adapting to radical changes introduced by emerging software and hardware technologies. Novel computer architectures and programming techniques will transform the simulation environment, and ASC must be at the forefront of capitalizing on technological advancements. By meeting this challenge and others in this objective, the ASC program will maintain its relevance to the overall NNSA mission by providing credible simulations at the needed fidelity levels and in a timely manner.

Future simulation environments require new programming models that can exploit novel architectural advances. Co-design collaboration methodology has demonstrated successful results in enabling ASC codes be ported to and perform on the next-generation architectures. As a result of elevating simulation needs in co-design, the cost of code development should decrease while simultaneously creating robust simulation capabilities that ultimately shorten design and qualification lifecycles. For example, computer architectures are evolving to a point where accelerator features can be designed into hardware and carried out as enduring requirements in system architectures across multiple system generations. The ASC program must develop roadmaps for simulations on non-classical hardware, such as neuromorphic, non–von Neumann, quantum, and AI-enabled technologies, because these hardware types may be deployed in subsequent generations of HPC systems, possibly at the end of this decade.

HPC capabilities provide a multitude of opportunities to enhance simulation execution. Essential to faster computational solutions is the creation of tailored algorithms for implicit or semi-implicit methods, multiscale physics coupling, high-order and hybrid high-order/low-order methods, and AI/ML methods. Devising faster and more efficient algorithms requires advances in computational mathematics and adoption of modern numerical techniques while exploiting new computing techniques

such as mixed-precision arithmetic, floating-point compression, and approximate and probabilistic computing. The computational power available in the near future has the potential to support in-situ techniques, such as embedded UQ, that can produce uncertainty estimates in a single calculation. Additionally, new computational science and engineering solutions must be developed to address issues of extreme levels of shared memory parallelism, memory latency, and concurrent multiphysics operators.

The ASC program will continue to advance computational methods by hardening the modular software architectures that started as R&D efforts in the ATDM portfolio. Next-generation capabilities will replace legacy capabilities as production codes and allow designers to continue to meet mission requirements by using tools that respond quickly to technological changes and evolving user requirements. Methods that abstract underlying architectural complexity to make it easier to port codes onto new architectures will also come with more consistent user interfaces that make the codes more accessible to users without code developer training. This accessibility translates into a code strategy that can easily be adapted in the near term to benefit the needs of the Design Agencies (DAs that are NNSA laboratories with "design" authority for specific weapon systems), and Production Agencies (PAs that are NNSA plants/sites with "production and manufacturing" authority).

> **Strategy**: To accelerate design and qualification, ASC will pursue programming models that efficiently exploit advanced computing architectures and facilitate the development of advanced algorithms that maximize the benefits of these new machines.

Objective 3: Simulation for an efficient production enterprise

Production and manufacturing of materials, components, and systems are a significant part of current activities that NNSA is conducting to modernize the stockpile. NNSA is confronted with numerous challenges when producing or procuring weapon components. Commercial industry has the option of achieving economies of scale and readily integrating novel technologies—a stark contrast to the options available to NNSA due to stringent security, safety, low-volume, and high-quality requirements. Regardless, technological advancements represent a significant pathway for achieving efficiency gains that can reduce costs and schedules, thereby providing risk-mitigation options. The investments in materials modeling previously described are applicable to addressing challenges to this objective.

ASC will develop simulation capabilities to model physical behaviors for key processes and technologies. Furthermore, the NNSA laboratories will employ more of the co-design collaboration philosophy and multidisciplinary team science to break down barriers to technology integration and adoption. Collaboration is an obvious requirement for leveraging, rather than duplicating, expertise while rapidly accomplishing production mission goals. Sociological solutions will be needed to address this cultural problem because this concept runs counter to a workforce culture born out of working on stringent NSE requirements and in a distributed nuclear weapons complex.

Developing models for manufacturing and production processes requires dedicated discovery experiments with sufficient diagnostics to obtain the relevant data necessary for predictive simulations. Performing experiments in production settings is challenging because these are difficult environments, due to inherent noise and scale, to obtain useful data for validating models and quantifying

uncertainties. In addition, these tasks could interfere with production activities that are already under severe schedule constraints. Success in developing and establishing experiments for these processes assumes a planned and sustained partnership with other programs that have funding authority over production activities and those who conduct experiments. Codes such as the LANL FLAG (Free LAGrange) code (see Figure 6) could potentially benefit the production missions greatly if ASC is provided sufficient lead time to build the new user requirements into its code base.

Objective 3 requires three major response pathways to delivering agile and reliable modeling and simulation capabilities to support the production complex:
- Deploy ASC tools for rapid iterations and assessments,
- Address material modeling needs in production simulations, and
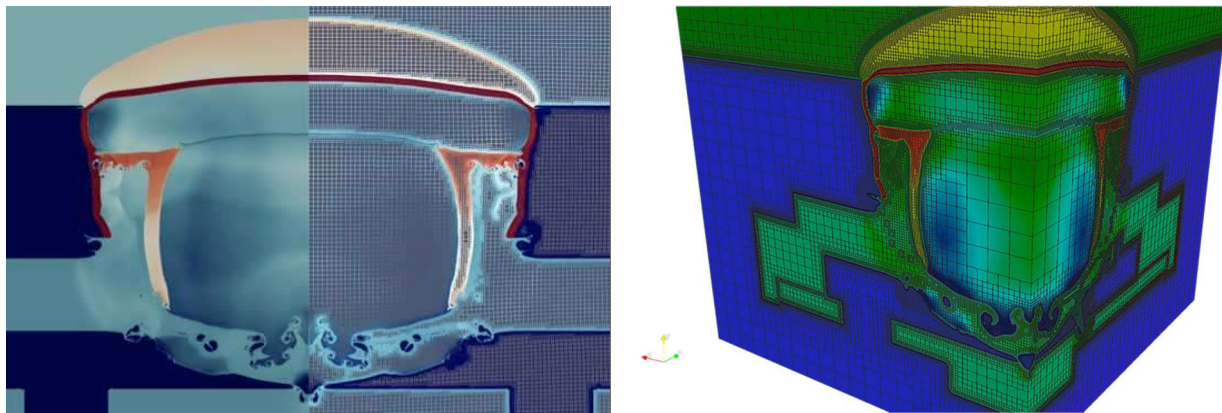- Develop full lifecycle models for production science.

Figure 6. Enabling 2D/3D end-to-end modeling of current and future detonators for the Nation's stockpile using LANL's FLAG code under ASC PEM High Explosives and IC Lagrangian Applications Project. More predictive detonator modeling has increased detonator production efficiency.

Pathway I: Deploy ASC tools for rapid iterations and assessments

To support cycle reduction, the ASC program will develop additional simulation capabilities for qualification evidence and those that enable rapid design. Simulation tools that can optimize design, production, risk assessment, and physical testing approaches need to be developed or enhanced further to reduce costs and schedules. An assessment of industry approaches and integration of commercial off-the-shelf tools can and should inform how to address the unique challenges of NNSA production needs. A systematic plan is needed to develop an integrated, multiscale modeling capability that links emergent material properties to the chemical compositions and manufacturing processes that would produce materials with properties of interest. Evaluating the impact of new materials and manufacturing processes on integrated device performance is a major challenge because novel materials require alternative modeling approaches to facilitate faster component qualification and certification. ASC tools must be adapted to model new materials and manufacturing processes to help inform and improve the quality and reproducibility of manufactured parts. This adaptation includes informing material property specifications and providing predictive, simulation-based estimates of allowable variability and tolerances for new components. Tools that provide realistic ranges of these values can lead to

efficiencies of managing material feedstocks and reducing waste associated with destructive analyses, as part of qualification and certification activities.

Model-based engineering (MBE) is a conceptual approach that reduces costly computations by exploring the design space with low-resolution models and training algorithms that converge on acceptable solutions. This can lower the computational cost for non-physical data and reduce waste of material feedstock on poor component designs. MBE can be used in concert with other methods, such as advanced manufacturing and design technologies, which include additive manufacturing and topology optimization. ASC must invest in developing the computational methods and infrastructure necessary to accelerate code development efforts to extend MBE to a variety of production mission needs. The concept of digital twins—a virtual replica of a physical item—is another approach in which success depends on new infrastructure and new methods for integrating simulated data with measurements. Data-centric workloads require significant computing capacity and solutions to address issues with data ingestion, curation, and management to enable workloads that are reconfigurable for optimizing performance. This complexity demands that technology gaps and investment plans be identified for agile computing capacity that will drive future advanced computational architecture investigations.

Applying modeling and simulation tools to identify and minimize the number of key performance parameters has the potential to reduce the number of physical prototypes required for rapid assessments of forging and encapsulation process parameters. Other early applications that are beneficial in mitigating design-induced production issues also show promise in identifying stress concentrations in metal parts during assembly and optimizing weld order to reduce thermally induced distortions, in addition to producing components with additive manufacturing (AM). CMFs mentioned previously need to be developed to capture best practices and standardized choices for modeling and simulation for production missions. These CMFs will also be informed by MBE practices to make them more interoperable between Design Agency (DA) and Production Agency (PA) environments and pave the way for the digital twin models for components and systems.

Collectively, leveraging existing infrastructure to collaborate with the PAs and developing physical models to support production processes, such as advanced manufacturing CMFs, will allow a rapid, physics-informed approach to support the production missions.

> **Strategy**: To deploy ASC tools for rapid iterations and assessments to support production and manufacturing activities, ASC will develop an integrated modeling capability, link material properties to production-relevant physical properties, and make HPC a ubiquitous tool for PAs.

Pathway II: Address material modeling needs in production simulations

Understanding physical behaviors to support modeling of as-built parts, manufacturing tolerances, part variability, and defects requires significant computational resources to model material response properties with predictive, ab initio approaches. Computing model response quantities using first principles in 3D represents an ongoing R&D challenge due to the complexity and scale of these types of problems. Further research will focus on specific materials and processes required for production challenges. The production mission requires a component lifetime modeling approach that enables product-based, rather than process-based, design and optimization, thereby driving toward the need for

an integrated, multiscale modeling approach that links the process-structure-properties-performance aspects of components. ASC must leverage collaborations with others in AI/ML for new physics models (e.g., materials informatics), faster and more accurate algorithms, and process automation technologies to provide timely answers to new production questions. ASC tools will be adapted to model new manufacturing processes to help inform and improve the quality and reproducibility of manufactured parts and the ability to assess and possibly accept off-nominal parts that may otherwise be needlessly rejected.

AM is an attractive alternative in manufacturing processes because it can create complex components via an additive process, instead of the traditional subtractive process of machining from bulk-produced materials, thereby reducing the number of process and machining steps in addition to material waste. Time and material savings are evident, but a need exists for simulation capabilities that model the material behavior of the components, capture process characteristics that influence material structure of the components, and determine whether adequate statistical variations between components can be maintained and controlled. Power variations, impurities of feedstock, and energy dissipation are just a subset of the parameters and relationships that influence the resulting material structure of components, and each must be captured by a model. Another related technical challenge that must be pursued simultaneously is whether simulated data could be accepted in qualifying and certifying components and whether these data are sufficient to inform or reduce costly destructive tests. To ensure success in meeting production and manufacturing targets for the nuclear security enterprise, close collaboration with experimental programs and PAs should occur before careful investments in capability development are made. Such an ongoing partnership exists between SNL and KCNSC, in which SNL researchers are working on a general laser weld modeling workflow that employs both high-fidelity and fast-running models (see Figure 7).

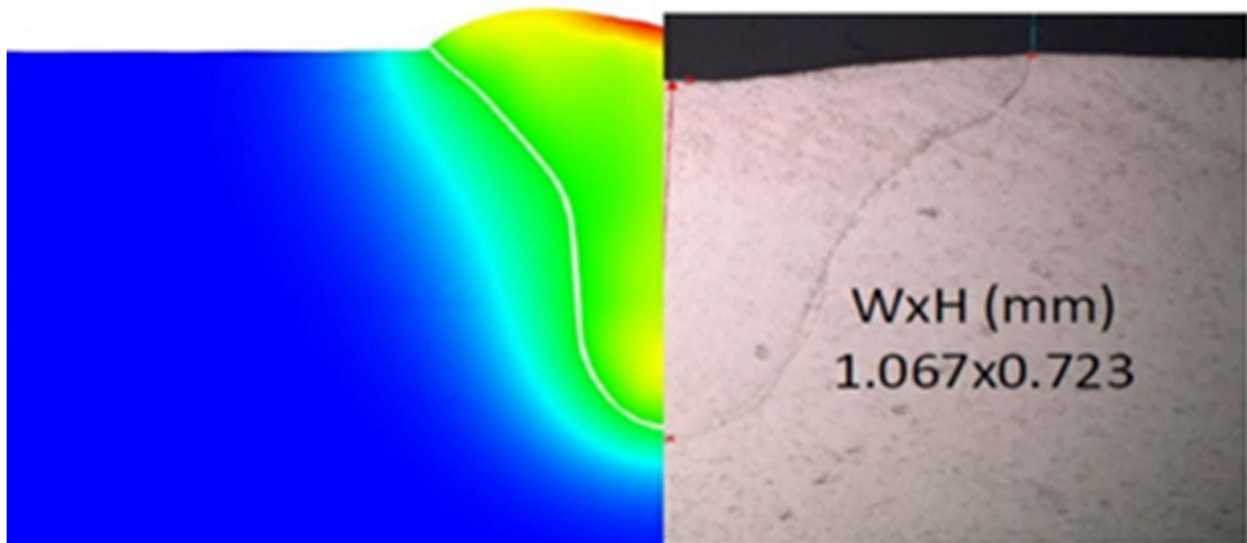*Figure 7. Developing reduced-physics models for quick turn-around analysis of production welds is critically important in numerous stockpile applications. On the left is a melt pool for a stainless-steel weld as predicted by a reduced-physics model calibrated to weld data on the right. This is an example of a challenging multiscale, multiphysics problem that requires fast-running tools for effective production work. (SNL)*

> **Strategy:** To improve material models for production simulations, ASC will increase the fidelity and accuracy of material models to account for unique conditions of the production process imparted through manufacturing processes and to quickly address production challenges.

Pathway III: Develop full lifecycle models for production science

A significant long-term goal for the ASC program is to develop full lifecycle models for predictive assessment of lifetime performance of systems in all environments and scenarios. Such a construct will represent the culmination of agile physics and data-centric model development and the computing capacity needed to execute full lifecycle models. It will also harmonize all previous elements described into a single construct, allowing scientists and engineers to evaluate the impact of manufacturing defects, as-built geometries, modeling approximations, surveillance data, etc., over the life of a weapon system.

The ASC program will develop a plan and execute on delivering continuous and autonomous execution of networked, multiscale, and multiphysics simulations that inform and respond to real-time measurements, all of which build on the concept of digital twins. Starting with hierarchical modeling approaches, the program will determine how to map multiple models of varying fidelity and scale and associated uncertainties to each other. These mappings could appear as databases that can be coupled to workflows that contain adaptively built systems of tractable models with their dependencies on experimental and computed data. Complex multiphysics environments then need to be emulated and coupled to create a full virtual environment in which multiphysics experiments are conducted in tandem with physical simulations of wear, aging, etc. Previous considerations on lifecycle modeling were targeted specifically from design to qualification. This lifecycle model approach extends to all activities—from conceptual design to surveillance—with matured design tools and real-time modeling capability. The nascent SNL Accelerated Digital Engineering initiative's vision depicted in Figure 8 portrays the ambitious endeavor to support future weapon system programs through an integrated digital-design ecosystem.
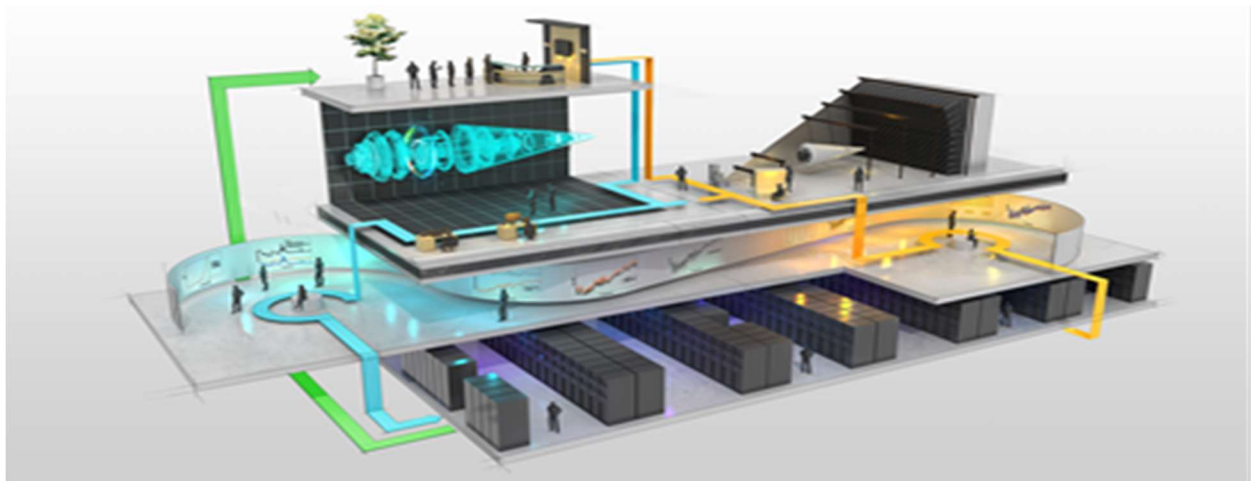

Figure 8. The Sandia Accelerated Digital Engineering initiative, initially began in the ASC program and broadened in FY 2022 to include Weapon Survivability and Delivery Environments, aims to accelerate engineering product realization via an integrated, digital-design ecosystem. The image is provided by

> *the Sandia Electrical Sciences SLICE team, who is developing a framework to deliver testing results combined with modeling and simulation results for electromagnetic applications.*

The lifecycle model approach needs an agile computing environment across the three laboratories, with significant capacity to handle the multi-physics coupling, hierarchical modeling, and autonomous exploration of coupling sensitivities needed to make these data useful to support decisions. ASC must coordinate requirements for future hardware architectures and manage the capacity, agility, heterogeneity, and reconfigurable requirements needed to support the investigation and integration of such data.

Strategy: To develop full lifecycle models, ASC will pursue an approach that predictively assesses the performance of systems throughout their lifetimes, spanning design, production, and surveillance phases.

Conclusion

This *ASC Simulation Strategy* has attempted to convey how the DAM portfolio will support the DP mission requirements via three objectives:

> *Objective 1*: Modeling and simulation for assessing the performance, safety, and security of an evolving stockpile;
> *Objective 2*: Modeling and simulation for optimizing design options and addressing threats; and
> *Objective 3*: Simulation for an efficient production enterprise.

To achieve these goals, ASC will leverage increased efficiencies in simulation and computing as described throughout this document. Moreover, innovation for efficiency and productivity emerges as a common theme applicable to addressing many future challenges.

The ASC program will design and develop tools and workflows to enable efficient, rapid, and auditable exploration of design options and trade spaces, with the end goal of increasing the responsiveness, collaboration, and overall productivity of the nuclear security enterprise. More sophisticated models of materials and phenomena known to be relevant to current and near-future concerns will address aging issues and challenges associated with the use of novel manufacturing technologies. These models must be adaptable to variations in microstructure, impurities, and other attributes not considered in the past, which requires accelerated techniques to explore options and incorporate new data. Capturing best practices in CMFs will create the apparatus needed for robust VVUQ across all applications of ASC simulation tools. Finally, all areas of modeling and simulation will leverage improvements in HPC and numerical methods to achieve these goals.

ASC will build on the success of the Stockpile Stewardship Program to meet the challenges of a sustained 21st century deterrent; UQ is central to these efforts. UQ will be an automated part of workflows and will be executed routinely by the broad base of scientists and engineers that comprises ASC. The focus on UQ will also drive numerous related efforts, such as data management, to archive the provenance of all data throughout user workflows, including designer decisions and other key metadata. Common formats and interfaces will improve access and sharing of data—such as those of underground tests, flight tests, environmental specifications, qualification tests, and test diagnostics. Success for ASC means

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that the program will aim to extract the maximum value from R&D investments, newly generated test data, and priceless historical test data.

ASC will strive to fulfill the three objectives of this 2022 *ASC Simulation Strategy* that will be executed by the outstanding workforce at NNSA Headquarters, national laboratories, and our partners. The ASC program looks forward to an exciting future of continuing to deliver for the NNSA missions.

Appendix A. Acronyms

AM	additive manufacturing
AMLI	Advanced Machine Learning Initiative
ASC	Advanced Simulation and Computing
ATDM	Advanced Technology Development and Mitigation
CDA	Code Development and Application
CSGF	Computational Science Graduate Fellowship
DA	Design Agency
DAM	Defense Applications and Modeling
DFT	density functional theory
DP	Defense Programs
HED	high energy density
HPC	high-performance computing
IC	Integrated Codes
ICF	inertial confinement fusion
LANL	Los Alamos National Laboratory
LLNL	Lawrence Livermore National Laboratory
MBE	model-based engineering
MD	molecular dynamics
MHD	magnetohydrodynamic
ML	machine learning
NNSA	National Nuclear Security Administration
NSE	nuclear security enterprise
PA	Production Agency
PEM	Physics and Engineering Models
PSAAP	Predictive Science Academic Alliance Program
QMU	quantification of margin and uncertainty
R&D	research and development
RDT&E	Research, Development, Test, and Evaluation
SNL	Sandia National Laboratories
UQ	uncertainty quantification
V&V	Verification and Validation
VVUQ	verification, validation, and uncertainty quantification

Appendix B. ASC National Work Breakdown Structure

ASC National Work Breakdown Structure
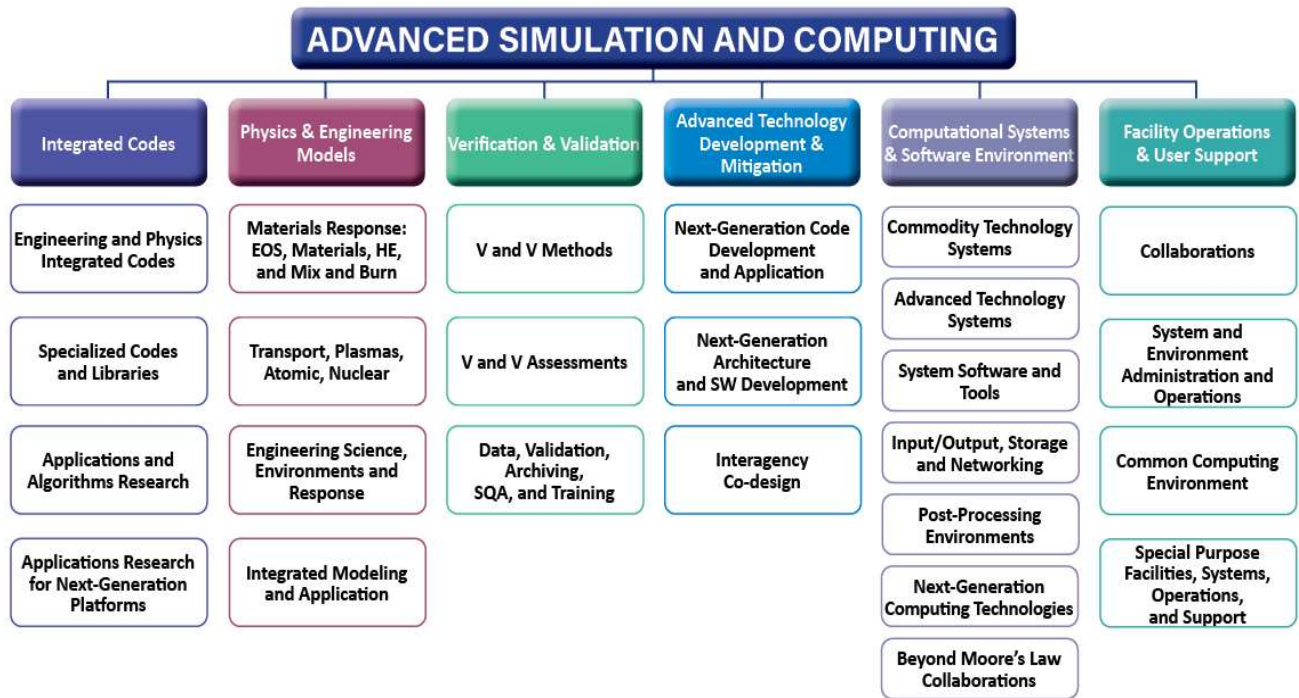
Back cover: Simulation of a confined turbulent jet impinging on a flat plate. Turbulent structures are shown in the vertical plane, colored by vorticity magnitude, with local heating shown in the horizontal plane. (SNL)

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