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Accelerated Strategic Computing Initiative (ASCI) Program Plan

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In response to the FY1994 National Defense Authorization Act establishing the Stockpile Stewardship Program, the U.S. Department of Energy (DOE) has taken a different approach to its responsibility to ensure confidence in the safety, performance, and reliability of our nuclear stockpile. In the past, confidence in the nation's nuclear deterrent was a product of computation, experimental science, and weapons physics. With the final judgements confirmed by nuclear test results, much simpler computer models could be used with the best available supercomputers to help design, modernize, and maintain the stockpile. Now, without nuclear testing as the final arbiter of our scientific judgement, weapons scientists must rely much more heavily on computers to simulate the aging process and its impact on our weapon systems, along with the impact of any required modifications.

DOE's Stockpile Stewardship Program was established to develop new means of assessing the performance of nuclear weapon systems, predict their safety and reliability, and certify their functionality. The program not only must fulfill its responsibilities without nuclear testing, but also must deal with constraints on non-nuclear testing, the downsizing of production capability, and the cessation of developing new weapon systems to replace existing weapons. Further complicating matters, weapon components are exceeding their design lifetimes, and manufacturing issues and environmental concerns will force changes in fabrication processes and materials of weapon components.

All of this must be resolved within a fast-approaching deadline. Not only are the weapons aging, so are the scientists and engineers who form the basis of our experience with underground nuclear tests and nuclear weapon design. Since the U.S. conducted its last nuclear test in 1992, our experience base is declining; those who participated in the design of our enduring stockpile are fast approaching retirement. As a result, the Accelerated Strategic Computing Initiative (ASCI) Program was established to be the focus of DOE's simulation and modeling efforts aimed at providing high-fidelity computer simulations of weapon systems that will enable scientists to continue to make the necessary judgements to maintain the credibility of the nuclear deterrent. The 2004 — 2010 timeframe is the key target for having usable, working ASCI computer systems and codes available so a smooth transition from "test based" certification and assessment can be made. To achieve this goal, planning must be done to link experimental data from aboveground test facilities, archival nuclear test data from fifty years of nuclear tests, and improved scientific understanding to provide high-confidence predictive simulation capabilities to support decisions about the enduring stockpile.

Integrated program planning has been conducted since ASCI was established in 1995 to bring together DOE's three national security laboratories as a single national program with strategic partnerships involving computer manufacturers and several of the nation's major universities. That program planning is being updated here in this document for FY2000 through FY2005. This plan is organized around the major program elements and the strategies employed within those elements to achieve ASCI's objectives in the areas of performance, safety, reliability, and renewal:

- **Performance**: Create predictive simulations of nuclear weapon systems to analyze behavior and assess performance in an environment without nuclear testing.
- **Safety**: Predict with high certainty the behavior of full weapon systems in complex accident scenarios.
- **Reliability**: Achieve sufficient, validated predictive simulations to extend the lifetime of the stockpile, predict failure mechanisms, and reduce routine maintenance.
- **Renewal**: Use virtual prototyping and modeling to understand how new production processes and materials affect performance, safety, reliability, and aging issues. This understanding will help define the right configuration of production and testing facilities necessary for managing the stockpile throughout the next several decades.

Starting with FY2000, ASCI's program elements have been restructured to reflect the way the challenge has evolved. The new "Materials and Physics Modeling" element grew out of "Advanced Applications Development" as a separate program element to address the integration of physical science into the ASCI codes. "Production Computing" was integrated with the program to achieve a unified computational and simulation effort. The result is the following list of integrated program elements organized into five categories. Brief descriptions of those elements follow.

Integration

• Program Integration:
— One Program — Three Laboratories
Planning and implementation of all ASCI efforts conducted in concert with participation from DOE headquarters and the three Defense Programs (DP) laboratories

Defense Applications and Modeling

• Applications Development
— Accelerated development of higher performance software to implement 3D, high-fidelity-physics simulation and prototyping
• Verification and Validation (V&V)
— Achieving high confidence in the computational accuracy of ASCI codes and their underlying models
• Materials and Physics Modeling
— Promoting capabilities to predict the physical properties of matter under conditions found in nuclear explosions
— Development of underpinning physics and prediction of material properties under STS environments through nuclear explosion

Simulation and Computer Science

• Problem Solving Environment (PSE)
— A computational infrastructure enabling execution of ASCI applications and access from the desktops of scientists
• Visual Interactive Environment for Weapons Simulation (VIEWS)
— Developing "see and understand" technologies for ASCI simulations, enabling scientists to view the 3D results of their stewardship calculations
• Distance and Distributed Computing and Communication ($DisCom^2$)
— Supporting high-end computing to remote sites and an integrated computing environment distributed across the nuclear weapons complex
• PathForward
— Accelerating commercial development of technologies needed for 30-teraOPS platforms and beyond

Integrated Computing Systems

• Physical Infrastructure and Platforms
— Developing powerful ASCI platforms in partnership with industry
• Operation of Facilities
— Operating ASCI computers and conducting innovative computing R&D

University Partnerships

• Academic Strategic Alliances Program (ASAP)
• Institutes and Fellowships
— Involving the U.S. academic community in ASCI science and computing

In addition to these program elements, this document describes two other important areas: a management plan and a description of the relationship of ASCI's simulation and modeling efforts to the Stockpile Stewardship Program.

ASCI is a large, complex, multi-faceted, and highly integrated R & D effort. Managing such an effort, planning and implementing inter-connected mileposts while pursuing new developments in simulation science and technology, is a great challenge. The ASCI approach to that challenge involves the coordinated use of multiple management structures — the staff at DOE Headquarters, the Tri-Lab Executive committee, and subject-area teams staffed from the three laboratories. The "Management" section describes that effort. The program has at its core the overarching objective to meet the science and simulation requirements of the Stockpile Stewardship Program. That relationship is described in the section "Relationship to Stockpile Stewardship/Management."

Ushering in a New Era

On August 11, 1995, President Clinton announced the United States intention to pursue a national policy of nuclear stockpile stewardship in the absence of nuclear testing. This decision ushered in a new era in the way the United States ensures confidence in the safety, performance, and reliability of its nuclear stockpile. The President said in his announcement,

> *We can meet the challenge of maintaining our nuclear deterrent under a [comprehensive test ban] through a science-based stockpile stewardship program without nuclear testing.*

Furthermore, the United States decision to halt new nuclear weapon designs was reaffirmed. This decision means that the U.S. stockpile of nuclear weapons will need to be maintained far beyond its design lifetime.

To implement this pivotal policy decision, the U.S. Department of Energy (DOE) established the Stockpile Stewardship Program. The goal of this program is to provide scientists with the means to maintain a credible nuclear deterrent *without* the use of the two key tools used to do that job over the past fifty years: underground nuclear testing and modernization through development of new weapon systems. Historically, U.S. policymakers were ensured confidence in the stockpile by the use of regular nuclear tests. They never had to rely on weapon systems that had exceeded their design lifetimes because older weapons were regularly replaced with new designs. With the cessation of these two practices, the U.S. committed itself to maintaining its existing weapon systems indefinitely, well beyond their intended lifetimes. Implementing this policy with credibility requires new scientific tools. The responsibility to develop those tools resides with the Stockpile Stewardship Program.

To meet this challenge, a new set of aboveground, non-nuclear experimental capabilities was required (see Fig. 1), environmentally benign fabrication capabilities were needed, and archived data from decades of nuclear tests had to be made available to weapon scientists. To make effective use of the interrelated scientific understanding that would result from this process, an unprecedented computational capability was needed to serve as the integrating force behind this effort. Simulation will clearly take on an unprecedented significance.

Figure 1. The Stockpile Stewardship Program requires non-nuclear aboveground experimental (AGEX) capabilities.

Realizing the Vision

The Accelerated Strategic Computing Initiative (ASCI) was established in 1995 as a critical element to help shift from test-based confidence to science- and simulation-based confidence. Specifically, ASCI is a focused and balanced program that is accelerating the development of simulation capabilities needed to analyze and predict the performance, safety, and reliability of nuclear weapons and certify their functionality—far exceeding what might have been achieved in the absence of a focused initiative.

To realize its vision, ASCI is creating simulation capabilities based on advanced weapon codes and high-performance computing that incorporate more complete scientific models based on experimental results, past tests, and theory. The result would be predictive simulations that enable assessment and certification of the safety, performance, and reliability of nuclear systems. Such simulations require much greater computing capabilities than industry supplies. Therefore, ASCI is partnering with industry to accelerate development of much more powerful systems and is investing in creating the necessary software environment.

ASCI is providing computational and simulation capabilities that will help scientists understand aging weapons, predict when components will have to be replaced, and evaluate the implications of changes in materials and fabrication processes to the design life of the aging weapon systems. This science-based understanding is essential to ensure that changes brought about through aging or remanufacturing will not adversely affect the enduring stockpile.

To meet the needs of stockpile stewardship in the year 2005 and beyond, ASCI must solve progressively more difficult problems as we move away from nuclear testing (see Fig. 2). To do this, applications must achieve higher resolution, higher fidelity, three-dimensional physics, and full-system modeling capabilities to reduce reliance on empirical judgements. This level of simulation requires high-performance computing far beyond our current level of performance. A powerful problem-solving environment must be established to support application development and enable efficient and productive use of the new computing systems. By 2005, the ASCI program is responsible for the following deliverables:

- Development of high-performance, full-system, high-fidelity-physics predictive codes to support weapon assessments, renewal process analyses, accident analyses, and certification,
- Stimulation of the U.S. computer manufacturing industry to create the powerful high-end computing capability required by ASCI applications, and
- Creation of a computational infrastructure and operating environment that makes these capabilities accessible and usable.

The ASCI program recognizes that the creation of simulation capabilities needed for performance simulation and virtual prototyping is a significant challenge. This challenge requires the science and technology resources available at the national laboratories and it will require close cooperation with the computer industry to accelerate their business plans to provide the computational platforms needed to support ASCI applications. Universities will also play a critical role in developing the computational tools and scientific understanding needed for this unprecedented level of simulation.

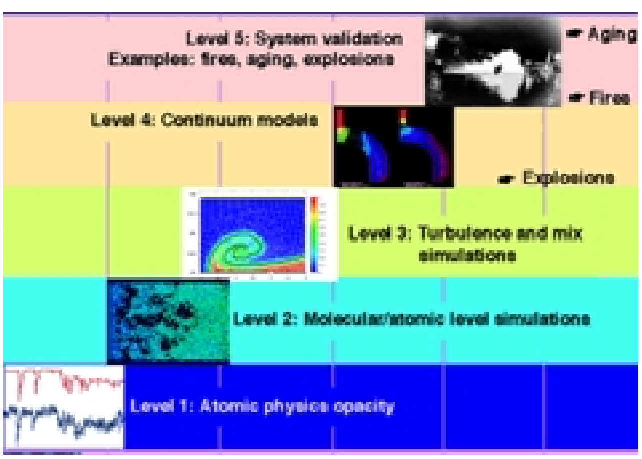

Figure 2. A hierarchy of models and modeling methods is needed to enable a predictive capability for the processes relevant to weapon performance.

The creation of sophisticated simulation capabilities also supports our need to maintain readiness to resume nuclear testing. The capability provided by ASCI significantly enhances our ability to design and understand tests in far greater detail than has been possible in the past. As a consequence, we could pursue new testing strategies, thus getting more useful information from each test.

Background

Over the past fifty years, the U.S. has based a significant portion of its national security on the credibility of its nuclear deterrent. In order to understand the significance of the Stockpile Stewardship Program and, specifically, the ASCI Program in the history of that deterrent, it is useful to review these areas:

- Test-based stockpile stewardship as practiced prior to 1992 and
- DOE's history of partnering with the U.S. computer industry.

These subjects provide some useful context for consideration of the approach taken by the ASCI Program in fulfilling the goals of the Stockpile Stewardship Program.

Test-Based Stockpile Stewardship

The U.S. has designed and maintained a stockpile of nuclear weapons for more than 50 years. Over that time, the U.S. government, through its national laboratories and production facilities, developed approaches to maintaining confidence in the performance, safety, and reliability of nuclear weapons. These approaches, both nuclear and non-nuclear, were generally test-centric. Scientists and engineers would attempt to apply the most complete physics understanding possible to designs or questions about the stockpile. Many times this would result in extensive mathematical predictions of a weapon's performance. As computer power increased, these predictions were incorporated into computer programs, which provided a higher level of information to weapon experts.

Because the physics understanding of the weapons was not complete, many empirically derived factors were incorporated into the computer codes to improve their fit to the test data. This led to a strong interdependence between the use of computational simulation and testing.

In the early days of the weapons program, the national laboratories consistently purchased the highest performance computers in the world. These computers were needed to continue to improve the designs of nuclear weapons, making the weapons smaller and lighter, while improving safety and reliability.

The computational power of these early computer systems was limited, and therefore codes continued to be one or two dimensional, requiring the use of many empirical factors in predicting weapon behavior. That was sufficient in an era where extensive testing was conducted. The computer codes would predict the test results, and then the test results would be used to make specific calibrations to the codes for each weapon. In this situation, code limitations were mitigated by the use of tests, which could serve as the final integrating factor.

This work was (and continues to be) supported by a wide array of aboveground test facilities and laboratory-scale experiments. The decision to pursue a stockpile stewardship program without nuclear tests has now stimulated a change in the mix of scientific capabilities required to maintain the nuclear deterrent. While ASCI is intended to replace test-centric approaches with computation-centric approaches, it does not imply that non-nuclear experimental data will cease to be important to weapon scientists. Aboveground and laboratory-scale experiments that would be allowed under a comprehensive test ban treaty will continue to be conducted, as permitted by laboratory budgets. In fact, ASCI anticipates an increase in this area of treaty-approved testing. Experimental facilities, like hydrodynamic testing facilities, pulsed-power accelerators, and the National Ignition Facility, will produce data that will increase in importance as weapon scientists begin the essential process of validating and verifying the physics models in the codes that, in turn, will predict the behavior of weapons in the enduring stockpile.

The ASCI Objectives

To meet the needs and requirements of the Stockpile, Stewardship Program, ASCI has specific program objectives in performance, safety, reliability, and renewal.

Performance: Create predictive simulations of nuclear weapon systems to analyze behavior and assess performance in an environment without nuclear testing.

Safety: Predict with high certainty the behavior of full weapon systems in complex accident scenarios.

Reliability: Achieve sufficient, validated predictive simulations to extend the lifetime of the stockpile, predict failure mechanisms, and reduce routine maintenance.

Renewal: Use virtual prototyping and modeling to understand how new production processes and materials affect performance, safety, reliability, and aging. This understanding will help define the right configuration of production and testing facilities necessary for managing the stockpile throughout the next several decades.

Enabling Science-Based Stockpile Stewardship

ASCI is a critical element of the Department of Energy's response to the decision ending nuclear testing. The Stockpile Stewardship Program will build on existing means and develop new means to assess the performance of nuclear stockpile systems, predict their safety and reliability, and certify their functionality. The Stockpile Stewardship Program not only must respond to the loss of nuclear testing, but also must deal with constraints on non-nuclear testing, the downsizing of production capability, and the cessation of new weapon designs to replace existing weapons. Of course, weapon components will continue to exceed their design lifetimes, and manufacturing issues and environmental concerns will force changes in fabrication processes and materials of weapon components.

The program will support efforts to develop the fundamental scientific understanding of nuclear weapons as the basis for surveillance, maintenance, assessment, and certification of the weapons. In the past, much of the integration of fundamental science into nuclear weapons relied on both underground nuclear and aboveground system testing.

In the future, ASCI simulation capabilities will link experimental data from aboveground test facilities (AGEX), archival nuclear test data, and improved scientific understanding to provide high-confidence predictive simulation capabilities needed to support decisions about the enduring stockpile. ASCI supports another element of the program, the Stockpile Life Extension Program (SLEP), by providing the computational parts of the capabilities needed to predict requirements for replacement of aged components and to ensure that those replacements do not introduce new problems into the stockpile. Finally, ASCI will complement and accelerate the ongoing efforts of the Defense Programs research and development program for advances in physics, material sciences, and computational modeling.

The Key ASCI Drivers

To crystallize planning for ASCI to support the Stockpile Stewardship Program, several key drivers have emerged. The primary driver is that, with the cessation of underground nuclear testing in 1992, the experiment-based experience and expertise of the program is declining due to the inevitable retirements of test-experienced weapons experts and the increasing length of time since the last nuclear test. This driver imposes a crucial target period of 2004 to 2010 for having usable ASCI computer systems and codes available for a smooth transition from “test-based” certification and assessment. The second key driver is the need for full three-dimensional simulation codes, which incorporate the complex physics required to model physical phenomena such as weapon performance, aging, and accident simulation. Finally, the last driver is the computer system speed and software required for this three dimensional high-fidelity physics and engineering modeling.

In response to these drivers, intermediate milestones have been established. In December 1999, ASCI successfully demonstrated the first-ever 3D simulation of a nuclear weapon primary explosion. By 2004, ASCI plans to have 3D working simulation codes with a 100-teraOPS (trillion floating-point operations per second) computer system to facilitate the transition to full operational capability by 2010. By 2005, ASCI plans to demonstrate an engineering simulation of the weapon response to the full stockpile-to-target-sequence (STS) environment. Along with the capacity to store very large data sets, the program must develop the capability to transfer high volumes of data at high speeds and to provide the scientific "visualization" of the results of ASCI calculations to weapon scientists. Achievement of these milestones will require the integrated success of the program elements described in this document.

ASCI Program Structure

- **Program Integration:**
  - One Program — Three Laboratories
- **Defense Applications and Modeling:**
  - Advanced Applications Development
  - Verification and Validation (V & V)
  - Materials and Physics Modeling
- **Simulation and Computer Science:**
  - Problem Solving Environments
  - Distance and Distributed Computing (DisCom^2)
  - PathForward
  - Visual Interactive Environment for Weapons Simulation (VIEWS)
- **Integrated Computing Systems:**
  - Physical Infrastructure and Platforms
  - Operation of Facilities
- **University Partnerships:**
  - Academic Strategic Alliances Program (ASAP)
  - Institutes and Fellowships

These elements are discussed in detail in the next section.

This section provides a description of each of the ASCI program elements followed by the top-level strategies each element will use to contribute to overall ASCI goals. The relative sizes of these program elements are illustrated in Fig. 3. The high-level mileposts for these program elements are listed and described in Appendix A. Beginning with FY1999, portions of the PSE effort were split to form Distance and Distributed Computing and Communication ($DisCom^2$), Visual Interactive Environment for Weapons Simulation (VIEWS), and Verification and Validation (V&V) as separate program elements. Funding for these program elements began in the FY1999 budget.

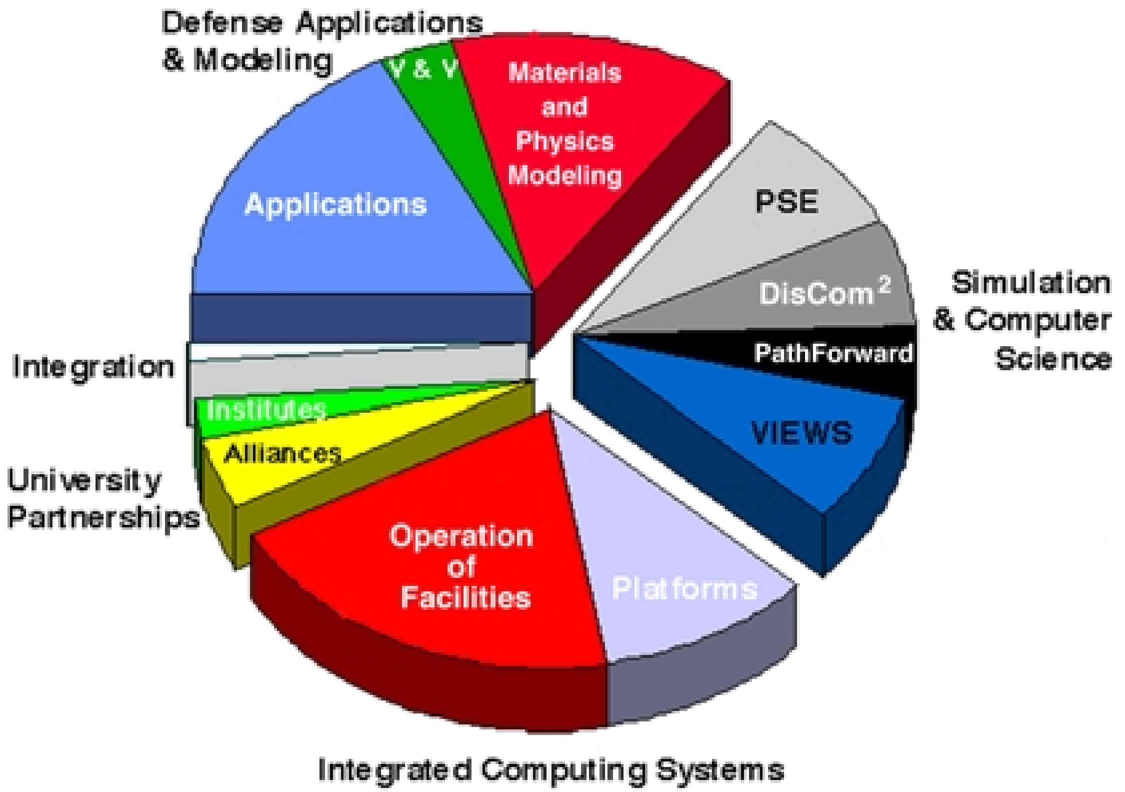

Figure 3. As of FY2000, ASCI has evolved into these groups of integrated program elements.

Program Integration:
One Program—Three Laboratories

The problems that ASCI will solve for the Stockpile Stewardship Program span the activities and responsibilities of the three Defense Programs national security laboratories (Los Alamos, Sandia, and Lawrence Livermore). Cooperation among the Defense Programs laboratories is essential to solving these problems in an efficient and effective manner. In accordance with this cooperative philosophy, representatives of the laboratories participated in the development of this plan. There has been, and will continue to be, unprecedented cooperation among the three Defense Programs laboratories. The ASCI program will be implemented by project leaders at each of the laboratories guided by DOE's Office of Research, Development, and Simulation through its Office of Advanced Simulation and Computing, under the Assistant Secretary for Defense Programs. The Defense Programs laboratories will share ASCI code development, computing, storage, visualization, and communication resources across laboratory boundaries in joint development efforts.

Integration Strategies

- Operate ASCI as a single, three-laboratory program activity with seamless management and execution across the laboratories
- Sponsor annual Principal Investigator Meetings
- Collaborate on development, and share hardware and software resources
- Take maximum advantage of standard tools, common system structures, and code portability to enable inter-laboratory collaboration

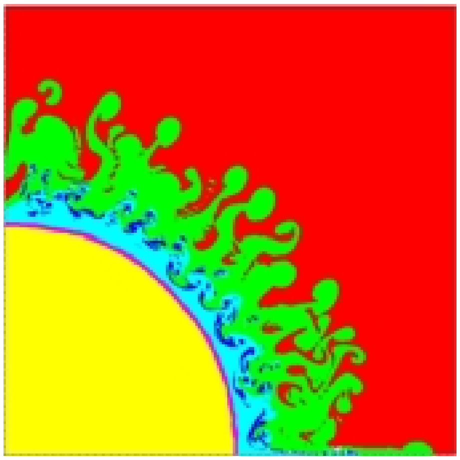

Figure 4. Based on the ALE (Arbitrary Lagrange-Eulerian) hydrodynamic method, this ARES simulation allows study of mixing phenomena in supernovae.

Defense Applications and Modeling: Advanced Applications Development

ASCI is developing, on an accelerated schedule, the progressively higher performance software applications needed to implement virtual testing and prototyping. The key to reaching Stockpile Stewardship Program objectives outlined for initial implementation in 2004 and full implementation in 2010 is the ability to achieve ASCI's critical simulation and applications code milestones in the intervening years. ASCI will provide simulations embodying the physical and chemical processes needed to predict the safety, reliability, performance, and manufacturability of weapon systems. It is a formidable challenge to replace the empirical factors and adjustable parameters used in current calculations with predictive physical models. Meeting this challenge will require large, complex computer applications codes, like the one shown in Fig. 4, that drive the scale of computing hardware and infrastructure. However, increased capability in hardware and infrastructure alone is insufficient. Much of the increased computational capability to be provided by ASCI must come from advances in the applications codes themselves. These applications will integrate 3D capability, finer spatial resolution, and more accurate and robust physics. Adding these new capabilities, however, will strain the limits of the algorithms used in today's simulation codes. In addition, the necessity to do full-system or scenario simulations will require the development of new algorithms for coupled systems. As a consequence, the development and implementation of improved numerical algorithms to address these new capabilities will be a critical component of the applications strategies. Tightly integrated code teams—large interdisciplinary work groups consisting of scientists and engineers, along with computational mathematicians and computer scientists, devoted to producing coherent software for efficient predictive simulations—will develop these codes.

Applications Strategies

- Focus on 3D, high-fidelity-physics, full-system applications
- Focus on full-system, component, or scenario simulations
- Design and implement numerical algorithms to meet the ASCI application requirements
- Accelerate code performance by developing computational techniques that exploit the new computer architecture

Verification and Validation (V&V)

The V&V Program will provide high confidence in the computational accuracy of ASCI and Stockpile Computing simulations supporting stewardship programs by systematically measuring, documenting, and demonstrating the predictive capability of the codes and their underlying models. Verification is the process of determining that a computational software implementation correctly represents a model of a physical process (Fig. 5). This program will evaluate current software engineering practices for application to the ASCI-scale simulations and establish minimum requirements for software projects. Validation is the process of determining the degree to which a computer model is an accurate representation of the real world from the perspective of the intended model applications. Validation makes use of physical data and results from previously validated legacy codes.

ASCI has placed special emphasis on V&V by establishing it as an independent program element. In the absence of new nuclear tests, the program needs more systematic, rigorous V&V methodologies to establish the increased confidence that will be expected of weapon simulations. This element has many interfaces with other stewardship elements and activities, requiring a great deal of coordination. For example, V&V will develop verification technologies and process guidelines, which in turn must be implemented by the Advanced Applications Development program element. The development and prototyping of verification tools supported by V&V will be supplemented by many PSE activities. These multiple interfaces represent a significant management integration challenge to bring ASCI applications and platforms to bear on stockpile stewardship problems of interest to weapons experts. The link between V&V activities, the experimental program, and Campaigns is crucial to the success of this effort.

Figure 5. Verification determines that a software implementation correctly represents a model of a physical process. Validation determines whether a computer model correctly representation the real world.

V&V Strategies

- Provide high confidence in weapons simulations supporting stewardship programs by systematically measuring, documenting, and demonstrating the predictive capability of the codes and their underlying models
- Provide requirements for experimental validation data within the Stockpile Stewardship Program
- Provide the basis by which computational uncertainties are evaluated and assessed
- Evaluate current software engineering tools and practices for application to ASCI simulations and establish minimum requirements for the code-development projects

Materials and Physics Modeling

In the past, physical properties of materials significant to the nuclear weapons program were often inferred from integral test data. Without the ability to conduct such integral tests, there is a high premium on the development of advanced capabilities – experimental, theoretical, and computational – to *predict* the physical properties of materials under conditions found in nuclear explosions.

At the heart of the development of these predictive capabilities is the determination of the physical properties of materials in regimes relevant to processes governing the performance, safety, and reliability of the nuclear stockpile. Of particular interest are the dynamic properties and response of materials under conditions of high strain and high-strain rates, impact, shock compression and quasi-isentropic loading. The dynamic response of materials is largely defined by the functional relationship between microstructure evolution, mesoscale properties, and macroscopic response. This is a topic of considerable scope that requires fundamental knowledge of materials properties and response, not only at vastly different length and time scales, but also in the linkage across these scales.

Laboratory experiments and high-performance simulations will provide the basis for the development of predictive models and validated physical data of stockpile materials. Consequently, ultra-scale scientific computing platforms, multi-physics application codes, and unique experimental facilities have been deployed and integrated to establish these predictive capabilities. For example, the high-pressure, high-temperature properties of key stockpile materials have already been elucidated and have led to the partial resolution of long-standing anomalies observed in certain nuclear tests. This example illustrates the powerful synergy between high-performance scientific computing and advanced experimental facilities as a strategy to provide a rigorous scientific basis for the development of predictive models and validated materials properties data. Timely insertion of these validated materials models and properties data into next-generation, high-fidelity-physics, full-system weapons codes will provide the basis to ensure confidence in the performance, safety, and reliability of the stockpile without nuclear testing.

High-performance simulations linking atomistic to continuum scales will lead to reliability predictions and lifetime assessment for corrosion, organic degradation, and thermal-mechanical fatigue of weapon electronics. The physics-based determination of materials response in hostile environments is another example of these advances.
Similarly, quantum-scale simulations and laser-driven shock compression experiments have validated the equation of state of hydrogen up to several Mbars, providing valuable insight both into weapons performance and inertial confinement fusion.

Materials and Physics Modeling Strategies

- Determine from first principles the multi-phase equation of state for Pu and other relevant metals, including melting and solid-solid phase transformations
- Determine from first-principles the equation of state for deuterium
- Develop physics-based, multiscale constitutive models of the dynamic response of Pu and other relevant metals
- Develop predictive models of materials failure, spall, and ejecta
- Develop nuclear and atomic data.
- Develop predictive models of interfacial dynamics in primary materials
- Develop physics-based models predicting the properties of Pu under aging due to self-irradiation
- Develop physics-based models of high explosives thermal and mechanical properties, including decomposition kinetics, detonation performance, properties of reaction products, and constitutive properties
- Develop physics-based, predictive models for corrosion, polymer degradation, and thermal-mechanical fatigue of weapon electronics
- Develop physics-based models of melting and decomposition of foams and polymers in safety-critical components
- Develop physics-based models of microelectronic and photonic materials under aging and hostile environments

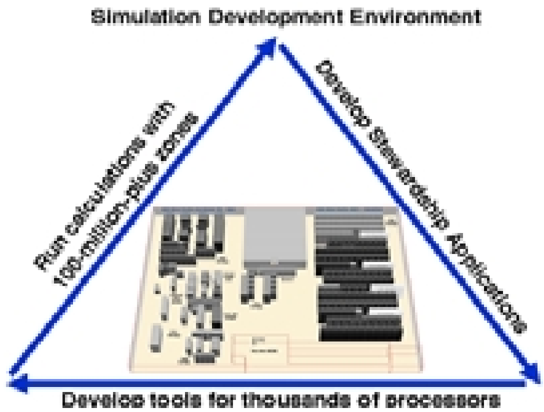

Figure 6. PSE has key responsibilities in pursuit of ASCI's most important milestones.

Simulation and Computer Science: Problem-Solving Environments (PSE)

ASCI's unprecedented code-development effort will require robust computing and development environments (as illustrated in Fig. 6) where codes may be developed rapidly. Through the Problem Solving Environment (PSE) program element, ASCI will develop a computational infrastructure to allow applications to execute efficiently on the ASCI computer platforms and allow accessibility from the desktops of scientists. This computational infrastructure will consist of local area networks, wide-area networks, advanced storage facilities, and software development tools.

PSE Strategies

- Creating a common and usable application development environment for ASCI computing platforms enabling code developers to quickly meet the computational needs of weapons designers
- Developing an environment that allows scientists to visualize, store, retrieve, and search data within the natural context of their work,, and
- Ensuring appropriate access to ASCI computers and other ASCI resources across the three weapons labs.

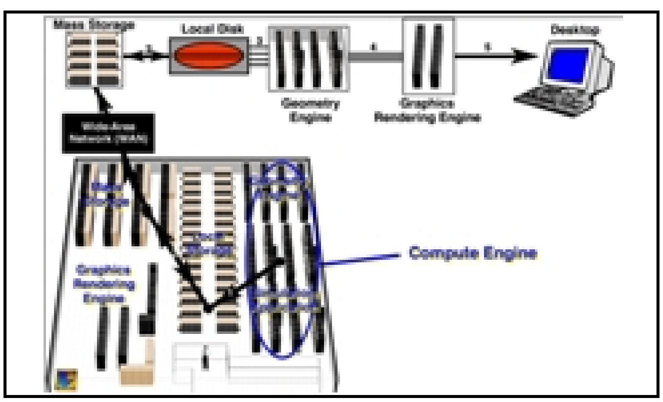

Figure 7. Beginning in FY1999, DisCom^2 emerged from PSE to form a separate program element.

Distance and Distributed Computing and Communication (DisCom^2)

DisCom^2 will assist in the development of an integrated information, simulation, and modeling capability to support the design, analysis, manufacturing, and certification functions of the Defense Programs complex through developments in two key strategic areas: Distance Computing and Distributed Computing. Distance Computing will extend the environments required to support high-end computing to remote sites. Distributed Computing will develop an enterprise-wide integrated supercomputing architecture that will support DOE's science and engineering requirements for stockpile stewardship. It will take advantage of the ongoing revolution in commodity, cluster-based, distributed high-performance computing. It will adopt, support, and augment (in key gap areas) the open software approach to distributed cluster computing. A product will be an evolving set of commodity computing solutions that compliment the ASCI tera-scale, ultra-computing platforms. These solutions will fit seamlessly into the ASCI computing environment as in the example of Figure 7.

DISCom^2 Strategies

- Extend the environments required to support high-end computing to remote sites
- Develop and deploy an integrated distributed computing environment
- Develop an enterprise-wide integrated commodity supercomputing architecture that will support DOE's science and engineering requirements for stockpile stewardship

PathForward

ASCI's strategy is to build future high-end computing systems by scaling commercially viable building blocks, both hardware and software, to 30 teraOPS and beyond. The PathForward program consists of multiple partnerships with computer companies to develop and accelerate technologies that are expected to either not be in the current business plans of computer manufacturers or not be available in either the time frame or the scale required by ASCI. The program is executing the PathForward program by entering into partnerships with U.S. industry to develop the key (critical path) technologies necessary to accelerate the development of balanced 30- to 100-teraOPS computer systems. Starting in FY2000, PathForward has grown out of the Platforms effort to become its own program element. Currently, the PathForward program element is investing in the development of technology in three critical areas: interconnect, storage, and software.

PathForward Strategies

- Stimulate development of interconnect technologies leading to a bandwidth-to-compute-speed ratio of 0.1 bytes per floating-point operation, or better, while maintaining low communication latency
- Maximize performance factors of density, agility, and steady-state data rate in development of advanced storage technologies
- Stimulate development of software to accelerate runtime system technologies and third-party alternatives for use in 100-teraOPS computing environments

Visual Interactive Environment for Weapons Simulation (VIEWS)

VIEWS, the "Visual Interactive Environment for Weapons Simulation,," is a new ASCI program element focused on the problem of "seeing and understanding" the results of multi-teraOPS simulations, and comparing results across simulations and between simulations and experiments. VIEWS brings together ASCI-supported research, development, engineering, deployment, and applications support in visualization, data management, and data exploration. Several efforts previously spread across a number of program elements are now consolidated within VIEWS. Through the creation of VIEWS, DOE Defense Programs intends to focus increased attention on the problem of exploring and understanding multi-terabyte scientific datasets. As R. W. Hamming succinctly stated, "The purpose of computing is *insight*, not numbers."

The goal of VIEWS is the creation of an infrastructure called a "Data and Visualization Corridor (DVC)." (The viewing area of LLNL's DVC facility is shown in Fig. 8.) One often thinks of the storage and I/O systems of supercomputers, and the graphics workstations attached to them, as a thin pipe through which data must be pumped. The idea of a "corridor" is meant to suggest the opposite metaphor, a wide path through which massive quantities of data can easily flow and through which scientists and engineers can explore data and collaborate. Thus, the corridor is precisely the kind of infrastructure needed to fully support the ASCI "see and understand" mission.

The corridor concept was outlined through a collaboration of DOE scientists, researchers from academia and industry, and leaders of multiple federal agencies. While the data exploration needs of a variety of agencies was taken into account, the ASCI imperative to understand the massive datasets resulting from teraOPS scientific simulation was, from the beginning, the driving force. The VIEWS program will implement the DVC concept within DOE/DP laboratories.

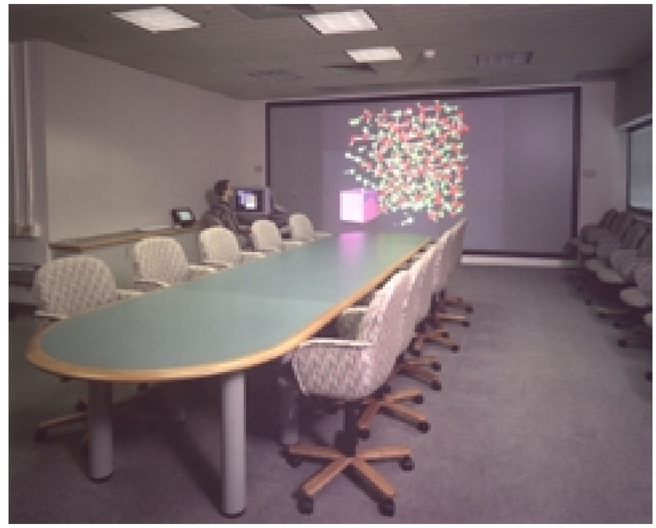

Figure 8. Data Visualization Corridor facilities, like this one at LLNL, enable scientists to view and use the results of high-fidelity 3D simulation.

There are several steps involved in implementing successful DVCs. In many cases, needed hardware and software technologies do not exist or are in their infancy.Hence, a major part of the VIEWS program has targeted research and development to create innovative technologies for scientific collaboration, data exploration, visualization, and understanding.

Keys to progress are well-defined technology roadmaps and well-engineered architectures. In general, the development of the DVC concept is focused on promising technologies that can have direct impacts on the ASCI program in a two- to four-year timeframe. Once prototype technologies exist, they need to be "hardened," integrated, tested, and evaluated by a representative set of users. Finally, these technologies need to be deployed in a generally available, operational and reliable environment for direct day-to-day use by ASCI users and applications.

VIEWS Strategies

VIEWS provides scientific understanding and insight through qualitative and quantitative data discovery, analysis, and assimilation by means of:

- Partnering with academia, industry, federal agency research and development
- Visual exploration and interactive manipulation of massive, complex data
- Orchestrated, effective data management, data extraction, and data delivery
- Efficient solutions for remote and collaborative scientific data exploration
- Deployment of highest-performance Data and Visualization Corridors (DVCs)

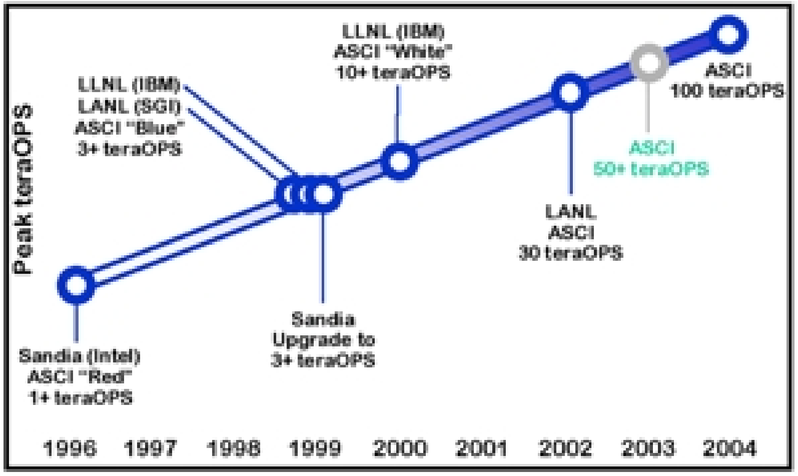

Figure 9. To satisfy the simulation requirements of the Stockpile Stewardship Program, ASCI is stimulating the computer industry to develop high-performance computers with speeds and memory capacities hundreds of times greater than currently available models.

Integrated Computing Systems: Physical Infrastructure and Platforms

The first supercomputers were developed for weapon applications in the 1960s as a partnership between the computer industry and the nuclear weapons laboratories. Throughout the 1970s and 1980s, this relationship continued. The Defense Programs laboratories were early user sites and a primary customer for new state-of-the-art high-performance computers and computing simulation capability.

In the late 1980s and early 1990s this relationship changed. The DP laboratories drastically reduced their partnerships with industry in developing computer systems. Due to budget exigencies, they also greatly reduced their purchases of supercomputers. As a result, the computing industry no longer viewed the DP laboratories as a primary customer for their most advanced computer designs. Moreover, the test-based weapon simulation capability did not require the highest performance and largest memory machines.

Today, more powerful computing platforms are needed to achieve the performance simulation and virtual prototyping applications that the Stockpile Stewardship Program requires. ASCI will stimulate the U.S. computing industry to develop high-performance computers with speeds and memory capacities hundreds of times greater than currently available models and ten to several hundred times greater than the largest computers likely to result from current development trends. ASCI will continue to partner with various U.S. computer manufacturers to accelerate the development of larger, faster computer systems and software that are required to run Defense Programs applications. ASCI partnerships have already brought about development and installation of the world's first teraOPS computer (the 1.8-teraOPS Intel machine at Sandia, Albuquerque, recently upgraded to 3 teraOPS), and two three-plus teraOPS machines at Los Alamos (in partnership with SGI) and Livermore (in partnership with IBM). An extension of the LLNL/IBM contract has set in motion the development of a 10-teraOPS machine to be installed in Livermore in the year 2000.

To ensure that high-end computer development does not fall behind the critical-path curve, the PathForward program element has grown out of the platform-development effort. PathForward is currently directed at developing specific key technologies necessary to accelerate availability of the next ASCI platform: a balanced 30-teraOPS system in 2002. Beyond the 30-teraOPS system, the strategy calls for a 100-teraOPS system in 2004, followed shortly by a 100+ teraOPS system (see Fig. 9).[†] The strategy is based on the plan to locate these systems at Los Alamos and Lawrence Livermore National Laboratories in a complementary fashion, ensuring that each site will have a high-end computing capability to support the stewardship mission. Under current plans, the computing needs of Sandia laboratories will be met by its utilization of one third of the computing resources of each of these ASCI platforms.

Platform Strategies

- Accelerate the development of scalable architectures
- Develop partnerships with multiple computer companies to ensure appropriate technology and system development

[†] The program has been investigating the addition of a 50+ teraOPS system in the FY2002/2003 timeframe. This additional platform would provide the capability needed to perform computational certification and DSW workload of weapons systems in FY2003 through 2006, as well as avoiding the increased risk inherent in dependence on only one commercial computer manufacturer instead of continuing to partner with at least two computer companies. However, the 50+ teraOPS system is not supported in current budget projections.

Operation of Facilities — "Operations," "Software," and R&D

The Operation of Facilities element is focused on making the computations resources needed to support stewardship available to the laboratories. While this element is structured differently at each of the laboratories, program-wide it is divided into three areas: "Operations," "Software," and "R & D." The "Operations" effort is focused on the operation of the computer centers at the three laboratories. In general, that effort has two mission elements: 1) to provide ongoing stable production computing services to laboratory programs, and 2) to foster the evolution of simulation capabilities towards a production terascale environment as ASCI computer platforms evolve towards the 100-teraOPS goal by the middle of the next decade. This effort consists of hardware platforms, software infrastructure, the networks, data storage, and output systems.

The Operation of Facilities "Software" effort supports the evolution of existing weapon simulation capability and provides ongoing support for the physical databases used by both legacy codes and the advanced ASCI weapon simulation codes. These efforts are structured to coincide with the programs associated with each of the codes.

The third part of the Operation of Facilities element is focused on underlying R & D to provide a continuing stream of new information and simulation innovation for ASCI and the stewardship effort.

Operation of Facilities Strategies

- Operate and maintain laboratory computing centers
- Maintain existing production codes for near-term Stockpile Stewardship use
- Use existing input data and codes for benchmarking, verification, and validation
- Provide the production simulation capabilities that support the enduring stockpile and serve as the foundation of future ASCI code development
- Enable, preserve, and advance existing computational capabilities to meet stockpile requirements
- Maintain the skills/knowledge base that ASCI will leverage to meet stewardship goal
- Maintain preparedness to apply ASCI's advanced simulation capabilities as they develop
- Conduct underlying R & D in computational sciences, networking, computational physics, and engineering sciences to support development of advanced ASCI codes
- Conduct underlying R&D to support development and deployment of advanced physics and engineering simulation and information environments within ASCI programs

University Partnerships: Academic Strategic Alliances Program

Historically, parts of the academic community have always had a close relationship with the DP laboratories. In fact, Los Alamos and Lawrence Livermore National Laboratories have been managed for the Department of Energy by the University of California for many years. The missions of the universities and the DP laboratories, however, are not closely aligned. The mission of the DP laboratories is focused on nuclear weapons, which requires very tight control of scientific information. Universities, on the other hand, generally encourage the free and open exchange of ideas and scientific knowledge. While this difference in the approach to handling information has sometimes led to tensions, ASCI and universities share a new common and critical interest. The success of ASCI depends on the ability to demonstrate that simulations can credibly be used as a means of ensuring stockpile confidence. Universities have a strong interest in improving the ability of simulations to credibly reflect reality. Simulation has already proven valuable in exploring and developing new scientific ideas. For example, the resolution of one of the most difficult and troubling problems in condensed-matter physics, the so-called "Kondo impurity" problem, was first provided by Prof. Ken Wilson of Cornell University. He did so by computational simulation using unique computing resources at Los Alamos. Thus, ASCI's efforts to revitalize this historic relationship between the national laboratories and the wider academic community have become an important part of the stockpile stewardship philosophy.

ASCI will require the technical skills of the best scientists and engineers working in academia, industry, and other government agencies in addition to those working in the national laboratories. The need to develop an unprecedented level of simulation capability requires strategic alliances with other leading research organizations. The purpose of the Alliances program is to engage the best minds in the U.S. academic community to help accelerate the emergence of new unclassified simulation science and methodology and associated supporting technology for high-performance computer modeling and simulation. These alliances will support the development and credible validation of this simulation capability. ASCI will also work with the larger computing community to develop and apply commercially acceptable standards. ASCI plans to initiate exchange programs to bring top researchers directly into the project while allowing laboratory personnel to expand their experience base in external projects. Finally, ASAP is viewed as an important step toward developing the next generation of scientists needed for the national security programs at the DP laboratories.

Figure 10. ASCI's Level One Strategic Alliances involve five of the nation's top research universities in the simulation effort.

These research projects are being implemented in three levels:

1. **Level One Strategic Alliances** established five major centers (see Fig. 10) engaged in long-term, large-scale, unclassified, integrated multidisciplinary simulation and supporting science and computational mathematics representing ASCI-class problems. The centers have a five-year funding commitment, each starting at about $3.7M per year with planned growth to about $5M per year, subject to contract renewal in the third year. These centers will collectively have access to up to 10% of the ASCI-class computing resources at the national security laboratories. They are:

— California Institute of Technology: Center for Simulating Dynamic Response of Materials
— Stanford University: Center for Integrated Turbulence Simulation
— University of Chicago: Center for Astrophysics Flash Phenomena
— University of Illinois, Urbana-Champaign: Center for Simulation of Advanced Rockets
— University of Utah: Center for Simulation of Accident and Fire Environments

1. **Level Two Strategic Investigations** established smaller discipline-oriented projects working in computer science and computational mathematics areas identified as critical to ASCI success. There are fourteen Strategic Investigation projects established in FY1999, each targeted for three years, with funding ranging from $200K to about $600K per year. Like Level One Alliances, these were selected by an open, peer-reviewed solicitation process.

3. **Level Three Individual Collaborations** establish focused projects initiated by individual ASCI researchers working on near-term ASCI-related problems. Typically, these specific projects are in the $50K to $100K per year range, funded out of laboratory ASCI budgets.

ASCI Institutes

In addition to the three-level Alliances Program, ASCI's academic collaborations will add a new component in FY2000 — The ASCI Institutes. The charter of the ASCI Institutes at the three DP laboratories is to create an environment for collaboration with academia on research topics in computer science, computational mathematics, and scientific computing that are relevant to the Stockpile Stewardship Program. These collaborations will be conducted through a variety of mechanisms, ranging from one-day seminars to multi-month sabbaticals at the laboratories.

Each of the three Institutes will have different topics of emphasis, depending on laboratory needs; however, they are expected to coordinate and leverage their activities to ensure maximum benefit to the ASCI program.

Hiring qualified and experienced computer and computational scientists is extremely challenging in today's job market. One of the objectives of this effort is to enhance the laboratories' ability to attract top-notch academicians to the laboratories.

Alliances/Institutes Strategies

- Encourage strategic alliances and collaboration
- Leverage other national initiatives
- Collaborate with the best R&D programs of other DOE departmental offices, other agencies, universities, and industry
- Attract top researchers in the key disciplines for weapon applications
- Form long-term strategic alliances with a small number of universities and academic consortia to fund critical efforts dedicated to long-term ASCI issues, such as high-confidence simulations
- Establish smaller scale collaborations with individual investigators and research groups to work on more narrowly focused problems, such as turbulence
- Link task-oriented collaborations closely with specific ASCI deliverables

This document is the next generation of the 1996 ASCI Program Plan. It builds on both the 1996 ASCI Plan and the Stockpile Computing Program, and integrates the results and experiences from the past three years. While the ASCI program has a multi-year plan, it is designed to be flexible in order to respond to changing technical developments and stewardship requirements. It has also responded to programmatic needs — specifically, a zero-based budget, a zero-yield Comprehensive Test Ban Treaty and a Stockpile Life Extension Program.

In fiscal year 1998, the ASCI applications effort focused directly on increasing the ability of laboratories to predict the integrated performance and safety of weapons through computational means. Additional code projects address materials aging and manufacturing issues and set the initial conditions for performance and safety codes. In the nuclear arena, the initial 3D-simulation milestone has been met as has the FY2000 burn-code milepost.

The burn-code milepost involved the first-ever three-dimensional (3D) simulation of a nuclear weapon "primary" explosion. Modern nuclear weapons consist of two main components: a "primary," or trigger, for the "secondary," the thermonuclear reaction. Demonstrating the ability to computationally visualize and analyze what happens to one of those components is the first critically important step taken in simulating an entire nuclear weapon's explosion in three dimensions. The complexity of the phenomena that were simulated by the burn code, as well as the fact that the computers, software tools, and numerical methods that made the burn-code computation possible had to be developed simultaneously with applications software, make this a major achievement.

In the virtual prototyping arena, ASCI is developing a simulation capability to design a variety of weapon components. Virtual prototyping allows us to simulate the potential performance of a part or system and the manufacturing processes required to produce it. It reduces development time, requires fewer physical prototypes, and requires fewer design tests. Furthermore, performance of the component or system in hostile environments can be examined in detail.

Virtual aging progress spans metals such as plutonium, to mixtures such as high explosives, to synthetics such as butyl O-rings. For plutonium, aging simulation tools for atomic forces and 3D structural phase transformations have been developed, and high-pressure elastic constants for body-centered cubic plutonium were calculated from first principles. For high explosives, a state-of-the-art high-explosive equation-of-state and detonation model combining thermo-chemistry and reaction-zone chemical kinetics was developed for safety and performance calculations. Successes have also been achieved over a wide range of other endeavors — necessary steps in the path to performance simulation based on basic principles, the cornerstone of science-based stockpile stewardship.

In the platform-development area (see Fig. 11), the initial platform contract was awarded to Intel in August 1995 and teraOPS-level operation was achieved in December 1996. The Intel machine has been nicknamed “Option Red” and is located at Sandia Albuquerque.

In a stepping-stone strategy, two more contracts nicknamed “Option Blue” were let in 1996 to pursue the 3-teraOPS goal with IBM and SGI/Cray. Both the IBM system and the SGI system have demonstrated peaks in excess of 3 teraOPS and have been integrated into the ASCI computing environments at LLNL and LANL, respectively, as is Sandia’s 3-teraOPS upgrade of the “Red” Intel machine. Higher computer processing capability leads to new challenges. To address these challenges, five partnerships were established under the “PathForward” program, all aimed at the technologies required for a 30-teraOPS system.

The next system to be built will be “Option White,” illustrated in Fig. 12. ASCI has extended its “Option Blue” contract with IBM to develop the 10-teraOPS “White” system to be installed at LLNL in the year 2000. A 30-teraOPS system to be sited at LANL is in its initial stages of development. The goal of the platform-development effort is to achieve 100-teraOPS by the year 2004.

Figure 11. ASCI has brought about development and installation of three of the world's fastest computer platforms. Intel's ASCI Red machine (upper left), located at Sandia Albuquerque, was the world's first teraOPS computer and was recently upgraded to more than three teraOPS. ASCI Blue Mountain (upper right) was installed at Los Alamos by SGI and has achieved a peak speed of over three teraOPS. ASCI Blue Pacific (bottom) was installed by IBM at Lawrence Livermore and has also broken the three-teraOPS barrier.

To support collaboration among ASCI researchers at the three laboratories, the first secure high-speed data network linking Los Alamos, Sandia, and Lawrence Livermore National Laboratories was established in 1996.

To support the understanding and interpretation of the results of these very large-scale simulations, a prototype visualization corridor was established in 1998. This system is intended to be the forerunner of systems developed under the VIEWS initiative.

The ASCI program initiated the Academic Strategic Alliances effort with establishment of long-term strategic alliances with five research universities to develop critical mass efforts dedicated to long-term multidisciplinary problems. The universities participating in the Academic Strategic Alliance Program are the California Institute of Technology, Stanford University, the University of Chicago, the University of Illinois at Urbana-Champaign, and the University of Utah. Fourteen Level-Two strategic investigations have been initiated and Level Three collaborations continue for FY2000.

The Computing and Simulation program will continue to advance during fiscal year 2000. Significant efforts will be required to continue the development of codes started in the initial phases of ASCI. The development plans for these codes include the delivery of initial capabilities needed to certify planned near-term stockpile modifications. The development of these codes requires a significant interface with Defense Programs experimental facilities for verification and validation.

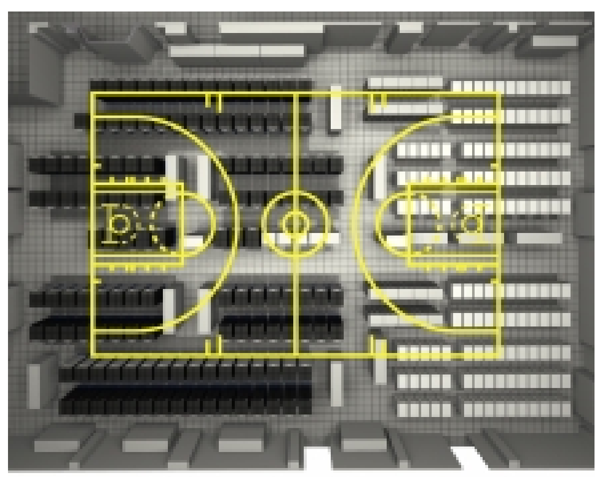

Figure 12. "Option White," the 10-teraOPS IBM computer to be installed at LLNL in the summer of 2000, will occupy 12,000 square feet of machine room floor space.

Program Management Objectives

ASCI program management has two important objectives:

1. Provide leadership. ASCI will develop computational capabilities that are critical to the Stockpile Stewardship Program. It must accomplish its mission on time and on budget. The ASCI management structure must enhance the work at the Defense Programs laboratories, keeping it focused on the ASCI mission. It must also ensure that resources are properly directed. The success of the program depends on the computer industry and universities. The ASCI management structure must provide leadership to engage the computer industry and universities in the quest for simulation capabilities that can credibly replace nuclear testing as a decision-making tool.

2. Facilitate the interactions among the laboratories. ASCI is breaking new ground in the degree of collaboration among the laboratories. The ASCI management structure must understand and break down artificial barriers that inhibit that collaboration.

Program Management Planning Process

ASCI program management will utilize the following planning process:

- **The ASCI Program Plan.** The Program Plan provides the overall direction and policy for ASCI. It serves as the strategic plan for the program and identifies the key issues and work areas for ASCI.
- **ASCI Implementation Plans.** These plans will be prepared annually and will describe the work planned at each laboratory to support the overall ASCI objectives. The implementation plans will be prepared by the strategy teams who will ensure that the work at each laboratory is closely coupled with the other labs. The implementation planning effort will begin in April and will conclude with a coordination meeting in July in anticipation of the beginning of the fiscal year on October 1.

Performance Measurement

ASCI managers realize that the successful development of modeling and simulation capabilities depends, in part, upon an effective and suitable performance-measurement program. Yet, measuring the overall impact of a collection of research and development activities has been frustrating because there is no widely recognized metric to measure their effectiveness. ASCI has adopted an approach that addresses this need by comparing actual output with planned output within a given year. This metric is referred to as the R&D Effectiveness Metric (EM). This method is not only consistent with the University of California approach to developing performance metrics, but also aligned with the Government Performance and Results Act of 1993. Developing realistic, but challenging, project milestones is the first step toward producing a meaningful EM. ASCI's annual implementation planning process ensures that project milestones are both cost-effective and fully integrated with all other ongoing and planned activities. Project metrics within a particular ASCI program element or strategy are aggregated showing overall performance for that strategy. Progress over time is demonstrated through the use of indexed metrics. Laboratory managers are responsible for both measuring and managing the performance of the projects within their purview. Each laboratory reports performance to DOE headquarters quarterly in the form of accomplishments and progress toward milestones.

The budget is reported and analyzed monthly by ASCI's laboratory-level resource analysts and by laboratory management. DOE's cost tracking procedures for ASCI projects are consistent with ASCI's fundamentally developmental nature. Funding and costs are tracked and reported at the program element level using DOE's official Budget and Reporting classification codes and Financial Information System. These tracking systems are extended in greater detail down to the level of individual projects.

Organization

ASCI's structure is designed to foster a focused collaborative effort to achieve program objectives:

- **Executive Committee**. This body consists of two high-level representatives (a primary and alternate) from each laboratory and from Defense Programs headquarters. The Executive Committee sets overall policy for ASCI, develops programmatic budgets, and provides oversight for the execution of the program.
- **Strategy and Program Teams**. These teams are responsible for the planning and execution (through the management structures of individual laboratories) of the implementation plans for each of the program elements: One Program/3 Labs, Applications, V&V, Materials and Physics Modeling, Problem-Solving Environment, DisCom^2, PathForward, VIEWS, Physical Infrastructure and Platforms, Operations of Facilities, Alliances, and Institutes. The strategy teams consist of two representatives (a primary and alternate) from each laboratory. The strategy teams are facilitated by representatives from the ASCI Headquarters (ASCI HQ) team.
- **ASCI Headquarters Team**. This team consists of Defense Programs Federal employees supported by representatives from the Defense Programs

laboratories. The ASCI HQ team is responsible for ensuring that the program supports the overall Stockpile Stewardship Program. The ASCI HQ team facilitates the program's interactions with other government agencies, the computer industry, and universities. Finally, the team sets programmatic requirements for the laboratories and reviews management and operating (M&O) contractor performance.

Program Collaboration Meetings

ASCI will regularly hold the following meetings as part of its leadership role and to facilitate collaboration among the three laboratories, industry, and universities:

- **Principal Investigator meetings**. These meetings will be held annually and will provide a forum for ASCI Principal Investigators to meet and discuss progress on their research areas. These meetings will help foster collaborations by allowing principal investigators at each laboratory to present and discuss their work with their peers at the other laboratories. The meetings (which will include participants from outside of the weapon labs) will also serve a peer-review function. These meetings will provide an annual technical review for the ASCI HQ team.
- **Executive Committee meetings**. Every 2 weeks, the ASCI Executive Committee will meet via teleconference to discuss important issues. These meetings will ensure that relevant issues are identified, discussed, and resolved in a timely manner. The biweekly teleconferences will be supplemented with quarterly face-to-face meetings.

The shift from test-based confidence to computation-based confidence in the enduring stockpile has far-reaching consequences in Defense Programs. This shift requires a new approach to the traditional methods used to ensure the performance, safety, and reliability of the nation's nuclear weapon systems. Defense Programs' Stockpile Stewardship and Management Plan describes this approach to assessing and certifying weapons as they move from their current full-scale, tested, and well understood state to a state where they have aged, been refurbished, or both. The ability to maintain confidence in the weapons as they move away from their current state will be provided primarily through advanced simulation capabilities and improved scientific understanding.

ASCI must maintain a close relationship with both the Stockpile Life Extension Program (SLEP) and the Defense Science Program. ASCI receives requirements from and provides capabilities to SLEP. ASCI in turn must look to the Defense Science Program to provide additional science and experimental data to support the development of the simulation capability. ASCI will also provide important computational capabilities to support experiment design and to explore revalidation in a simulation environment.

The following is a short summary of the ASCI relationship with other elements of the Defense Programs Stockpile Stewardship and Management Plan.

Stockpile Life Extension Program

The Stockpile Life Extension Program (SLEP) is the operational arm of Defense Programs that conducts the surveillance, maintenance, refurbishment, and production activities for the stockpiled weapons. It is the interface with the DoD user. This program is responsible for certifying and assessing the performance, safety, and reliability of aging weapons or weapons that are changed by refurbished parts that have been manufactured with new processes (for example, because of the inability to support the old manufacturing process due to cost or environmental concerns). ASCI supports SLEP by providing the advanced computational capabilities that facilitate these assessments and certifications in the absence of underground nuclear testing.

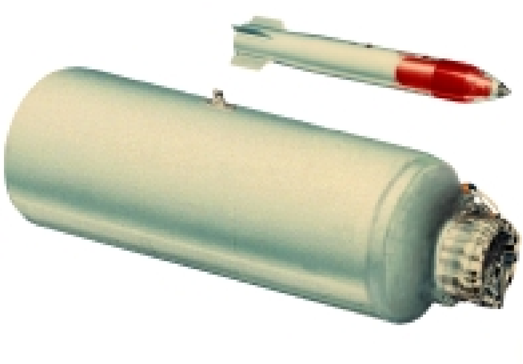

Figure 13. The B-83 Modern Strategic Bomb: one of the weapon systems that make up the current U.S. nuclear stockpile.

ASCI will also provide important capabilities to address two major concerns with the stockpile. Today the United States nuclear stockpile is considered to be safe and reliable. In the example illustrated in Fig. 13, the B-83 modern strategic bomb was built with all of the modern safety features when it entered the stockpile. In many cases, the weapons in the stockpile reached that safe and reliable state only after a period of time (shortly after the introduction of the weapon systems into the stockpile), when problems were identified and fixed. Defense Programs currently anticipates that the weapons will remain safe and reliable for many years. The concern, however, is that the weapons will develop problems affecting their performance and safety because of old age, just like any electromechanical appliance. Defense Programs is committed to identifying and correcting these problems long before they affect confidence in the stockpile. ASCI will provide vital computational capabilities to be used by the Enhanced Surveillance Program to help predict when stockpile refurbishment is required.

The second major concern that SLEP must address is the possible introduction of new problems into the stockpile by refurbishment activities designed to rectify aging problems. ASCI will provide simulation capabilities that will be used to help predict how stockpile refurbishments will affect the performance, safety, and reliability of the weapons. These capabilities will be critical to keeping the number of new problems introduced by SLEP to an absolute minimum. ASCI simulations are also critical to a more effective design process (for limited-life components) by assuring reduced costs and schedules.

Defense Science Program

The Defense Science Program is the traditional source of science development, testing (including, in the past, underground tests), and experiments needed to support the United States nuclear stockpile. In an era of test-based confidence, this program provided direct answers about the performance, safety, and reliability of the stockpile. The Stockpile Computing program was focused primarily at supporting the testing program. In this era without underground testing, with reduced aboveground tests, and with new manufacturing processes, the focus is shifting to computation-based confidence and the strong relationship between Advanced Simulation and Computing and Defense Science. The ASCI effort is conducted by the Advanced Simulation and Modeling Office of DOE's Research, Development, and Simulation Organization illustrated in Fig. 14.

Stockpile Stewardship provides the understanding in science and the physics models needed to understand weapon performance. ASCI provides the verified and validated codes, computer platforms, and simulation environment that make it possible to simulate the operation and aging of U.S. weapon systems. Stockpile Stewardship will also provide the experimental facilities, like the National Ignition Facility and the Dual Axis Hydrodynamic Testing (DAHRT) Facility, which will be used to develop new physics models and provide validation data. In addition, the Microsystems Engineering Sciences Applications (MESA) Facility will provide new engineering design and development capabilities. Finally, the Stockpile Stewardship Program will maintain and continue to develop and understand the archival data from past underground tests, which provide a critical link back to full-scale weapon tests.

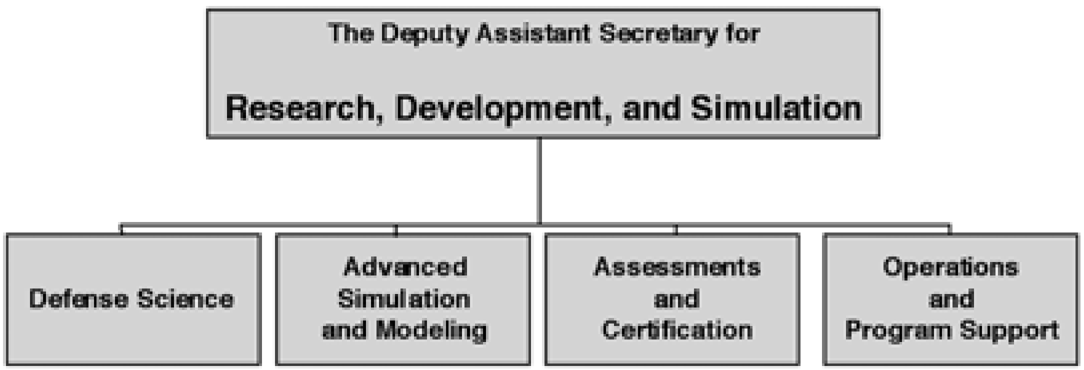

Figure 14. The ASCI effort is conducted by the Advanced Simulation and Modeling Office of DOE's Research, Development, and Simulation Organization.

In August 1995, the United States took a significant step to reduce the nuclear danger. The decision to pursue a “zero- yield” Comprehensive Test Ban Treaty will allow greater control over the proliferation of nuclear weapons and will halt the growth of new nuclear systems. This step is only possible because of the Stockpile Stewardship Program, which provides an alternative means of ensuring the safety, performance, and reliability of the United States’ enduring stockpile. At the heart of the Stockpile Stewardship Program is ASCI, which will create the high-confidence simulation capabilities needed to integrate fundamental science, experiments, and archival data into the stewardship of the actual weapons in the stockpile. ASCI will also serve to drive the development of simulation as a national resource by working closely with the computer industry and with universities.

ASCI mileposts are first listed in this section by an ID label, the quarter in which they are to be completed, and a title. Following that list, a brief description is provided of each milepost. Finally, the mileposts are graphically displayed in a timeline (see Fig. A1). The ID label identifies the milepost in the following way: Milepost "NA-0.1" is the first (".1") milepost to be completed in the area of Nuclear Applications ("NA") in the year 2000 ("0"). Full mileposts are indicated in **BOLD** type, major milestones are indicated in REGULAR type.

Nuclear Applications

NA-0.1	**FY00 Q1**	**Three-dimensional primary-burn prototype simulation**
NA-0.2	FY00 Q4	Three-dimensional prototype radiation-flow simulation
NA-1.1	**FY01 Q1**	**Three-dimensional secondary-burn prototype simulation**
NA-2.1	**FY02 Q1**	**Three-dimensional prototype full-system coupled simulation**
NA-3.1	**FY03 Q1**	**Three-dimensional high-fidelity-physics primary-burn simulation, initial capability**
NA-4.1	**FY04 Q1**	**Three-dimensional high-fidelity-physics secondary-burn simulation, initial capability**
NA-4.2	**FY04 Q4**	**Three-dimensional high-fidelity-physics full-system simulation, initial capability**

Nuclear Safety

NS-2.1	**FY02 Q4**	**Three-dimensional safety simulation of a complex abnormal explosive-initiation scenario**

Non-Nuclear Applications

NN-0.1	**FY00 Q2**	**Three-dimensional prototype hostile-environment simulation**
NN-0.2	FY00 Q4	Architecture for coupled mechanics running at all NWC sites
NN-1.1	**FY01 Q4**	**Mechanics for normal environments**
NN-2.1	FY02 Q4	Coupled multi-physics for hostile (nuclear) environments
NN-3.1	**FY03 Q4**	**Coupled multi-physics for abnormal environments**
NN-5.1	**FY05 Q1**	**Full system STS simulation**

Verification and Validation

VV-1.1	FY01 Q1	Establish and deploy a common set of acceptable software engineering practices applicable to all advanced application-development activities
VV-1.2	**FY01 Q2**	**Demonstrate initial validation methodology on the then-current state of application modeling of early-time primary behavior**
VV-2.1	FY02 Q4	Demonstrate initial validation methodology of the then-current state of ASCI code modeling for normal and abnormal STS environments behavior
VV-5.1	**FY05 Q1**	**Demonstrate initial uncertainty quantification assessments of ASCI nuclear and non-nuclear simulation codes**

Physical and Materials Modeling

PM-2.1	FY02 Q2	Microstructure-level shock response of PZT 95/5
PM-2.2	**FY02 Q4**	**Delivery of initial macro-scale reactive flow model for high-explosive detonation derived from grain scale dynamics**
PM-3.1	FY03 Q4	Meso-scale model for corrosion of electrical components
PM-5.1	FY05 Q4	Delivery of an advanced multi-phase equation of state for plutonium
PM-5.2	FY05 Q4	Delivery of validated multi-scale constitutive models of the dynamic response of Pu and other metals

VIEWS

VU-0.1	**FY00 Q1**	**Prototype system that allows weapons analysts to see and understand results from 3D prototype primary-burn simulations**
VU-2.1	FY02 Q4	64M pixel display driven by a scalable rendering system.
VU-4.1	**FY04 Q4**	**Ability to do realtime analysis on a 200-TB ASCI dataset**

PSE

PS-1.1	**FY01 Q1**	**Initial software development environment extended to the 10-teraOPS system**
PS-5.1	FY05 Q3	Production-quality uniform user and application interfaces available on all ASCI high-end computing platforms

DisCom^2

DC-1.1	**FY01 Q2**	**Distance-computing environment available for use on the 10- teraOPS ASCI system**
DC-3.1	**FY03 Q4**	**Complex-wide infrastructure that integrates all ASCI resources**

Physical Infrastructure and Platforms

PP-0.1	**FY00 Q3**	**10-teraOPS (Option White) final system delivery and checkout**
PP-2.1	**FY02 Q1**	**30-teraOPS final system delivery and checkout**
PP-4.1	**FY04 Q3**	**100-teraOPS final system delivery and checkout**

Milepost Descriptions

Nuclear Applications

NA-0.1 FY00 Q1

Three-dimensional primary-burn prototype simulation

The ASCI project will calculate the explosion of a primary with three-dimensional engineering features. The simulation will produce relevant information, including a yield, to be compared to a nuclear test.

(A more detailed description of this milepost is available on request from the DOE Office of Advanced Simulation and Modeling.)

NA-0.2 FY00 Q4

Three-dimensional prototype radiation-flow simulation

The ASCI project will calculate a radiation flow simulation with three-dimensional engineering features. The simulation will produce relevant information that will be compared to a nuclear test.

(A more detailed description of this milepost is available on request from the DOE Office of Advanced Simulation and Modeling.)

NA-1.1 FY01 Q1

Three-dimensional secondary-burn prototype simulation

The ASCI project will calculate the explosion of a secondary with three-dimensional engineering features. The simulation will produce relevant information, including a yield, to be compared to a nuclear test.

(A more detailed description of this milepost is available on request from the DOE Office of Advanced Simulation and Modeling.)

NA-2.1 FY02 Q1

Three-dimensional prototype full-system coupled simulation

The ASCI project will make a prototype calculation of a full weapon system (primary + secondary) with three-dimensional engineering features. The simulation will produce relevant information, including the primary and secondary yield, to be compared to a nuclear test.

(A more detailed description of this milepost is available on request from the DOE Office of Advanced Simulation and Modeling.)

NA-3.1 FY03 Q1

Three-dimensional high-fidelity-physics primary-burn simulation, initial capability

The ASCI project will make a high-fidelity-physics calculation of a primary system with three-dimensional engineering features. The simulation will produce relevant information, including the primary yield, to be compared to a nuclear test.

(A more detailed description of this milepost is available on request from the DOE Office of Advanced Simulation and Modeling.)

NA-4.1 FY04 Q1

Three-dimensional high-fidelity-physics secondary-burn simulation, initial capability

The ASCI project will make a high-fidelity-physics calculation of a secondary with three-dimensional engineering features. The simulation will produce relevant information, including the secondary yield, to be compared to a nuclear test.

(A more detailed description of this milepost is available on request from the DOE Office of Advanced Simulation and Modeling.)

NA-4.2 FY04 Q4

Three-dimensional high-fidelity-physics full-system simulation, initial capability

By December 31, 2004, the ASCI project will make a high-fidelity-physics calculation of a full system (primary + secondary) with three-dimensional engineering features. The simulation will produce relevant information, including primary and secondary yields, to be compared to a nuclear test.

(A more detailed description of this milepost is available on request from the DOE Office of Advanced Simulation and Modeling.)

Nuclear Safety

NS-2.1 FY02 Q4

Three-dimensional safety simulation of a complex abnormal explosive-initiation scenario

By the third quarter of fiscal 2002, the ASCI project will calculate a 3D nuclear safety simulation of a complex abnormal initiation of the high explosive in a nuclear weapon using advanced high explosive models. The hypothetical initiation scenario will be more complex than in previous nuclear safety simulations. The simulation will produce information that will be compared with relevant nuclear and nonnuclear test data.

(A more detailed description of this milepost is available on request from the DOE Office of Advanced Simulation and Modeling.)

Non-Nuclear Applications

NN-0.1 FY00 Q2

Three-dimensional prototype hostile-environment simulation

This milepost will be a demonstration of ASCI software for 3D dynamic response of a re-entry vehicle system to hostile radiation and blast environments. This initial simulation capability will include 3D weapon geometry, but with limited physics, and limited physics and mechanics coupling. Included are models for the following hostile environments: (1) blast and impulse loading which can potentially result in structural damage to the weapon system and components; (2) photon radiation transport which can penetrate the weapon structure, depositing energy at critical component locations which can potentially result in thermal-mechanical damage; and (3) photon radiation transport which can penetrate the weapon structure, producing electrons which can potentially result in electrical damage to the components.

In this simulation we will demonstrate ASCI software for a typical re-entry vehicle in nuclear environments, but with limited physics to three scenarios above:

- Full 3D re-entry vehicle structural response to blast and impulse loading with mesh discretization in sufficient detail to predict internal component shock response.
- 3D Monte Carlo determination of dose, and thermal-mechanical response of a typical weapon component.
- Simulations will be performed on the ASCI Red TOPS Supercomputer utilizing at least 2000 processors.

Verification of software will continue within ASCI Applications code team, and gathering of experimental data for mechanics and physics validation will continue as the central thrust of the Hostile Certification Campaign 1. This milepost is critical to successful completion of a succeeding milepost for full STS hostile simulation capability.

NN-0.2 FY00 Q4
Architecture for coupled mechanics running at all NWC sites

This milestone will be a first-release of ASCI architecture for adaptive, coupled mechanics applications for engineering analysis of STS environments. The software will be running at all NWC sites. SIERRA is a broadly applicable, scalable software architecture written in modern programming language. Emphasis is placed on reusable software and utilization of existing libraries and algorithms. SIERRA version 1.0 will be released in FY00Q4. This release will include

- Parallel I/O
- Distributed Mesh Services
- Finite Element Services
- Dynamic Load Balancing Services
- Parallel Mechanics Transfer Services
- Linear Solver Services
- H-adaptivity

The SIERRA V1.0 distribution will include source code, online documentation, build environment and software configuration management.

This milepost is critical in that it will provide the development and production platform for succeeding milestones in Non-Nuclear Applications.

NN-1.1 FY01 Q4
Mechanics for normal environments

This milepost will be a demonstration of ASCI software for 3D dynamic response of a re-entry vehicle system to normal flight environments. This initial simulation capability will include 3D weapon geometry, but with limited mechanics and physics. Included are:

- 3D nonlinear structural response including implicit dynamics algorithms.
- 3D aerodynamics including re-entry shield heating and ablation.
- 3D re-entry vehicle geometry with mesh discretization in sufficient detail to resolve weapon component and physics package response.
- Simulation will be performed on the ASCI 10-teraOPS computer utilizing a majority of machine processors.

Verification of software will continue within ASCI Applications code team, and gathering of experimental data for mechanics and physics validation will continue as the central thrust of the Hostile Certification Campaign. This milepost is critical to successful completion of a succeeding milepost for full STS hostile simulation capability.

NN-2.1 FY02 Q4
Coupled multi-physics for hostile (nuclear) environments

This milestone will be a demonstration of ASCI software to compute the coupled response of a weapon system in hostile (nuclear) environments. This simulation will include:

- Coupled 3D blast and impulse loading and structural response,
- Coupled 3D Monte Carlo radiation transport and thermal-mechanical response,
- Coupled 3D deterministic radiation transport and electromagnetic response for cavity SGEMP.
- Problem geometry will be full 3D model of re-entry vehicle with mesh discretization sufficient to resolve energy deposition, shock response, thermal-mechanical response, and cavity SGEMP in critical weapon components.
- Simulation will be run on the ASCI 30-teraOPS computer utilizing a majority of processors.

Physics and mechanics modules will be integrated into an architectural framework which will accommodate the various alternative solver strategies and datasets employed. After this first release, verification of software will continue within ASCI Applications code team, and gathering of experimental data for mechanics and physics validation will continue as the central thrust of the Hostile Certification Campaign. This milepost will lead to successful completion of a succeeding milepost for full STS hostile simulation capability.

NN-3.1 FY03 Q4
Coupled multi-physics for abnormal environments

This milepost will be a demonstration of ASCI software to simulate the coupled "crash and burn" scenarios and weapon and component response for safety assessment of STS environments.

A coupled, multi-physics simulation will be performed for a typical accident scenario which will include:

- 3D open pool fuel fire environment, including turbulent, buoyantly driven incompressible flow, heat transfer, mass transfer, combustion, soot, and participating media thermal radiation.
- 3D transient dynamic response of solids, including arbitrary contact, multi-element formulations, and nonlinear material models.
- 3D quasi-static response of solids, including arbitrary contact, shell multi-element formulations, and nonlinear material models.
- 3D heat transfer including convection, contact, enclosure radiation, multi-element formulations, and nonlinear material response.
- Reaction chemistry for foam decomposition.
- Simulation will be performed in the Sierra framework and will demonstrate adaptive meshing, data transfer between meshes, and solution steering.
- Problem will be fully three-dimensional, with mesh discretization in sufficient detail to model thermal-mechanical response of safety critical weapon components.
- Simulation will be performed on the ASCI 30-teraOPS machine utilizing a majority of machine processors.

After first release, verification of software will continue within the ASCI Applications code team, and gathering of experimental data for mechanics and physics validation will continue as the central element of the Engineering Certification Campaign. This milepost is a necessary and significant step towards successful completion of a succeeding milepost for full STS simulation for abnormal environments.

NN-5.1 FY05 Q1
Full system STS simulation

This milepost will be a 3D demonstration of initial production ASCI software for engineering simulation of weapon response for full STS environments. This demonstration will address coupled response of a weapon system in combined normal, hostile and abnormal environments. This simulation will include:

- Coupled 3D blast and impulse loading and structural response,
- Coupled 3D Monte Carlo radiation transport and thermal-mechanical response,
- Coupled 3D deterministic radiation transport and electromagnetic response for cavity SGEMP,
- 3D open pool fuel fire environment, including turbulent, buoyantly driven incompressible flow, heat transfer, mass transfer, combustion, soot and absorption, and participating media thermal radiation.
- 3D transient dynamic response of solids, including arbitrary contact, multi-element formulations, and nonlinear material models.
- 3D quasi-static response of solids, including arbitrary contact, shell multi-element formulations, and nonlinear material models.
- 3D heat transfer including convection, contact, enclosure radiation, multi-element formulations, and nonlinear material response.
- Reaction chemistry for organic decomposition.
- Simulation will be performed within an architectural framework and will demonstrate adaptive meshing, data transfer between meshes, and solution steering.
- Problem geometry will be fully three-dimensional, with sufficient mesh discretization to model component response.
- Simulation will be performed on the ASCI 100-teraOPS machine utilizing a majority of machine processors.

Thi.s milestone is critical for simulation-based design, manufacture and certification of stockpile refurbishment. Code software will continue to be verified by the ASCI code teams. Experimental data for mechanics and physics validation, at both the single physics and integrated scale, will be performed in the Engineering and Hostile Certification Campaigns.

Verification and Validation

VV-1.1 FY01 Q1
Establish and deploy a common set of acceptable software engineering practices applicable to all advanced application development activities

This milepost represents the selection and implementation of highest benefit software quality and development process guidelines across ASCI code development projects at all three laboratories. The milepost would focus on two distinct areas. The first area would bring all code development activities in application projects up to common, agreed upon levels of software quality and software engineering practices. Such practices would include source management, version control, regression testing, and bug tracking. The second area is the development, selection and analysis of a few, small physics domain-specific suites of verification test problems. At a minimum, all relevant code projects will use this common set.

VV1.2 FY01 Q2
Demonstrate initial validation methodology of the current state of ASCI code modeling for early-time primary behavior

This milepost is a demonstration of the validation assessment methodology of the current state of ASCI code modeling capabilities applied to modeling of early primary behavior. The intent of the milestone is to demonstrate a validation assessment methodology early enough in the ASCI Code V&V process that this type of process can be productively applied to other modeling areas in the early phases of the FY00-FY05 ASCI Applications development timeframe. This assessment will involve one ASCI code at each nuclear laboratory.

This assessment will include comparisons of the code results to an agreed upon data suite. The current state of the physical models will be employed, and because the milepost occurs fairly early in the ASCI timeline, the models may not yet have many of the advanced physics or materials models in place. Quality of comparisons will be measured against current design/analysis standards for legacy codes.

Validation is a continuous process that occurs as new physics models and code features are incorporated and tested against theory or data. Therefore, the validation methodology is expected to evolve and improve over the course of the ASCI Program.

The validation methodology and the results of the application of this process to the primary modeling capabilities will be documented.

VV-2.1 FY02 Q4
Demonstrate initial validation methodology of the then-current state of ASCI code modeling for normal and abnormal STS environments behavior

This milepost is a demonstration of the validation assessment methodology of the current state of ASCI code modeling capabilities applied to modeling of Normal and Abnormal STS Environments behavior. The intent of the milestone is to demonstrate a validation assessment methodology early enough in the ASCI Code V&V process that this type of process can be productively applied to other modeling areas in the early phases of the FY00-FY05 ASCI Applications development timeframe. This assessment will involve at least one ASCI stockpile application at each laboratory.

This assessment will include comparisons of the code results to an agreed upon data suite. The current state of the physical models will be employed, and because the milepost occurs fairly early in the ASCI timeline, the models may not yet have many of the advanced physics or materials models in place. Quality of comparisons will be measured against current design/analysis standards for legacy codes.

Validation is a continuous process that occurs as new physics models and code features are incorporated and tested against theory or data. Therefore, the validation methodology is expected to evolve and improve over the course of the ASCI Program.

The validation methodology and the results of the application of this process to the Normal and Abnormal STS Environments modeling capabilities will be documented.

VV-5.1 FY05 Q1
Demonstrate initial uncertainty quantification assessments of ASCI nuclear and non-nuclear simulation codes

This milepost represents a demonstration of the process of uncertainty quantification of predictive capability based on several validation studies for selected ASCI nuclear and non-nuclear simulation codes. Such analysis would be physics domain specific and would involve sets of ongoing validation comparisons that drive uncertainty quantification analysis. Nuclear performance and nuclear safety codes would concentrate on NTS experiments, local experiments, and their diagnostics, while the non-nuclear codes would use appropriate engineering tests and experiments. These sets of validation studies would provide a basis for estimates of error bounds in ASCI simulations of selected problems of direct programmatic importance.

Materials and Physics Modeling

PM-2.1 FY02 Q2
Microstructure-level shock response of PZT 95/5

The overall goal of this effort is to develop and apply a numerical simulation capability to resolve issues surrounding the performance of lead zirconate titanate (PZT) ceramic as a power supply for neutron generators. A successful simulation capability will be able to relate microstructural characteristics to ferroelectric performance in the power supply application. These simulations will support the PZT Supply team and the Neutron GeneratorPower Supply Design team.

At this milestone, we will demonstrate a grain-scale simulation capability that includes generating physically-based microstructures of porous ceramics, meshing the microstructure for finite element analysis, and performing coupled transient dynamics - quasistatic electric field (QSE) finite element method (FEM) calculations of the response of a ferroelectric specimen (PZT 95/5) to shock wave loading. The microstructure generation simulations will include the following behavior: normal grain growth; densification; pore migration by surface diffusion and bulk diffusion. The microstructure will be represented by an all-hexahedral element mesh that resolves the crystal grains as flat-sided polyhedra or with a 1-irregular mesh (i.e. initial refinement of a structured mesh). The FEM calculations will treat the fully coupled electro-mechanics of an initially poled ferroelectric specimen in the QSE approximation. Additionally, they will treat thermal run-away electrical breakdown and explicitly depict cracking in the polycrystalline specimen. The material model will describe the elastic, inelastic, thermal, and phase behavior of the ferroelectric with the inelastic response including domain switching effects as well as inelasticity due to plasticity or damage.

PM-2.2 FY02 Q4

Delivery of initial macro-scale reactive flow model for high-explosive detonation derived from grain scale dynamics

High explosives can have reactions resulting from external stimuli ranging from mild pressure bursts to full detonation. The ability to predict these responses is important for understanding the performance as well as the safety and the reliability of these materials. Currently, we have only relatively simple phenomenological computational models for the behavior of high explosives under these conditions. These models are limited by the assumption that the explosive is homogeneous. In reality the high explosive is a highly heterogeneous composite of irregular crystallites and plastic binder. The heterogeneous nature of explosives is responsible for many of their mechanical and chemical properties.

We will use computational models to simulate the response of explosives to external mechanical stimuli at the grain level. The ultimate goal of this work is to

- understand the detailed processes involved with the material response, so that we can
- develop realistic material models which can be used in a hydrodynamics/multi-physics code to model real systems.

The new material models will provide a more realistic description of the explosive system during the most critical period of ignition and initiation.

The focus of this work is to use the results of such simulations to develop an advanced macroscopic reactive flow model that is consistent with our understanding of the grain scale details, and can incorporate such information quantitatively.

PM-3.1 FY03 Q4

Meso-scale model for corrosion of electrical components

Atmospheric corrosion of copper, silver, and aluminum electrical components is the leading degradation mode observed in the stockpile. The end goal is to develop a physics-based understanding of corrosion and eventual prediction of the reliability of electrical components for design lifetimes. Application will include future components at the microsystem level.

This milestone will demonstrate a validated type-I corrosion continuum (solid-state transport and reactive chemistry in a gas-liquid-solid heterogeneous system) simulation capability, based on theory and novel combinatorial and in-situ corrosion sensor experiments, and perform first science-based assessment of electrical component lifetime. Consistent with the *MESA* concept, successful completion of this milestone will rely on a strong coupling between computation materials scientists, weapon engineers, and physics and chemistry experiments at the nano-to-micro scale.

PM-5.1 FY05 Q1

Delivery of an advanced multi-phase equation of state for plutonium

By the end of calendar year 2004, we will have developed and tested an advanced, multiphase plutonium equation of state (EOS) for high-fidelity weapons simulations. This milepost will represent the confluence of several coordinated projects concerned with the development and application of state-of-the-art theoretical/empirical methods (validated by fundamental material tests) to calculate accurate cold, ion-thermal, and electron-thermal components of EOS and melt. The result will be a robust multi-phase EOS based on a full description of the Pu phase diagram, including all relevant solid phases and the liquid. Both the phase diagram and the new EOS will be validated as thoroughly as possible by experimental data generated in the Materials Dynamics Campaign.

PM-5.2 FY05 Q4

Delivery of validated multi-scale constitutive models of the dynamic response of Pu and other metals

This milestone is coordinated with MTE 2.2 in Campaign 2 and represents the successful integration of ASCI simulations and experimental activities. Constitutive models are dynamic models, either in analytic or tabular form, that can be incorporated into large-scale application codes to predict the performance of nuclear weapons. For materials that have not previously been tested or at pressures or temperatures that are inaccessible to direct measurement, these models must be calculated from simulations that use our knowledge of the atomic forces and microstructure to predict the dynamic response. This milestone calls for the development of an accurate process to perform such simulations and to produce the resulting multiscale constitutive models for Pu and other relevant metals; the milestone also requires that these simulations be validated by experiments. In other words, this requirement means that key steps in the process of up-length-scale flow of information in the ASCI methodology have been validated experimentally so that the process itself is reliable. For example, this includes constitutive model development of results from Kolsky Bar, Taylor tests and Gun Tests. The milestone also means that the predictions of the multi-scale constitutive model, either on Pu or other materials, have been tested to the degree possible. An example of this would the validation of atomic calculations of elastic moduli at high pressure by diamond anvil experiments that measure the elastic constants of Ta and Pu at high pressure, or the predictions of yield strength of Pu at high pressures with diamond anvil experiments of yield strength of Pu at these pressures. Similarly, underlying assumptions of the models must be tested. An example would be testing the dislocation dynamics codes and assumptions about source terms, etc. by observing the dynamics of dislocation lines in low strain, low-strain-rate experiments; another example is the validation of homogenized values of strength parameters produced by the grain-level test sample constructed on ASCI codes. It is not realistic to expect that there will no further need for improvements in the development of multi-scale models or further testing as this milestone is reached. But it is realistic to expect that great progress will have been made and useful, physics-based models will be in place in application codes.

VIEWS

VU-0.1 FY00 Q1

Prototype system that allows weapons analysts to see and understand results from 3D prototype primary-burn simulations

The ASCI burn code milepost depends upon critical STS PSE and technologies for success. The focus of this milepost is on delivering data management, data delivery and data visualization services for end-user weapons designers that allow them to see and understand the multi-terabyte datasets produced by the ASCI simulation codes.

Weapons designers must be able to:

- Efficiently store and access multi-terabyte ASCI simulation results.
- Organize and manage these datasets.
- See and understand complex simulation results via graphical visualization and analysis tools.
- Share results with other weapons designers and code developers.

Key FY00 PSE and VIEWS products and services in support of this milepost are:

PSE

- Archival storage (DTS/archival storage):
  - Deployment and Integration of HPSS Release 4.1 to include integrated MPI-I/O, DFS, and server scalability functionality in the unclassified environments by the end of 4QFY99 and the classified by 1QFY00.
  - Identify "bottlenecks" and develop mediating strategies for scaling parallel data transfers to utilize parallel paths to ASCI visualization and compute platforms.
  - Additional ports of the CLient Application Program Interface (CLAPI) will be available for Sun Solaris and SGI with HPSS Release 4.1.1. LANL will continue to develop and enhance its high-performance parallel user interface PSI. This work will include enhancements to the ACLs provided in FY99 and better optimization within PSI for performance.
- Parallel IO (DTS/SIO)
- Optimized I/O libraries critical to the performance of ASCI simulation and visualization applications. Improved end-to-end performance of DMF/FBK/CDMlib/HDF5/MPI-IO layers,
- Easy-to-use, high performance I/O systems, whose throughput rates and capacity are in balance with the computational speed and memory size of ASCI platforms,
- Optimized data transfer between simulation and visualization applications, and archival storage.
- High speed interconnect (DTS/HSI)\
  - Continued support of the cluster internal high speed interconnect in collaboration with platform partners to improve the reliability and performance. LANL focus is on the HiPPI 800 interconnect in support of the burn code milepost.

VIEWS:

- Deploy state of the art Data and Visualization Corridors that provide high-resolution powerwall displays (5 million pixels or larger) in shared laboratory environments and high bandwidth data and visualization services in designer offices.
- Deploy, support and enhance common visualization tools (CEI/Ensight, IBM Data Explorer, AVS/Express, MeshTV) as appropriate.
- Develop, deploy and support scalable visualization and rendering tools that allow high performance interaction with extremely large ASCI data sets.
- Develop and deploy a common data model and file format for ASCI scientific data that allows interchange of data between code teams and between laboratories.
- Develop and deploy meta-data management tools that allow weapons designers to create, edit and search meta-data describing created ASCI data sets.

VU-2.1 FY02 Q4
64 M pixel display driven by a scalable rendering system

This major milestone focuses on delivery of technology in two of the critical areas in the ASCI/VIEWS program that are needed to enable effective "seeing and understanding" of ASCI data, namely:

- High resolution displays – As ASCI simulations take on higher and higher fidelity, it is equally important to provide visual display systems that are well-matched to that fidelity. Large numbers of pixels are needed to maximize the visual bandwidth to the human brain, with the ideal being at full visual acuity (i.e., pixel resolution that matches the maximum resolution perceivable by the human brain). This display quality is needed to ensure that intricacies in a data-visualization are not artificially cloaked by display limitations. This is particularly important as the complexity of systems being simulated rises, in turn complicating the exploration process of discovering information in the simulation data.
- Scalable Rendering – The demands of ASCI simulations cannot be met without the massively parallel computational capabilities that are being deployed for ASCI. The ability to meet computational requirements is heavily reliant on the use of scalable computation technologies. While parallelism is being used at modest levels in today's highest performance graphics systems, the delivered performance fails to provide desired levels of interactivity, even with today's ASCI data sets. ASCI visualization requirements have been identified that project a need for one thousand times the performance of the highest-performing, hardware-accelerated graphics pipeline in the year 2004. Cost-effective technologies that scale for rendering, as well as computation, must be developed if such requirements are to be met.

The milestone will be met when a 64 Mpixel display, driven by a scalable rendering system, is demonstrated against data from one or more tri-lab weapons applications.

64 Mpixel display

This display resolution is consistent with the 8K x 8K resolution identified on the ASCI Visualization Curve for the year 2002. This effective resolution will be achieved via the integration of multiple displays, each of which is likely to have a pixel resolution in the range of 4 – 10 Mpixels. The ASCI tri-labs are working with industry to deliver high-resolution, single displays, as well as with industry, academic (including Princeton and the University of Minnesota) and other research partners to develop scalable display technologies that use multiple displays. Note that the targeted display quality is desired for office environments as well as larger collaboratories.

Scalable Rendering

This technology is tied to multiple requirements on the ASCI Visualization Curve in the 2001-2002 timeframe. A very high-performing, scalable rendering (both polygonal-surface rendering and volume rendering) capability will be needed to enable “realtime interaction with a 300 GB timedump”, at “40 Hz interaction” rates, on “8K x 8K displays”. One alternative for achieving such scalability is through the use of clustered, commodity-based graphics architectures that leverage parallel use of cost-effective hardware acceleration. This investigation will be performed collaboratively by the tri-labs with academic (including Stanford and Princeton) and industrial partners. Important issues related to the effectiveness of such scalable rendering architectures will be the ability to feed data to the rendering system efficiently, using parallel data streams, together with efficient, scalable data manipulation infrastructure for extraction and/or generation of the data to be rendered (e.g., isosurface generation).

VU-4.1 FY04 Q4
Ability to do realtime analysis on a 200-TB ASCI dataset

The focus of this milepost is on delivering Data and Visualization Corridors that allow weapons designers to do realtime analysis of a 200TB ASCI simulation dataset to enable them to see and understand the simulation results. One often thinks of the storage and I/O systems of supercomputers, and the graphics workstations attached to them, as a thin pipe through which the data must be pumped. The idea of a “Corridor” is meant to suggest the opposite metaphor, a wide path through which massive quantities of data can easily flow, and through which scientists and engineers can explore data and collaborate. Thus, the Corridor is precisely the kind of infrastructure needed to fully support the ASCI “see and understand” mission.

A robust and efficient data handling system will be required that will allow a 200TB ASCI simulation dataset to be stored and accessed effectively and manipulated, compressed, filtered and subsetted down to a smaller size that can be efficiently handled by visualization and analysis tools at interactive rates. Subset operations may be in the form of one timeslice, selected variables across some set of timeslices, spatially cropped data, and sliced data (reduced dimensionality). Manipulations will include data resampling, derivations, multi-resolution processing, and geometry extraction. Based on the ASCI curves, it is expected that the data will need to be reduced to 2.0TB to allow real-time interaction.

Key technologies required to meet this milepost include:

- High bandwidth interconnects connecting the simulation platform, hierarchical storage management, data engines and visualization engines within a laboratory and between laboratories.
- A robust set of data services that enables efficient manipulation and subsetting of data for subsequent realtime analysis.
- Data discovery and multi-resolution analysis preprocessing systems that allow key user defined features of the datasets to be extracted in a compressed form.
- High performance browsing tools that allow high-speed interaction with the preprocessed compressed data and allow selection of smaller subsets for further detailed analysis.
- Detailed visualization and analysis tools that can be applied to subsets of the original uncompressed data sets.

Problem-Solving Environment

PS-1.1 FY01 Q1
Initial software development environment extended to the 10-teraOPS system

(A more detailed description of this milepost is available on request from the DOE Office of Advanced Simulation and Modeling.)

PS-5.1 FY05 Q3
Production-quality uniform user and application interfaces available on all ASCI high-end computing platforms

By Q3 FY05, PSE will deliver production quality uniform user and application interfaces on all ASCI high-end computing platforms. Included here are development tool interfaces and APIs to run-time systems invoked by ASCI applications.

Development tools and run-time systems will need to support whatever platform architecture and programming model is deployed in the '05 time frame. The intent is to leverage existing technology that is being developed to support clustered SMPs with deep memory hierarchies. The extent this is possible depends on how far future architectures and programming models move from what is in use today. Specific tool requirements and solutions will firm up as this becomes known, but it is expected that future machines and programming models will not vary fundamentally from what is in use today.

It is anticipated that the Etnus/TotalView debugger will continue to evolve as the standard multi-platform parallel debugger in the ASCI program. The software path-forward Ultra-scale Tools Initiative and follow-on programs will ensure the development of needed advanced parallel debugging capabilities on all ASCI platforms. Procurement contracts will ensure cooperation from platform partners. PSE TotalView R&D will accelerate the development of advanced features and provide risk mitigation through the development of lab staff familiar with TotalView internals.

Common performance tool capabilities will emerge from PSE development of portable performance tools based on a common parallel tool development infrastructure. PSE R&D initiated in FY00 will continue to provide scalable portable performance tool capabilities for the ASCI program. The common infrastructure strategy leverages performance tool work done by alliance partners and platform vendors to establish a common base for the development of portable performance tools.

PSE, path-forward, and alliance research efforts will be directed toward the creation of a common integrated development tool and run-time environment where, for example, the performance tool extracts low level performance information from the run-time system given knowledge of internals, or the compiler generates detailed symbol table information required by the debugger. We hope to extend the Ultra-scale Tools Initiative to include run-time and performance tool technologies as a driver to moves third party ISVs toward an integrated solution in collaboration with PSE and alliance R&D.

PSE, working in partnership with platform partners and third party ISV's, will continue to provide and support common parallel programming models and languages. It is expected that Fortran and C++ will continue to evolve and be the base programming languages. PSE will participate in standards effort (such as the current OpenMP) to ensure programming languages and parallel extensions continue to meet ASCI needs. It is expected that MPI will continue to be the standard message-passing interface and a scalable/high-performance implementation will be made available on all platforms. A common API to lightweight, high performance thread packages will be deployed allowing mixed message passing/thread programs. Common object-oriented development and run-time frameworks such as POOMA, Sierra and their follow-ons will be deployed on all platforms.

Equation solver interface (ESI)-compliant high-performance scalable linear and non-linear solvers will be developed and deployed on all ASCI platforms providing a common API to ASCI applications.

DisCom^2

DC-1.1 FY01 Q2
Distance computing environment available for use on the 10-teraOPS ASCI system

The Distance Computing element of DISCOM2 extends the functionality and capability of ASCI resources to remote users. The environment will integrate the user environment components with secure, reliable, parallel data communications to meet the bandwidth requirements to provide 10 TOPS of remote computational capabilities.

Based on an analysis of the ASCI applications, 10 Gigabits/Second of network bandwidth will be made available to utilize 10 TOPS of computational resources. The requisite NSA approved type 1will be made available. The filters and gateways that limit the effective bandwidth between the ASCI resources will be eliminated in accordance with an approved DOE security plan.

The DISCOM2 project has developed several data movement applications that can effectively utilize a parallel network. These applications are based on the standard tools that users are currently utilizing. (e.g. HPSS, SCP, FTP) Initial implementations of these applications are available today. Production releases of these applications will be delivered by Q2 FY01.

There will be significant additional support requirements for both the remote user environment and the distance bandwidth. All of these areas will be in production operation by Q2 FY01.

The DisCom will synchronize the features within the distance computing environment to provide new capability in a stable environment to the user community. The environment addresses the user needs in the areas of problem setup, compilation, execution, visualization, as well as the I/O required. A system design activity will provide the interface for the DisCom projects, operational & support projects, as well as other ASCI projects to provide the communication necessary for a tri-lab integrated release. For example, the synchronization will ensure that the parallel file I/O capability/feature and the parallel network capability/feature will be integrated appropriately for the user needs in the areas specified above.

DC-3.1 FY03 Q4
Complex-wide infrastructure that integrates all ASCI resources

By Q4 FY03, DisCom2 will develop and deploy infrastructure that integrates all of the ASCI computing resources into a flexible and adaptable distributed computing environment. The system will support a wide spectrum of the high-end modeling and simulation needs for design, analysis, manufacturing, and certification of nuclear weapons. The computing system spans high-end applications, resource management, ultra-computers, parallel wide-area and system-area networks, capacity clusters, visualization, and data services required by weapons simulations.

Meeting this milestone requires:

- Deployment of a secure production high-performance parallel wide-area network that interconnects the system-area networks in the machine rooms of the laboratories.
- Deployment of a robust distributed resource management system that brokers all of the required computing services.
- Deployment and integration of capacity clusters that complement the ultra-computers by providing simulation, visualization, and data services.
- An integrated approach to configuring the environments and to managing the allocation of the system's resources.

Each of these elements is described below.

By Q4 FY03, a wide-area parallel network will be deployed with over 30 Giga-bit-per-second aggregate bandwidth among the three laboratories. This bandwidth will be aggregated from multiple lower bandwidth channels running in parallel. The parallel network architecture is composed of multiple simultaneous channels in parallel, low-cost high-performance network interface cards, OS bypass mechanisms, and wave division multiplexing in the wide area. Interim milestones in DisCom2 provide for the development and integration of these capabilities into a manageable network that extends the high-end secure system-area networks for the ASCI machines across the wide area.

By Q4 FY03, a distributed resource management (DRM) will be deployed among the three laboratories that simplifies the way users interact with simulation and supporting resources. DRM will provide the resource management infrastructure complex-wide for the discovery, reservation, allocation, monitoring, and control of geographically distributed resources. The resources comprising the complex-wide secure intranet include heterogeneous computing, communication, storage, visualization, data, and software resources. Users must receive consistent, fair, and responsive access to resources regardless of location. DRM must achieve high utilization of all resources. This service may be limited due to enhanced security requirements and new policy limitations.

By Q4 FY03, a robust and broad set of simulation services will be deployed in commodity clusters. Clusters at both Sandia sites will be tightly integrated together and have an aggregate computing capacity of over 3000 nodes. Commodity web and computing technologies will be configured to utilize the clusters to provide integration of many product and process design tools. This will enable delivering the capabilities of the interconnected design tools and data to the designer's desktops in both classified and unclassified network environments. Bringing together simulation, product design data, and computational services will help to reduce product cycle time, cost, and defects. Collectively, these resources provide an “information and simulation nuclear weapons complex intranet”.

By Q4 FY03, DisCom2 will coordinate an integrated approach to configuration management and system allocation. At a minimum, the features supported by the system will be documented to provide understanding to the user community of what is available and additionally will provide a mechanism for reporting and tracking bugs. A tri-lab configuration management process will be coordinated to ensure technical integration of the resources.

Physical Infrastructure and Platforms

PP-0.1 FY00 Q3
10-teraOPS (Option White) final system delivery and checkout

The Option White MuSST SMP cluster (multiple sustained stewardship teraOPS, symmetric multi-processor) cluster forms the third major step along the ASCI Platforms curve. Developed by IBM and being sited at Lawrence Livermore, the MuSST PERF system will enjoy in excess of 10.2 teraOPS of computing capability, 4.0 TB of memory and 150 TB global disk to the ASCI program classified ultra-scale code development and programmatic activities.

Installation of Option White will proceed in a phased manner for both hardware and software. During the second quarter of FY00, the vendor will demonstrate the operation of the MuSST system, with 4.0 TB of SDRAM memory, meeting the requirements with a laboratory supplied benchmark. The demonstration milepost represents an early exhibition of system capability. In the following quarter, checkout and testing will occur using compact applications run in parallel on the entire system, and the system will be exercised with selected nuclear weapons application(s) and selected verification problem(s).

PP-2.1 FY02 Q1
30-teraOPS final system delivery and checkout

The delivery and installation of the 30-teraOPS system to Los Alamos National Laboratory is the fourth important milestone in the implementation of ASCI’s platform strategy. The 30-teraOPS system will be delivered and installed at Los Alamos during the first quarter of FY02. Once installed, the system will be tested and demonstrated in two important ways.

First, a set of compact applications will be run in parallel on the entire installed system. This initial test will serve as a test of the operational status of the full system.

Second, the system will be exercised with selected nuclear weapons application(s) and selected verification problem(s). These tests will serve as an initial check of system functionality.

It should be noted that this milepost assumes a specific contract delivery date and corresponding peak performance rate. Options exist for later delivery with corresponding higher performance. If one of these options is selected, the specifics of this milepost will be modified.

PP4.1 FY04 Q3
100-teraOPS final system delivery and checkout

The delivery and installation of the 100-teraOPS system by FY04 is the milestone that completes the ASCI platform goal of implementing a 100+teraOPS computing platform. Once installed, the system will be tested and demonstrated in two important ways.

First, a set of compact applications will be run in parallel on the entire installed system. This initial test will serve as a test of the operational status of the full system.

Second, the system will be exercised with selected nuclear weapons application(s) and selected verification problem(s). These tests will serve as an initial check of system functionality.

It should be noted that this milepost assumes a specific contract delivery date and corresponding peak performance rate. System delivery dates are expected to differ between various potential vendor partners, depending on the individual vendor's business plans. The performance and delivery dates noted here is a nominal strategy. Exact dates and performance values will be obtained in the procurement process, and later deliveries are anticipated to result in higher performance numbers.

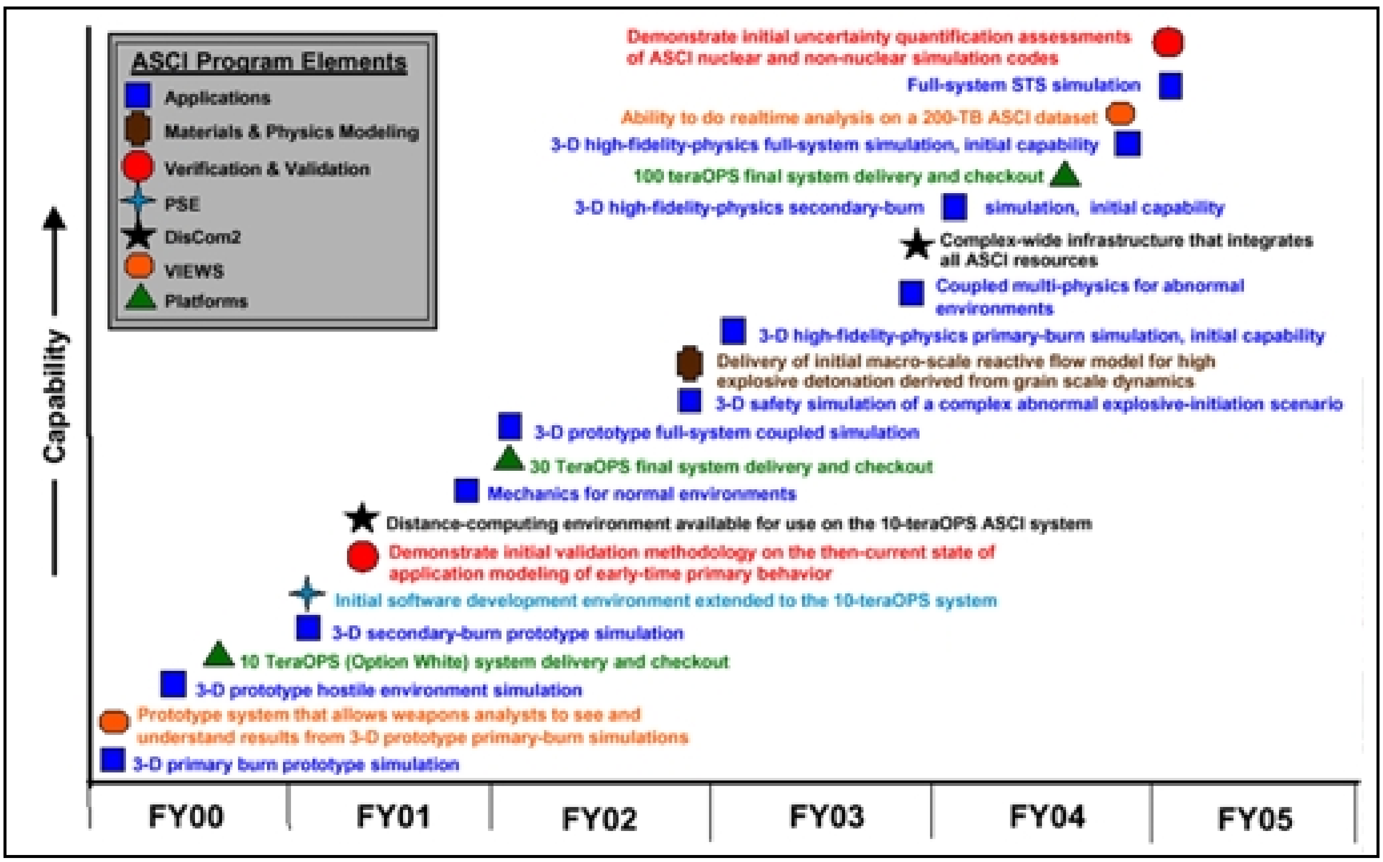

Figure A1. ASCI mileposts in the FY2000-2005 timeframe.