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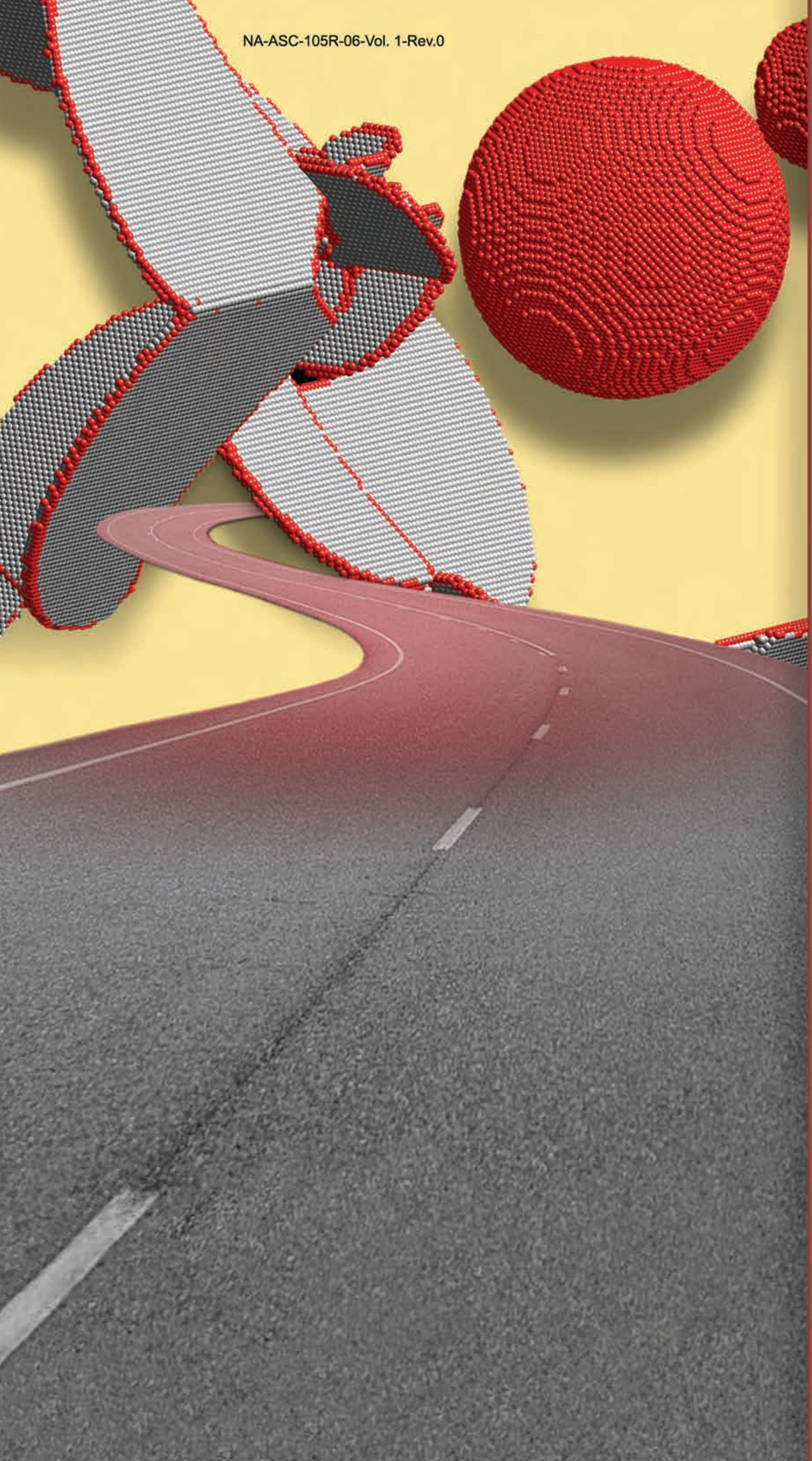
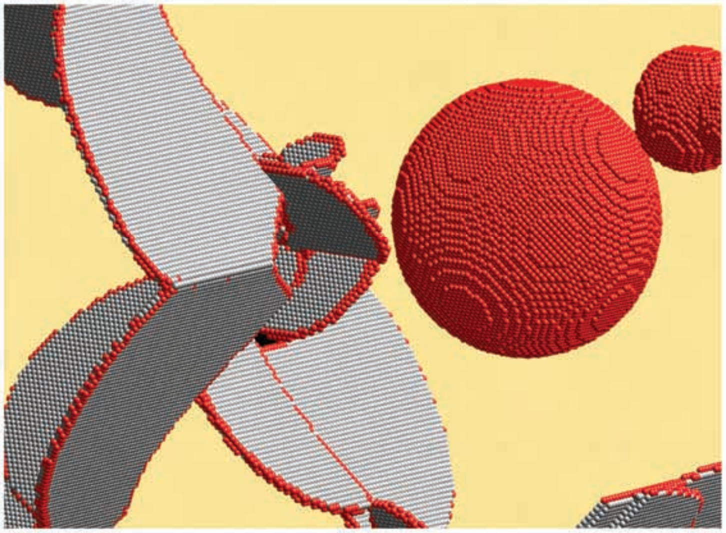


ASC™ ROADMAP

National Nuclear Security through Leadership in Weapons Science

National Nuclear Security Administration



ON THE COVER:

Dynamic void collapse in single crystal copper by dislocation emission. Shown is a small section of a 2.13-billion atom molecular dynamics simulation of a shock-compressed copper single crystal with a 0.41% preexisting void density. The simulation was performed using the SPaSM application running on BlueGene/L. Atoms in pristine fcc lattice sites are not shown, atoms in hcp stacking faults are grey, and other atoms (including surfaces and dislocation cores) are red. Untouched voids ahead of the shock front are visible in the upper right, while the complete collapse of voids leads to an array of planar stacking faults (grey) bounded by partial dislocation loops (red) behind the shock front. SPaSM is used to simulate many aspects of material phenomena, including response of materials to shock waves and the growth of instabilities and turbulence. The ASC Program uses results from such simulations to better understand these phenomena for its programmatic needs.

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Advanced Simulation & Computing ROADMAP

National Nuclear Security through Leadership in Weapons Science

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Dr. Njema Frazier, NA-114

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NNSA Defense Programs

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The *ASC Roadmap* is the third in a series of governing documents for NNSA's Advanced Simulation and Computing Program (ASC). Like the first two, *ASC Strategy: The Next Ten Years* and the *ASC Business Model*, the *ASC Roadmap* has benefited from the dedicated efforts of more than 30 senior-level experts. Most importantly, the patience and thoughtful guidance of NA-114, Office of Advanced Simulation and Computing, and the support of the ASC Execs have made this effort a success. Our gratitude, therefore, goes to all individuals involved and particularly to the following:

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FOREWORD

First and foremost, I believe that computational science and computer simulation are the only means to integrate our national understanding of weapons and their various behaviors and effects. Theory and experiment are critical to developing component models and checking the veracity of the computational predictions produced by those models, but only through integrated, multiscale simulation can we explore the precise conditions we want, at the scale we want, as thoroughly and quickly as needed. As we move into a more complex global future, our need to respond will hinge on our ability to simulate various scenarios and weapons issues.

An obvious question, then, is to ask to what extent leading-edge scientific technology will be needed as we move into an era with a smaller active stockpile, composed in significant numbers of a reliable replacement warhead, which is supported by a modern production complex. For the first time in the history of nuclear weapons, our nuclear deterrent will rely upon devices that, though carefully compared with the underground test data, have not been tested in their nuclear regimes. I believe that sustaining the testing moratorium requires that we transition to a point of sustainability at which our confidence in science-based simulations exceeds our confidence in simulations calibrated by underground test data.

Today's stockpile is overseen by seasoned experts, whose knowledge is grounded firmly in our test experience and complemented by modern tools and simulation. With the likelihood of maintaining weapons far into the future, well beyond the loss of our first-hand understanding, we must ask how we will train today's grade school children to certify and assess in 2030. How will they develop the experience under weapons conditions to assess the unknown issues or threats of the future, from effects and outputs, to issues inherent in an older stockpile and a collection of untested systems? Decisions today are based on not just the test data, but also on the experience and expertise of trained scientists and engineers that understand how design modifications and seemingly innocuous changes can lead to surprising results.

I see the *Roadmap* as an essential blueprint for transformation. With it, we can embark into this era of a reliable replacement warhead, aging weapons, young designers, and new national security applications with a plan for developing the transition to a sustainable scientific competency for the nation.

Dr. Dimitri Kusnezov,

Director, NA-114

EXECUTIVE SUMMARY

This *Roadmap* commits to goals that drive us to a future in which we will be able to sustain credible assessment of systems in the stockpile while maintaining the testing moratorium. Since the devices in the stockpile change in their characteristics as they age, and since refurbishments alter their properties, we cannot continue indefinitely to base our assessments on calibrations tuned to the parameter space defined by the as-designed test data. To be sustainable, stockpile stewardship must be grounded in science-based simulations and data, and the program must move to a point when science-based prediction overtakes calibration and enables us to accurately assess the state of the devices in the stockpile.

This direction follows from the program's *ASC Strategy: The Next Ten Years*. The *Strategy* outlines the following agenda:

> *The strategy for the next ten years…will set high-level directions and emphasize a deeper understanding of the underlying science, a continual replacement of the phenomenology in the weapon simulation codes by better theoretical models, and a quantification of their limitations.*

For the strategy to be realized, the program has to determine the high-level steps to be taken. Thus, the *ASC Strategy* and *Roadmap* work in concert, with the *Strategy* providing broad guidance to the weapons laboratories on scientific development areas required for meeting mission commitments with greater confidence, and the *Roadmap* providing details of the actual steps that must be taken to achieve significantly greater confidence in the calculations. Both documents support leadership in weapons science and the science-based simulation required for the nation to meet a multitude of diverse needs—from maintaining an aging stockpile (keeping systems from having to be pulled out of the weapons arsenal), to supporting the broad range of Homeland Security issues associated with national nuclear security (enabling interdiction, supporting dismantlement of devices that make their way onto our shores, and providing forensics and attribution of a nuclear device), to avoiding technological surprise (examining what-if scenarios to understand what options nuclear-nation states might be exploring).

This transformation to simulating a broader range of applications with greater confidence is already happening. Take, for example, the Reliable Replacement Warhead (RRW). The capabilities used in RRW development will be the primary support for the Complex's transformation (i.e., Complex 2030) and the future stockpile. Modern machining, safe dismantlement, and the development of further incarnations of the RRW will be made possible by accurate simulations. The cost savings over trial and error in manufacturing and experimental design and overly conservative approaches to refurbishment will repay past investments many times over.

To support the aggressive timelines for transformation of the Complex, the growing issues related to the aging stockpile, potential nuclear threats to the nation, and the nation's commitment to maintaining a capability-based nuclear deterrent into the future, the *Roadmap* features four major components, or *focus areas*, to meet these challenges and achieve the high-level *Strategy* goals:

- Address national security simulations needs;
- Establish a validated *predictive capability* for key physical phenomena;
- Quantify and aggregate uncertainties in simulation tools;
- Provide mission-responsive computational environments.

These focus areas are the four key elements by which ASC will measure progress, impact, and effectiveness. Each focus area has supporting goals and targets with time lines to measure progress toward a well-quantified predictive capability with computational environments to support the larger-scale, intensive computations.

1.0 SIMULATION AND THE CESSATION OF NUCLEAR WEAPON TESTING

For more than fifty years, the US nuclear program, spearheaded by the test program in Nevada, satisfied the nation's nuclear weapons mission needs. During this time, the Atomic Energy Commission (AEC) and its eventual successor, the Department of Energy (DOE), maintained a successful program of testing, surveillance, and simulation to ascertain the behavior of nuclear weapons.

This paradigm shifted in 1992, when Congress initiated a one-year test moratorium as part of the FY1993 Energy and Water Development Appropriations Bill, which President Bush later signed into law[1] on October 2, 1992. From that point to this, the US Congress and each administration have supported the extension of the moratorium indefinitely.

In the years following the nuclear testing moratorium, the DOE Office of Defense Programs faced several major challenges:

1. The population of weapons scientists with direct experience of underground tests (UGTs) would inevitably decrease as those scientists and engineers retired from the national laboratories. Although they would be replaced by talented physicists and engineers, the new weapons scientists would not be able to develop their intuition and knowledge as their predecessors had from a cycle that included calculation, testing, recalibration of the codes, and calculation again.

2. Code-development efforts would have to address the need for three-dimensional representations of nuclear weapons phenomena. Earlier codes were one and two dimensional and depended on assumed symmetries of the weapon system. However, since devices are inherently three dimensional and age in unforeseen ways, the codes would be required to assess the three-dimensional time evolution of weapons behavior to predict reliability and safety.

Major Cost Benefits Enabled Through ASC Simulations

- A $30B W76 system can remain active
- W88 weld thinning anomaly resolution saves several hundred million dollars in manufacturing
- Machining anomaly in the B61 system resolved
- Determination that the $4B W88 system could get increased yield margin through a simple engineering solution rather than employing a costly remanufacturing solution
- Time to complete the Phase II study of system development for RRW was six months, as compared with several years as well as a nuclear test, historically

3. More powerful computing systems would be needed to support the new requirement to run three-dimensional simulations. Specifically, the requirements called for systems many orders of magnitude more powerful than those that existed in 1994.

These considerations led to the establishment of Accelerated Strategic Computing Initiative (ASCI) in 1996 as an essential element of a Science-Based Stockpile Stewardship (SBSS) Program. ASCI's main objective was to provide high-fidelity, three-dimensional nuclear weapons simulation and modeling capabilities on an "accelerated" time line to meet the emerging needs of a stewardship program required to sustain an effective deterrent in the absence of nuclear testing.

In 2000, ASCI transitioned from an initiative to a program, and it was renamed the Advanced Simulation and Computing (ASC) Program. The establishment of ASC affirmed simulation and modeling as key decision-making tools and cemented their long-term role as integral components of the Stockpile Stewardship Program (SSP).

The SSP—with the ASC Program:

- Allows the US to continue an underground nuclear test moratorium and still maintain a reliable nuclear weapons stockpile.
- Ensures that all aspects of nuclear weapons stockpile operations are safe and secure—from design and engineering through dismantlement.
- Generates a large return on investment by providing cost-effective, simulation-based solutions (without testing) to issues facing the nuclear weapons stockpile—resolving significant finding investigations (SFIs), conducting annual assessments for certification, enabling stockpile lifetime extension programs, and responding to

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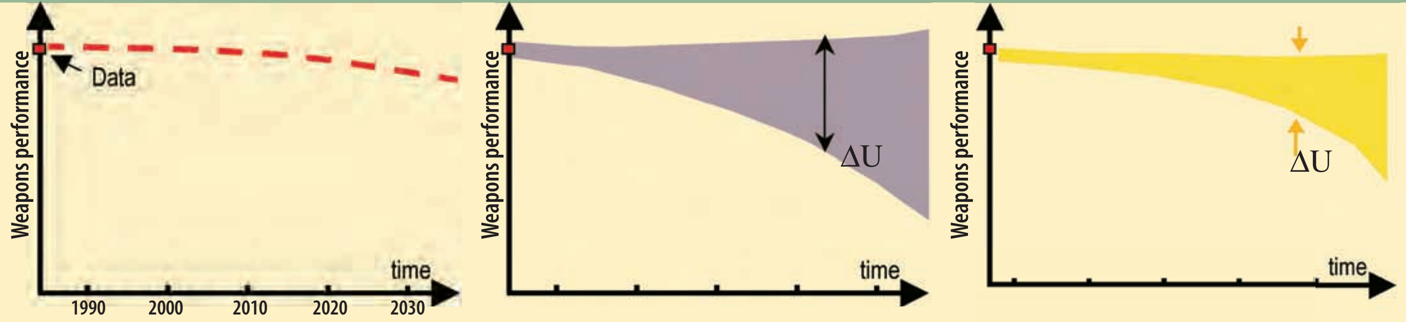
[1] NNSA L. 102-377 mandated the following: (1) banned testing before July 1, 1993, (2) set conditions on a resumption of testing, and (3) banned testing after September 1996 unless another nation tested. On July 3, 1993, President Clinton extended the moratorium at least through September 1994 and subsequently extended the moratorium twice more past the September 1996 benchmark.

emerging requirements, such as the Reliable Replacement Warhead (RRW).

Lastly, as the US maintains its moratorium on underground nuclear tests, the Complex cannot continue to base its simulation and modeling efforts solely on data that are increasingly removed from the reality of the aged-weapons' performance. Previously, both the limited computational tools and the near-term commitments to support the stockpile necessitated this approach. Now, however, we have a development path for the needed software and hardware tools to move towards a quantified predictive capability (Figure 1). This *Roadmap* is designed to focus the ASC Program's efforts over the next decade on providing new levels of predictive capability to the SSP. It defines focus areas and supporting goals and targets required to achieve predictive capability in modeling and simulation, and it articulates a sequential, priority-based approach to achieving a new level of fidelity, adding confidence to SSP decisions and supporting a capability-based nuclear deterrent into the future.

NEAR-TERM WEAPONS SUPPORT



(a) Actual weapon performance with time

The red dashed line represents the time evolution of the weapons-system characteristics from aging. This curve represents the actual characteristics of the weapon that would be observed if weapons tests were to be done to measure the effects of aging.

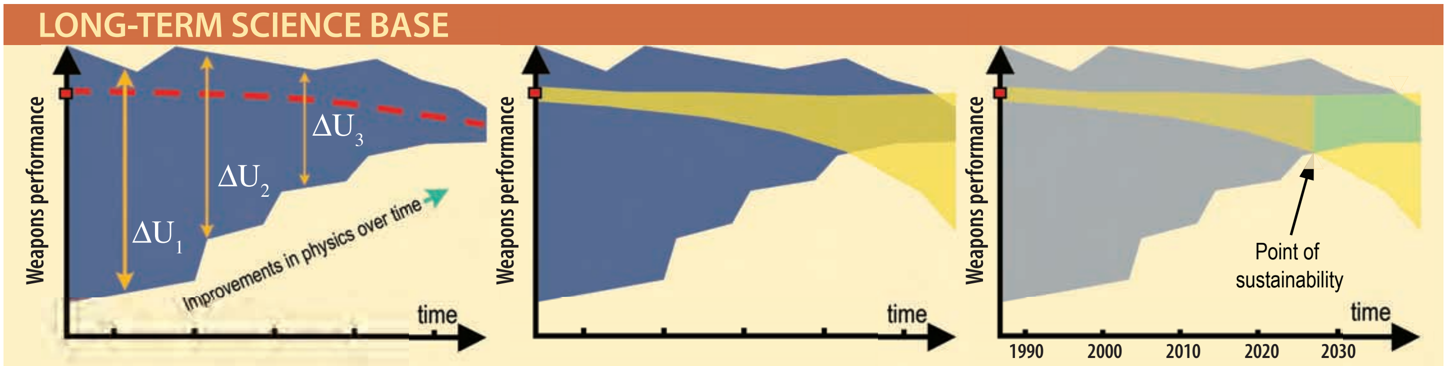
(b) Uncertainty bounds on Legacy codes calibrated to underground test (UGT) data

Without nuclear tests, we must simulate the changes in weapons characteristics as they age using simulation codes that are "tuned" to the initial data. As a result, our confidence in the results of the simulation decreases with time (represented here by the increase in the uncertainty in the calculation over time).

(c) Reduced uncertainty bounds on modern, 3-D codes calibrated to UGT data

To meet current stockpile commitments, we are continually improving the codes and acquiring more powerful computers to increase confidence in their results. However, these higher-fidelity codes are still "tuned" to test data, and in the absence of predictability, simulation uncertainty still increases with time.

LONG-TERM SCIENCE BASE



(d) Reduction in cumulative uncertainty in "un-tuned" scientific models over time

This schematic reflects the direct relationship between improved fidelity of the physics models and reduced uncertainty in the codes over time. Improving our scientific understanding enables us to better simulate the performance of aging weapons systems that may no longer be well characterized by prior nuclear tests.

(e) Code uncertainty overlaid with scientific model uncertainty

Improvements to the codes decrease the uncertainty in simulations, thereby enabling more confident predictions. As the science-based models become more accurate predictors of weapon performance, we can reduce our reliance on "tuned" calculations.

(f) Crossover points (▲▼) from growing uncertainty in extrapolated predictions, to a sustainable science-based capability

The indicated crossover points show when the uncertainties in science-based codes are smaller than uncertainties in codes tuned to underground test data. At the point of sustainability, modeling and simulation will transition to a sustainable base for the national security mission.

Figure 1—Near-term weapons support and long-term science base.

2.0 THE CASE FOR FUTURE SUSTAINABILITY

Computer simulation is, and will continue to be, the only means to responsively address emerging issues related to systems under nuclear conditions. This continued capability is crucial, then, to the nation's commitment not to conduct underground nuclear tests. We are following two paths that allow us to maintain the testing moratorium: the traditional path of fitting our computer models to underground test data and performing simulations in regimes that are minimally removed from the applicable parameter space, and the rigorous, science-based path intended to address a diverse portfolio of current and future nuclear applications.

As Figure 1 illustrates, aging and refurbishment push nuclear weapons behavior into an area where the uncertainty associated with traditional approaches becomes progressively larger. To credibly address this space and predict performance further from the as-tested configurations, we must create modern physical models with capabilities enabling confident calculation in these new and more applicable regimes.

2.1 NEAR TERM: THE LIFE EXTENSION PROGRAMS

To meet the needs of the SSP in the near term, ASC has aggressively pushed computational capabilities and enhanced simulation tools. By using test data to calibrate the major approximations (the "knobs") in the models, code developers and designers have built effective computer representations to probe scenarios at and near the area of our test experience. The process of calibration allowed for credible interpolation between different nuclear tests and for small extrapolations to untested conditions. However, this same process conceals the unknown science and engineering issues—since it allows for compensating errors in various approximations that can mask reality.

The traditional approach contains a number of severe limitations:

- Confidence in our predictions decreases as the weapons systems change because of aging and refurbishment. Put another way, the uncertainty increases, as illustrated in Figure 1(b)-(c), as the test data become less and less relevant to the aging and refurbished weapons we maintain. As a consequence, we are increasingly less confident that our calibrations to match the underground nuclear data provide accurate representations of nuclear behavior.
- We cannot provide credible error bars for our predictions if the simulations are adjusted by design to match the data against which we are attempting to quantify the uncertainties.

As an interim approach, during the transition between the traditional and scientifically grounded paths, we have succeeded in reducing the rate at which confidence decreases by increasing dimensionality of the weapons codes from 1-D and 2-D to 3-D; performing much higher-resolution simulations to surface engineering and physics details that were previously not discernible; and speeding up the codes through faster computers and better algorithms. The cumulative effect of these actions allows a clearer understanding of our interpolations and extrapolations. However, in the long term, this approach will continue to lead to *reduced confidence with time* as illustrated in Figure 1(b)-(c), or equivalently increased uncertainty, because the underlying approximation is still calibrated to the test data.

2.2 LONG TERM: FUNDAMENTAL SCIENCE-BASED REPRESENTATIONS OF WEAPONS BEHAVIOR

Reliance on simulations calibrated to the test data is not feasible indefinitely. Inevitably, issues will arise that were neither anticipated nor explored in the days of UGT. It is clear that a parallel long-term activity, focused on better scientific understanding and well-grounded approximations that enable the computer models to provide improved confidence with time, is critical. By systematically attacking the major scientific hurdles, the program will gradually remove the need to calibrate to the test base. The RRW effort provides significant motivation to shift the emphasis from the near-term approach that we have been following, Figure 1(b)-(c), to a sustainable effort based on solid science and engineering, Figure 1(d)-(f).

There are several clear advantages to the replacement of "knobs" with credible scientific models:

- Confidence in our predictions will improve with time.
- The nuclear test base will be used to confirm our simulation predictions, rather than as a calibration point.
- Simulation will be a robust, responsive, and versatile tool in which uncertainty bounds can accompany predictions.

2.3 THE TRANSITION TO SCIENCE-BASED SIMULATIONS

The *Roadmap* time line and focus areas are driven by the need to ensure that the transformed stockpile of 2030 poses a credible nuclear deterrent. To this end, we are emphasizing long-term science and the removal of the "knobs." This is illustrated notionally by the crossover point of the two uncertainty curves shown in Figure 1(f). This is the point in time when our confidence in approximations based on scientific understanding exceeds the confidence we have from test base calibration. We refer to this as "The Point of Sustainability"—when our decisions are based on science-based computation not codes calibrated to past nuclear tests. Reaching this point will allow the SSP to sustain a credible nuclear deterrent because it will rely upon a simulation capability that is science based and relevant to the regimes of crucial importance. Clearly, if we delay, the blue envelope of uncertainty in Figure 1(d)-(f) will grow, and the transition to the science-based path (at the point of crossing) will be pushed into the future. The *ASC Roadmap* defines the actions we plan to take to enable making this transition achievable in time to ensure that the transformed stockpile is a credible nuclear deterrent.

3.0 PATH TO PREDICTIVE CAPABILITY

As NNSA undergoes a transformation towards a responsive nuclear weapons infrastructure—as called for in the Nuclear Posture Review[2]—simulation is recognized as a key enabling technology for this transformation. An increasing emphasis on reliability, surety, and enhanced manufacturability places heavy demands on the ASC simulation tools. The stockpile of tomorrow will contain Legacy weapons, refurbished Legacy weapons, and reserves from which either parts or entire weapons can be used for augmentation of the active stockpile—including systems with enhanced surety features, such as the RRW.

The *ASC Roadmap* describes the four focus areas deemed essential for achieving the mission and strategic goals of the program:

1. *Address national security simulation needs* by delivering the capability to support the current and future SSP mission and by retaining the flexibility and robustness to respond to unanticipated events.

2. *Establish a validated predictive capability* by investigating key physical phenomena, developing a fundamental understanding of the underlying physical processes, deploying enhanced science-based models to reduce uncertainties, and reducing the reliance on ad hoc[3] models.

3. *Quantify and aggregate the uncertainties in simulation tools* associated with material data, physics models, algorithm choices, and numerical discretization inherent in simulation of complex phenomena, and thereby increase confidence in simulations.

4. *Provide mission-responsive computational environments* that meet stockpile stewardship needs and achieve the scale required for predictive capability through a balanced portfolio of capacity, capability, and advanced computing, as well as greater integration of the user environment and improved cost effectiveness.

As delineated above, the focus areas are the broad descriptions of the high-level, high-priority activities for the program. Each focus area is accompanied by goals and targets that span the next decade. The *goals* are designed to inspire longer term innovations aimed at making challenging, or "stretch," outcomes achievable at some future time. While it might be hoped to achieve a stretch goal either partially or fully within a defined time frame, the timing of the achievement of the stretch goal cannot be guaranteed—it can only be striven for through focused programmatic effort. The targets are clear, quantifiable, challenging deliverables against which we can measure the progress towards *Roadmap* goals and achievement of the focus area objectives. These goals and targets are described in more detail below, with out-year targets, in particular, being represented in the ASC Targets insert.

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[2] Nuclear Posture Review: http://www.defenselink.mil/news/Jan2002/d20020109npr.pdf

[3] Ad hoc: tailored or calibrated to experimental results—such as 'ad hoc models' or 'ad hoc parameters'

FOCUS AREA 1. ADDRESS NATIONAL SECURITY SIMULATION NEEDS

This focus area centers on the simulation tools required to support the current and future SSP mission, in particular to assess and maintain the existing and future nuclear deterrent—including the RRW—in the absence of UGT.

It is crucial that the ASC Program possess computational flexibility and robustness to respond to unanticipated future needs. ASC simulation tools will continue to support the resolution of SFIs and enable Stockpile Life Extension Programs (SLEPs) for the stockpile. The activities associated with each goal below will improve confidence in the ability to extend beyond the current design base. This ability is essential for certification of the future stockpile as it ages and continues to depart from the UGT database. Additionally, ASC will develop its capabilities for application to broader national security applications in collaboration with other government agencies such as the Department of Defense (DoD), Department of Homeland Security (DHS), and Defense Threat Reduction Agency (DTRA). These activities will also increase the robustness and flexibility of the simulation tools and demonstrate an ability to respond to evolving national security needs.

There are four goals within this focus area.

1.1 DELIVER SIMULATION CAPABILITY FOR NUCLEAR WEAPONS NEEDS (2007–2009)

In conjunction with Directed Stockpile Work (DSW) and the Campaigns, ASC will identify and deliver the physics, engineering, and computational capabilities to meet current and anticipated SSP needs. Particular emphasis will be given to delivering the capabilities required to establish baselines using ASC tools for all weapon systems, including the RRW, by 2009.

1.2 DELIVER SIMULATION TECHNOLOGY FOR BROADER NATIONAL SECURITY NEEDS (2007–2012)

In addition to meeting SSP needs, ASC will demonstrate the ability to apply ASC stockpile simulation technology and resources to broader national security challenges (e.g., nonproliferation and threat reduction). Thrust areas will be identified and mutually beneficial partnerships established with external organizations to help address their challenges. Use of ASC simulation capabilities in collaboration with partner organizations to address several key national security applications will be made by 2012.

1.3 INVESTIGATE AND UNDERSTAND OFF-NORMAL SYSTEM PERFORMANCE AND FAILURE/ANOMALY ISSUES IN THE TEST DATABASE (2008–2013)

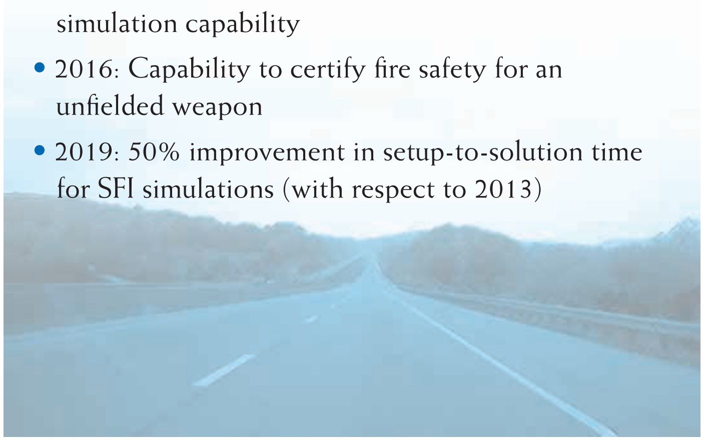
In a collaborative effort, DSW, Campaigns, and ASC will analyze off-normal system performance by simulating selected tests using best-practice models and methodologies. Based on these analyses, improvements to physics models will be investigated, and evidence will be gathered to identify unresolved physical processes.

1.4 DELIVER ENHANCED SIMULATION CAPABILITY FOR FUTURE NUCLEAR WEAPONS NEEDS (2010–2015)

Quantification of Margins and Uncertainties (QMU) assessments, discoveries from the Campaigns, and developments from other ASC activities will determine the physics, engineering, and computational requirements and the necessary simulation tools that need to be developed to increase confidence in stockpile weapons assessment, certification, SLEP evaluation, and SFI closures. This enhanced predictive capability will be verified and validated to the level needed to address evolving DSW requirements and SSP issues.

TARGETS FOR FOCUS AREA 1

- 2008: National code strategy
- 2009: Modular physics and engineering packages for national weapons codes
- 2012: Tested capability to address emerging threats, effects, and attribution
- 2013: 50% improvement in setup-to-solution time for SFI simulations (with respect to 2007)
- 2014: Full-system engineering and physics simulation capability
- 2016: Capability to certify fire safety for an unfielded weapon
- 2019: 50% improvement in setup-to-solution time for SFI simulations (with respect to 2013)



FOCUS AREA 2. ESTABLISH A VALIDATED PREDICTIVE CAPABILITY FOR KEY PHYSICAL PHENOMENA

To reach the goal of predictive capability in simulation/analysis codes, the SSP must establish an experimentally validated theoretical understanding of the physical processes that impact the performance of nuclear weapons. This effort begins by identifying key physical phenomena from which physics and engineering models are developed, progresses through simulation verification and validation, and concludes with the delivery of a predictive capability to be adopted in the ASC integrated performance codes. Delivery of this capability is therefore the shared responsibility of the ASC Program and the Campaigns to perform the required scientific discovery and DSW, and the verification and validation.

This focus area has three major aims: (1) discover the underlying physical phenomena behind the models that have been calibrated to experimental results, that is, the ad hoc models; (2) replace the ad hoc models with computationally effective, physics-based models as alternatives; (3) reduce the uncertainty in any physics-based model or database to the degree that is needed by QMU and validation studies.

To ensure that these aims are met, ASC will exploit the most recent simulation capabilities and work closely with the Campaigns as they use their ever-improving suite of experimental capabilities and data-acquisition techniques. Maximum progress will be achieved in these investigations through focused, well-integrated, coordinated activities. ASC will establish a Center to coordinate activities across ASC (laboratories and *Alliance Centers*[4]), with the Campaigns, and with external collaborators. This Center will employ a broad variety of capabilities, including theoretical studies and direct numerical simulation (DNS),[5] to explore isolated physical processes, experimental data analysis to validate models, and performance and analysis codes to perform integrated simulations. Ultimately, predictive capability is achieved through incorporating improved physics and engineering models in the integrated ASC codes and validating these simulations against relevant above-ground experiments and nuclear test data.

There are four goals in this focus area.

2.1 DELIVER A PROGRAM PLAN AND ESTABLISH A COLLABORATIVE CENTER TO ACHIEVE PREDICTIVE PHYSICS CAPABILITY (2007–2008)

By 2008, ASC will collaborate with the Campaigns and deliver a national program plan defining the path to an enhanced predictive simulation capability. Included will be a prioritized list of the major uncertainties that need to be reduced and a list of the ad hoc models that need to be replaced. Additionally, candidate physical processes will be identified that may explain and allow the removal of the ad hoc models. A center focused on predictive capability will be established to ensure coordination and collaboration among the participants, including the relationship with the Campaigns and external collaborators. Roles and responsibilities for all participants will be defined along with proposals for the scientific work that will be needed. In 2007, ASC will support efforts with the Thermonuclear Burn Initiative (TBI)—a pilot for the Virtual Collaborative Center model—to focus on one of the critical hurdles to predictive capability.

2.2 APPLY THEORY, SIMULATIONS, EXPERIMENTAL DATA, AND INTERIM MODELS TO CONFIRM DOMINANT PHYSICAL PHENOMENA (2008–2009)

As efforts progress toward an enhanced predictive capability, ASC will deploy improved interim models with theoretical and experimental backing. Detailed assessment of the candidate physical processes using numerical, theoretical, and experimental means will have commenced and will inform the improvements in the interim models. These studies, supported by peer-review, will identify a subset of the candidate physical processes currently represented by ad hoc models, deploy interim improvements to reduce reliance on ad hoc models, and identify essential experiments to confirm these conjectures.

2.3 DEMONSTRATE IMPROVED PHYSICS UNDERSTANDING BASED ON RELEVANT EXPERIMENTAL RESULTS (2009–2013)

In collaboration with the Campaigns, experimental programs will be proposed to validate the representative models for physical processes that describe the key physical phenomena. The conclusion of this activity will be to confirm which candidate processes are eligible to

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[4] Alliance Centers: http://www.sandia.gov/NNSA/ASC/univ/univ.html

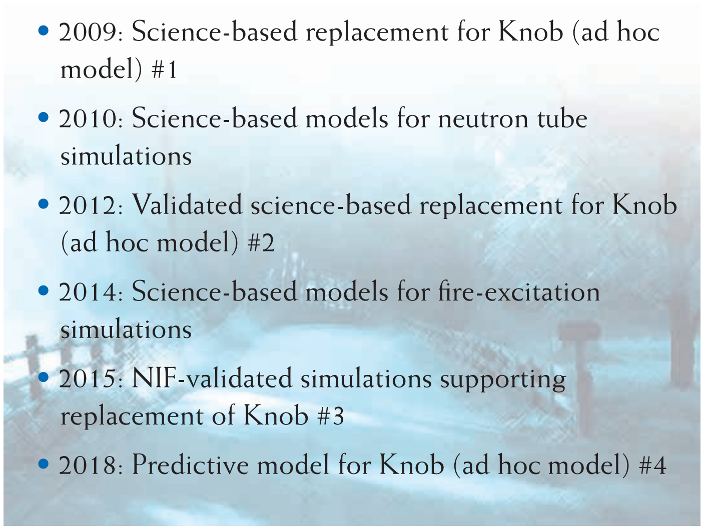
[5] Direct Numerical Simulation (DNS): simulation in computational fluid dynamics in which the (Navier-Stokes) equations are numerically solved without any turbulence model. Thus, the whole range of spatial and temporal scales of the turbulence must be resolved. DNS tends to be computationally expensive because of the high resolution required.

replace the old ad hoc models and the quantification of the extent to which they have reduced uncertainty. Progress depends critically on availability and alignment of experimental priorities at the major experimental facilities (e.g., Dual Axis Radiographic Hydrodynamic Test Facility [DARHT], Z-Pinch Refurbishment Project [Z-R], National Ignition Facility [NIF]).

2.4 DEVELOP AND DEPLOY VALIDATED PREDICTIVE MODELS FOR KEY PHYSICAL PHENOMENA (2010–2015)

Accurate, effective numerical methods will be derived, and scalable algorithms will be implemented to represent the new science-based models in the integrated codes. Model parameters and physical data will be extracted from the supporting theory, simulation, or experiment. The integrated codes will be validated against relevant experiments and then be delivered to DSW to be used on stockpile problems.

TARGETS FOR FOCUS AREA 2



- 2007: Launch Thermonuclear Burn Initiative collaboration
- 2008: Realistic plutonium aging simulations
- 2009: Science-based replacement for Knob (ad hoc model) #1
- 2010: Science-based models for neutron tube simulations
- 2012: Validated science-based replacement for Knob (ad hoc model) #2
- 2014: Science-based models for fire-excitation simulations
- 2015: NIF-validated simulations supporting replacement of Knob #3
- 2018: Predictive model for Knob (ad hoc model) #4

FOCUS AREA 3. QUANTIFY AND AGGREGATE UNCERTAINTIES IN SIMULATION TOOLS

The aims of this focus area are (1) to establish a comprehensive methodology for quantifying and aggregating the uncertainty in weapons calculations and (2) to establish and maintain a prioritized list of model and parameter uncertainties in these simulations. To achieve these aims, it is important to identify the approximations, assumptions, and adjustments in weapon calculations. The subsequent steps will be to assess the sensitivity of the simulation to these factors and then to quantify their uncertainty from both physical and numerical sources. Both will require verification problems of increasing physical and geometric complexity and the identification of additional experiments to validate the codes and assess the uncertainty of specific models. Identifying the priority of these models and parameters will help guide the uncertainty reduction efforts in Focus Area 2.

Simple procedures are available for assessing calculational sensitivity to individual parameters, although these procedures can be computationally intensive. The SSP requires an ability to assess the overall calculational uncertainty by aggregating the effect of the uncertainties in all aspects of the calculation. It is vital, therefore, not only to gain an appreciation for the uncertainties in each part of the calculations, but also to identify, assess, and validate procedures for aggregating these uncertainties. These methodologies will be demonstrated by application to the stockpile and utilization in QMU assessments in design processes.

This focus area has three goals.

3.1 ESTABLISH AND PRIORITIZE THE PARAMETERS MATRIX (2007–2008)

ASC will establish a detailed, hierarchical list of the major parameters and modeling options introduced in weapons calculations—along with their feasible ranges and distributions. A tri-lab status-ranking mechanism for physics and engineering codes based on sensitivity (likelihood) and consequence (impact) will be defined with an initial status for each list item. This peer-reviewed, prioritized list will then define the priorities for future work in reducing the uncertainties in ASC simulations.

3.2 ESTABLISH NATIONAL AND COLLABORATIVE FORUMS TO DEVELOP UNCERTAINTY AGGREGATION METHODOLOGIES AND BENCHMARKS (2008–2009)

In addition to identifying sources of uncertainties, ASC will establish national and collaborative forums to develop methodologies and benchmarks required for verification, validation, and quantification and aggregation of uncertainty in weapons simulations. In particular, quantification is needed for the effects of mesh resolution, numerical discretization, material data uncertainties, physics models, and algorithmic approximations on calculations. Advances will also be made on methods for combining fundamental data and model uncertainties with integral uncertainties obtained in more integrated experiments. Uncertainty quantification and aggregation during a calculation is an evolving science, and several candidate methodologies need to be developed and assessed on relevant problems, with leading candidates selected for further development and application.

3.3 DELIVER UNCERTAINTY AGGREGATION FOR QMU APPLICATIONS (2008–2014)

By 2014, ASC will deliver an uncertainty aggregation process for application by DSW. This will include uncertainties for all relevant material properties data, numerical discretizations, physics models, and algorithms. Algorithms and frameworks required for uncertainty quantification and aggregation will be defined and applied to targeted stockpile calculations in support of QMU-based stockpile activities.

TARGETS FOR FOCUS AREA 3

- 2008: National verification & validation strategy
- 2008: Assessment of major simulation uncertainties
- 2009: Shared weapons physical databases
- 2010: Uncertainty Quantification (UQ) methodology for QMU
- 2012: 20% reduction in overall prediction error bars (with respect to 2006)
- 2013: Re-assessment of major simulation uncertainties
- 2014: Demonstrated uncertainty aggregation for QMU
- 2017: 20% reduction in overall prediction error bars (with respect to 2012)

FOCUS AREA 4. PROVIDE MISSION-RESPONSIVE COMPUTATIONAL ENVIRONMENTS

The objective of this focus area is to provide the computational environments for carrying out the SSP mission. Broadly, this includes providing the appropriate balance of capacity, capability, and advanced computing resources to match the needs of the weapons program. Thus, efforts will focus on improving the usability of the computational environment, improving the cost performance of both software and hardware, and making strategic investments so that ASC can continue to meet the requirements of the SSP at an acceptable cost.

Both the complex and diverse demands that ASC performance and analysis codes place on the computational environment and the scale of the required simulations have positioned the ASC Program far in advance of the mainstream high-performance computing community. To achieve predictive capability goals, the ASC Program must continue to invest in, and influence, the evolution of computational environments. This will require radical innovation, tempered by the understanding that computing environments must be stable and should not require applications to be substantially rewritten or reinvented without realizing significant returns.

Immediate priorities include moving toward a more standard user environment, deploying more capacity[6] platforms, and developing petascale[7] computing to support the scientific investigations needed to achieve predictive capability and to perform aggregated uncertainty quantification studies.

In accordance with the Complex 2030 vision, ASC will look to operate capability computing as a national user facility, accessible complex-wide, to address the most challenging and pertinent stockpile stewardship issues. Partnering with computer vendors to develop advanced architectures that show promise to meet the future computing needs of the Complex, developing a common user environment, and reducing the footprint of weapons program capability computing to two sites.

This focus area has three goals.

4.1 DEPLOY COMPUTATIONAL ENVIRONMENTS FOR UNCERTAINTY QUANTIFICATION (UQ) ANALYSES (2007−2008)

Extensive Verification & Validation (V&V) and UQ simulations impose new requirements on the tools, infrastructure, and computing platforms. In collaboration with DSW and the Campaigns, ASC will gather requirements, identify solutions, and deliver the computational environments needed to meet deliverables in the 2009 time frame. Particular attention will be given to the balance between capacity and capability[8] computing. An important development will be improving the usability of capacity computational environments through common tools and interfaces. Productivity will be enhanced by reducing time to solution through increased performance, improved turnaround time, decreased problem and grid setup time, and enhanced problem analysis.

4.2 DEPLOY COMPUTATIONAL ENVIRONMENTS AND USER FACILITIES FOR WEAPON SCIENCE STUDIES AND OTHER CAPABILITY COMPUTING NEEDS (2008-2012)

The computing resources needed to support the *ASC Roadmap* focus areas, as well as DSW and Campaign deliverables, in the 2013–2015 time frame will be identified and delivered. (In 2005, a national ASC study, in support of an NNSA Defense Programs Level 1 Milestone, established that a number of weapon science studies require a petascale computing environment.) The demands on these architectures will be used to drive leading-edge hardware and software technology with progress in Advanced Systems likely to be required. Algorithms, tools, and system software will be developed to increase scalability, manage petascale data sets, and take full advantage of evolving Advanced Systems technologies. ASC will continue to engage in partnerships with advanced architecture vendors to achieve higher efficiency and improve balance across the range of hardware components. Application performance analysis and modeling will be applied to identify gaps, guide the path for algorithm development, and determine the desired architectural balance for future computing systems.

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[6] The use of smaller and less-expensive high-performance systems to run parallel problems with more modest computational requirements, in contrast to capability computing. The main figure of merit, metric, in capacity computing is the cost/performance ratio.

[7] Anything greater than about 200 teraFLOPs

[8] The use of the most powerful supercomputers to solve the largest and most demanding problem, in contrast to capacity computing. The main figure of merit, metric, in capability computing is time to solution.

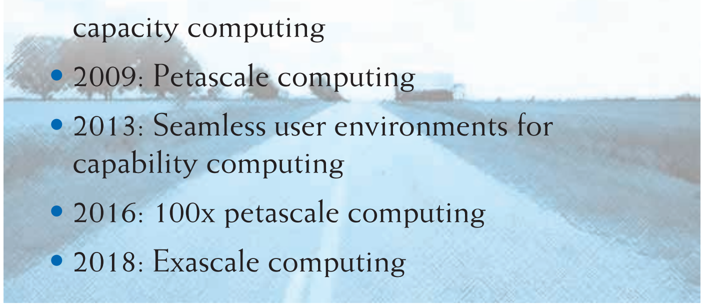
Additionally, a user facility model will be implemented to ensure that the most challenging problems of the Complex receive essential computing services. Implementing the Capability Computing Campaign (CCC) user model will serve as the foundation for computing resource delivery across the Complex. The User Facility Model will be cost-effective remote computing consistent with the Complex 2030 transformation plan.

4.3 DEPLOY COMPUTATIONAL ENVIRONMENTS FOR ENHANCED PREDICTIVE CAPABILITY IN 2015 (2011–2014)

ASC will deploy the computational environment necessary to perform the most complex and predictive weapon simulations ever achieved using integrated ASC codes. ASC will collaborate with industrial, academic, and government partners to build on the "weapons science" computational environments to deliver balanced computing resources supporting program deliverables in the 2015 time frame. Supporting infrastructure will be implemented for moving, managing, storing, and analyzing data generated at the petascale. System software, solvers, algorithms, and enabling technology will be developed to enhance user productivity and achieve the required scalability. Work in this time frame will establish the technological foundation to build toward exascale computing environments, which predictive capability may demand.

TARGETS FOR FOCUS AREA 4

- 2007: Initiate new National User Facility model for capability supercomputing
- 2008: Seamless user environments for capacity computing
- 2009: Petascale computing
- 2013: Seamless user environments for capability computing
- 2016: 100x petascale computing
- 2018: Exascale computing



4.0 CONCLUSION

The *ASC Roadmap* will serve as (1) a guidance document; (2) an input to program plans; (3) an organizing tool for defining progress, and (4) a basis for judging the evolution of simulation capabilities. Most importantly, it describes—for both internal and external stakeholders—the future direction of the ASC Program for the next decade and beyond.

This document represents a significant development not only for the ASC Program, but also for Defense Programs and NNSA. The three laboratories have collaborated on a unified strategy to meet the programmatic mission. We expect this *Roadmap* to deliver on its full potential as it is becomes more tightly integrated with the Campaigns and DSW. Moreover, it will drive changes to organizational behavior and business processes within ASC and influence change in other programs.

Finally, while the next steps involve distribution and discussion of the *Roadmap* and development of ASC program plans and implementation plans that are consistent with the needs defined in the *Roadmap*, this document will continue to evolve. Even within the ten-year scope of this *Roadmap*, the process—and the intellectual content—must be dynamic. Beyond the ten-year scope, we must position ourselves to deal with future national security needs. Ten years ago it was clear that the Complex needed 3-D, physics-rich simulation codes that could be supported by terascale platforms in order to certify stockpile weapons in the absence of UGTs. Today, it is clear that challenges associated with Responsive Infrastructure and RRW, the aging stockpile, and emerging nuclear-nation states call for a predictive simulation capability supported by petascale capability. As the future unfolds, it is likely that yet another set of requirements will arise as we strive to maintain a credible nuclear deterrent and use all of NNSA's nuclear competencies to guard against technological surprise and other threats to the nation.

GLOSSARY

Many of the terms used in this document have a specific meaning within the context of the Stockpile Stewardship Program and the ASC Program.

Baseline:	The model of a weapons system calibrated against available data sets. A baseline matches a subset of the data as well as possible through a process of adjusting the free parameters of the models in the codes used to perform the baseline.
Capability machines:	A classification of the large parallel computing systems wherein the system is dedicated to, or capable of being dedicated to, a single calculation. Capability machines are characterized by a job mix with few simultaneous jobs, with individual jobs utilizing 40% or more of the system's compute nodes.
Capacity machines:	A classification of parallel computing systems that are not used as capability machines. A job mix of many simultaneous jobs characterizes capacity machines. Historically, today's capability platforms become tomorrow's capacity machines as technology progresses.
Legacy code:	Application codes that existed prior to the start of the ASC Program, before 1995. In many cases, Legacy codes are no longer being actively developed.
Modern code:	Application codes first developed under the ASC Program, starting after 1995. Some codes that would have been classified as Legacy codes have been significantly redesigned under the ASC Program and are therefore classified as modern codes.
Validation:	A process applied to the model of a phenomenon, where it is determined to what degree the model accurately represents that phenomenon.
Verification:	A process applied to an application code, where it is determined that the computer calculation for a particular problem accurately represents the solution of the mathematical model.