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ADVANCED SIMULATION AND COMPUTING (ASCI) PROGRAM PLAN

2002-2003



U.S. Department of Energy National Nuclear Security Administration Defense Programs

Lawrence Livermore National Laboratory Los Alamos National Laboratory Sandia National Laboratories



On the cover: Sandia National Laboratories' arming, fuzing, and firing assembly (AF&F) is depicted in various stages of increased model fidelity. Over the past decade, an explosion of computer hardware and software technologies has increased the sophistication of structural dynamics modeling.

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Advanced Simulation and Computing PROGRAM PLAN 2002-2003



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E X E C U T I V E S U M M A R Y

Our nation's nuclear deterrent was historically a product of weapons physics, experimental science, and computation. The regularity of nuclear test experiments did not require a strong reliance on the understanding of the wide variety of physical processes involved. Consequently, 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 judgment, weapons scientists and engineers have a greater reliance on computers to simulate the aging process and its impact on our weapon systems, along with the impact of any required modifications.

The Advanced Simulation and Computing program (which continues to retain its historical name ASCI) creates simulation capabilities through the development of advanced weapons codes and high-performance computing that incorporate high-fidelity scientific models validated against experimental results, past tests, and theory. The goal is to meet the science-based simulation requirements of the Stockpile Stewardship Program (SSP), which encompasses all National Nuclear Security Administration (NNSA) efforts to meet its nuclear weapons responsibilities. This includes the means to assess and certify the safety, performance, and reliability of nuclear weapons.

At the dedication of ASCI's Strategic Computing Complex in May 2002, former NNSA Administrator General John Gordon remarked that a predictive capability through Stockpile Stewardship depends strongly on "first principles science and highresolution calculations that only these supercomputers

can provide."

The ASCI program is actively addressing stockpile issues, developing and using simulations to study problems ranging from advanced design and manufacturing processes, to understanding accident scenarios, to weapons aging and the resolution of Significant Finding Investigations (SFI). The diversity of the needs requires a balanced system of hardware, software, and computer science solutions. The 100-teraOPS platform, which has historically been the desired entry-level system to support realistic three-dimensional, high-fidelity weapon simulation and visualization, is now close at hand. Computer platforms beyond this scale, essential to support SSP activities, are planned.

In the past year, the ASCI program has spent significant effort reassessing and redefining the major milestones, in collaboration with weapons designers, the Directed Stockpile Work community, and with the Science Campaigns. Major accomplishments have ranged from the installation of new platforms and their

subsequent use for the first prototype three-dimensional full-system weapons simulations, to the resolution of SFIs and the redesign of weapons components because of changes in mission requirements. This plan updates the program planning for FY2002 through FY2007, and includes a discussion of the Level 1 milestones. Our programmatic approach involves the coordinated use of multiple management structures—the staff at ASCI Headquarters, the Tri-Lab Executive Committee, and subject-area teams staffed from the three NNSA national laboratories. The plan is organized around major program elements and the strategies employed within those elements to achieve ASCI's objectives. As ASCI has matured, the program elements have been restructured to reflect the changes in the current technological environment and in the challenges we face.



ASCI scientists worked closely with the production complex on the W87 Life Extension Program (LEP). The W87 LEP produced the first U. S. warhead with a modified physics package in the past seven years. Close interaction between ASCI engineers and production plants has been essential to the success of this program.

OVERVIEW

OVERVIEW

On October 2, 1992, underground nuclear testing ceased by Presidential decree. Until that moment, monitoring of the nuclear weapons stockpile was achieved through (1) underground nuclear testing and (2) "modernization" (i.e., through development of new weapon systems). Well over fifty types of nuclear weapons have undergone a full life-cycle of development, deployment, and destruction in this manner. One of the consequences of the nuclear test ban was that the safety, performance, and reliability of U.S. nuclear weapons must be ensured far beyond their original design lifetimes in a manner fundamentally different than in the past. This would involve a new emphasis on continuing assessment and certification of weapons resident in the stockpile.

In 1993, the Stockpile Stewardship Program (SSP) was established with the mission of developing the next generation

of assessment and certification tools. Overseen by the National Nuclear Security Administration (NNSA), SSP is of significant interest to the Departments of Energy and Defense, Congress, and the nation at large.

The Nuclear Posture Review was also established in 1993 to address the effects of changes in the worldwide security environment and their military implications upon the United States nuclear weapons strategy and stockpile. The final report noted that "The United States will continue to set the highest international standards of stewardship for nuclear safety and security, command and control, use control, and civilian control." ASCI is developing the tools for the SSP to accomplish its goals of safety and security.

The Advanced Simulation and Computing program evolved from the merging of the Accelerated Strategic Computing Initiative (ASCI) and the Stockpile Computing program. For historical reasons, the use of the acronym "ASCI" has continued following this programmatic merger.

ASCI's goal is to provide the means to assess and certify the safety, performance, and reliability of nuclear weapons and their components (Figure 1). The schedule for developing three-dimensional weapons simulation capabilities is integrated with the certification of refurbished, lifeextended weapon systems. The simulation and modeling tools have already made an impact on the assessment of stockpile issues,

Design **l**esting Manufacturing **Transportation/Storage Surveillance** Delivery **Countermeasures** "Button to Boom" **Initiation Yield** Dismantling Figure 1. Simulations contribute critically throughout the entire life-cycle of a nuclear weapon.

far in advance of the planned schedules. Weapon designers, scientists, and engineers now require ASCI simulation and modeling capabilities and technologies to study how weapons age in the stockpile and to assess and certify planned refurbishments of weapon-system components. By 2010, ASCI envisions two essential outcomes. First is the creation of predictive simulation capabilities necessary to support weapon systems certification and refurbishment schedules. Second is the provision of the computing environment to accomplish the science-based Stockpile Stewardship mission.

Role of ASCI in Stockpile Stewardship

ASCI is steadily progressing toward the goal of delivering predictive computer codes based on multi-scale modeling, small-scale experimental data, nuclear test data, engineering analysis, and expert judgment. Integration of all these is provided through the ASCI codes and is an essential component of the rapidly evolving certification methodology that will direct future assessment of nuclear weapons and their components.

Assessments, essential to the Directed Stockpile Work (DSW), are based on simulation and modeling. With the help of ASCI tools, assessments can have an immediate impact on DSW by applying analyses of small-scale experiments, theoretical models, and Nevada Test Site data to the Stockpile Life Extension Program (SLEP) and to Significant Finding Investigations (SFI). The significance of this impact is considerable, given the variety of weapons in the stockpile (Figure 2). ASCI is also a principal player in the evolving intellectual framework being developed by NNSA, Lawrence Livermore, Los Alamos, and Sandia National Laboratories to bring greater rigor to the certification methodology applied annually to nuclear weapons. This methodology seeks to identify and quantify the tolerances and related uncertainties associated with the time-dependent performance of nuclear systems. This systematic procedure will permit the detailed examination and evaluation of weapon component performance and the associated confidence yet to be addressed in detail by the nuclear test program. The DSW, along with SFI

analysis and resolution, provides increased assurance to the nation of the safety, reliability, and sustainability of the U.S. nuclear stockpile.

Because the weapons in the stockpile continue to age, the material properties of the nuclear and non-nuclear components also have the potential to change; thus, surveillance and refurbishment must be part of a program for a sustainable stockpile. Our understanding of past, current, and future manufacturing processes depends in considerable measure on our ability to understand and to simulate the effects of these changes. ASCI capabilities will increasingly be needed and used to model manufacturing processes for weapon components. Advanced modeling and simulation will provide the quantitative basis to modify existing processes (when necessary) and define new manufacturing processes that offer improved safety and environmental compliance. However, the program cannot rely on theory and codes alone. Confidence in the ASCI code predictions will continue to rely heavily on a robust experimental program that provides validation data for physics and materials models. By utilizing the powerful simulation capabilities of ASCI, the experimental program can improve not only the analyses of data but also the design of experiments to maximize the relevance and value of the data to our code-validation efforts. The partnership of ASCI and the experimental program provides an increased level of confidence in the design and function of weapon components and in the performance of the entire system.

UNIT	TED STATE	S Veapons st	TOCKPILE		1
ROMR	DESCRIPTION	CARRIER		MISSION	MILITARY
B61 - 3/4/10	Tactical Bomb	F-15 F-16	Los Alamos/Sandia	Air-to-Surface	Air Force
B61 - 7/11	Strategic Bomb	B-52 & B-2	Los Alamos/Sandia	Air-to-Surface	Air Force
WARHFAT	DESCRIPTION	CARRIER	LABORATORIES	MISSION	MILITARY
W62	ICBM Warhead	Minuteman III ICBM	LUNL/Sandia	Surface-to-Surface	Air Force
W78	ICBM Warhead	Minuteman III ICBM	Los Alamos/Sandia	Surface-to-Surface	Air Force
WARHEAD) DESCRIPTION	CARRIER	LABORATORIES	5 MISSION	MILITARY
W76	SLBM Warhead	C4 & D5 Missiles, Trident	Los Alamos/Sandia	Underwater-to- Surface	Νανγ
W88	SLBM Warhead	Submarines D5 Missiles, Trident Submarines	Los Alamos/Sandia	Underwater-to- Surface	Νανγ
WARHEAD) DESCRIPTION	CARRIER	LABORATORIES	MISSION	MILITARY
W87	ICBM Warhead	Peacekeeper ICBM	LLNL/Sandia	Surface-to-Surface	Air Force
BOMB	DESCRIPTION	CARRIER	LABORATORIES	MISSION	MILITARY
B83 - 0/1	Strategit Bomb	B-52 & B-2	LLNL/Sandia	Air-to-Surface	Air Force
BOMB	DESCRIPTION	CARRIE <u>R</u>	LABORATORIES	MISSION	MILITARY
W80 - 0	TLAM - N	Attack Submarine	Los Alamos/Sandia	Underwater-to- Surface	Νανγ
W80 - 1	ALCM/ACM	B-52	Los Alamos/Sandia	Air-to-Surface	Air Force

Figure 2. The Stockpile Stewardship challenge is to maintain stockpile confidence as changes occur.

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Relationship of ASCI to Directed Stockpile Work

Continual collaboration between ASCI developers and DSW users of simulation tools is a major strength of the SSP. Joint efforts in software development, code validation and verification, and tool suite application all are good examples.

Software Development

ASCI code project priorities are guided and coordinated with designers via specific tasks and schedules to meet DSW requirements and thereby accommodate weapon systems' modifications as part of SLEPs.

Code Verification and Validation

The verification and validation (V&V) of ASCI codes is conducted by ASCI and DSW as part of the formal Stockpile Stewardship V&V process. Experiments designed to address specific weapons issues are used to validate codes. Codes are also verified against idealized scenarios whose solutions are known.

Tool Suite Application

Weapons designers use the ASCI simulation and modeling tool suite to assess unresolved surveillance SFIs by using three-dimensional simulations and new numerical techniques in the ASCI simulation codes previously unavailable. These capabilities are vital to SLEP activities because they provide simulation and modeling tools needed to certify the performance, safety, and reliability of aging or refurbished nuclear weapons. There are many examples of these activities:

 Los Alamos and Lawrence Livermore National Laboratories are using the ASCI tools and technologies to address physics and engineering issues associated with the W88, W76, B61, and W80 devices.

- Sandia National Laboratories was able to reduce the number of developmental tests in a stockpile-engineering product because of the high confidence in validated ASCI simulations. This reduction in development tests allowed an acceleration of the development schedule and an improved allocation of existing resources.
- ASCI simulations and tools are being used to refine and optimize the casting and manufacturing processes. As a result of collaborative efforts with manufacturing experts and a strong V&V process, increased confidence in the casting simulations has resulted in improved mold designs and manufacturing processes.

Coordination between ASCI and DSW is a significant part of the execution of redesign studies during which modifications are made to a system, and models must be incorporated into the codes that account for changing parameters or system specifications.

Simulations are also needed to model previous manufacturing processes for weapon components and to define new, cost-effective, safe, and environmentally compliant manufacturing processes that will allow consistent nuclear weapon performance, safety, and reliability in the future.

The relationship maintained between ASCI and the DSW programs provides the means by which the simulation tools and requirements may be matched to meet the needs of the stockpile assessment program.



Relationship of ASCI to the Defense Programs' Science Campaigns

The development of predictive capabilities relies on a strong experimental program to support the assessment of stockpile issues and provide materials and physics data needed to validate new scientific models and theories being incorporated into the simulation codes. ASCI maintains a close relationship with the Defense Programs' Science Campaigns.

The Defense Programs' Science Campaigns provide the science development, testing, and experiments needed to manage the nuclear weapons stockpile. In the previous era of test-based confidence, this program provided direct answers about the performance, safety, and reliability of the stockpile. In the current era, the focus has shifted to a computation-based confidence, which requires a close connection between ASCI and the Defense Programs' Science Campaigns.

Using Stockpile Stewardship facilities such as the National Ignition Facility (NIF) at Lawrence Livermore, the Dual Axis Radiographic Hydrodynamic Testing (DARHT) Facility at Los Alamos, and the Microsystems and Engineering Sciences Applications (MESA) Facility at Sandia, the Science Campaigns accumulate vast quantities of physics data. These experimental data provide ASCI with the understanding necessary to improve physics models used to better characterize weapons' performance and aging.

ASCI Coordination with the DOE Office of Science

Certain technical problems that arise in terascale computing are generic to scientific simulation and apply equally to other applications within the NNSA and Office of Science. This includes the management of large scientific data sets, the analysis and visualization of petabyte data sets, the operating systems for high-performance computing, and mathematical algorithms and software for solving complex problems. While there are significant differences in the detailed nature of the problems being addressed, there is still much to be gained by exploiting the natural synergy between the high-performance computing program within the Office of Science and ASCI. Both programs are collaborating to identify areas of common interest and to establish appropriate coordination of efforts.

The ASCI Strategy

The overall ASCI strategy is made up of five components that are also individual divisions in its organizational structure. The first is Defense Applications and Modeling (DAM), which develops applications necessary to achieve the ASCI goal mentioned in the Overview. The second is Integrated Computer Systems (ICS), which provides the computing platforms and centers necessary to achieve the ASCI goal. The third is Simulation and Computer Science (S&CS), which provides the infrastructure necessary to connect the applications and platforms into an integrated system capable of achieving the ASCI goal. The fourth component, University Partnerships, supports the first three strategic divisions. The fifth component provides overall program integration.

ASCI funding is allocated to cover a mix of people, hardware, and contract costs incurred by the ASCI divisions. In Figure 3, the current distribution for the program is shown. Roughly 70% supports people, the scientific foundation of the program. While the platforms receive much of the media attention, these major procurements make up only a portion of the 22% currently devoted to hardware.



Figure 3. Nearly 70% of the ASCI investment is in people and intellectual capital.



DAM Strategy

The DAM strategy for ASCI has been to transform a two-dimensional simulation paradigm into one that is fully three dimensional. This paradigm shift incorporates improved physics-model-based codes that are formally verified and validated.

ICS Strategy

In order to accommodate the paradigm shift taking place through the DAM strategy, ICS acquires powerful ASCI platforms in partnership with U.S. industry and operates computing centers necessary to run the codes.

S&CS Strategy

The S&CS strategy is developing the infrastructure necessary to utilize the new codes and systems provided by DAM and ICS. This strategy requires creating tools and environments that bring together DAM and ICS.

The progress of the three strategies, along with the support of University Partnerships and Program Integration, may be seen illustrated in Figure 4 with the W76 Arming, Fuzing and Firing subsystem (AF&F). The degree of detail with which one can model the AF&F has increased dramatically from codes, computers, and environments circa 1980s to those of today. The higher resolution and fidelity allow much more realistic simulations of the behavior of the system under various conditions that would otherwise not be possible. Ever-improving fidelity of the codes, validated against experimental data, provides increasingly realistic tools to address the need of the SSP.



Figure 4. The immediate benefit of increasing computer speed is the ability to develop more realistic simulations of weapon systems. The study of the W76 AF&F is shown above with the resolution enabled by the best computers available at the time. The current simulations on ASCI White (right) afford more than one hundred times the resolution than those at the time of the test ban. With the ever-increasing fidelity comes a much greater predictive ability of the behavior of the system under different scenarios, which could otherwise not be addressed.

The ASCI strategy is implemented within a tri-lab-based framework that enables the program to systematically plan, implement, monitor, and evaluate the most desirable integrated course needed to address the simulation needs. Given the changes in requirements, the tri-lab framework provides the environment to meet the increasing role and requirements of simulation and computing in stockpile stewardship.

Restoring the Weapons Program Computational Capability

Computers and computer simulation have always provided an important tool set for nuclear weapons research. The history of supercomputer purchases at the NNSA national laboratories for the past two decades is shown in Figure 5. Platform procurements in the 1980s were erratic. After a policy decision in 1990 that ended new



Figure 5. The history of computer hardware purchases at the NNSA national laboratories from 1982 through 2001 is shown in constant dollars and 2001 dollars. The trend of the 1990s was reversed with the emergence of the ASCI program in 1995. After the test ban, simulations have replaced underground testing, and the need for a sustained simulation effort has become of central importance to the SSP.



weapons design work, there was a period of very low platform expenditures. Following the 1992 test ban, an alternative to testing was needed; simulation was deemed integral and new platform procurements followed. ASCI's tri-lab strategy directs a carefully planned platform procurement schedule that is part of the Integrated Computing Systems strategy. This plan is carefully evaluated and approved by the tri-lab program. This process has led to a more consistent and methodical platform procurement profile than existed in the past. The resulting benefits of a planned procurement schedule have yielded tremendous performance to the SSP. Building on the heritage of ASCI's Red, Blue Pacific, Blue Mountain, and White, Los Alamos continues to receive delivery of Q hardware, and Sandia and Lawrence Livermore have made progress in procuring ASCI's next-generations of platforms, Red Storm and Purple.

ACCOMPLISHMENTS







Zapotec is a code developed at Sandia National Laboratories to couple complex structural and continuum dynamics phenomena. Events that can benefit from this type of simulation tool include material penetration, blast interactions with structures, and certain manufacturing processes. The sequence of six pictures shows the ability obtained through Zapotec calculations to simulate penetration of complex geologic targets required for predicting earth penetrator weapon performance at realistic target sites.

ACCOMPLISHMENTS

In the first five years since its inception, the ASCI program has improved physics models and algorithms, developed terascale computing platforms, and enhanced visualization with the high-speed infrastructure necessary to support such a program. The following sections outline the program's principal accomplishments for 2001 as evidenced in their meeting of scheduled Level 1 milestones—the highest programmatic yardsticks. Many of these accomplishments are results of collaborative (tri-lab) efforts among the three NNSA national laboratories: Lawrence Livermore, Los Alamos, and Sandia National Laboratories.

Defense Applications and Modeling

In their 2001 Level 1 milestone, Los Alamos and Lawrence Livermore demonstrated a proof-of-principle capability for three-dimensional, full-system studies of weapons systems. These high-quality prototype simulations shed new light on the complex coupled dynamics of weapons, producing relevant information for comparison with nuclear test data, including the primary and secondary yields. These calculations show that it is possible to simulate an entire explosion, both primary and secondary, in three dimensions with a single computational code.

The calculations were conducted on the 12 teraOPS ASCI White computer at Lawrence Livermore. The Los Alamos code team utilized the secure Distance Computing and Communication (DisCom) link and network to connect both sites. The Lawrence Livermore calculations took approximately 40 days and ran on more than 1000 processors of ASCI White. Additional calculations were performed to explore parallel scaling efficiency using up to 4000 processors and to study related physics issues relevant to stockpile applications. The ASCI Burn Code review panel met in January 2002 and declared the milestone successfully completed. Both laboratories finished well ahead of schedule.

In September 2001, Sandia National Laboratories successfully completed its Stockpile-to-Target Sequence Normal Environment Prototype Simulation Level 1 Milestone. This was a demonstration of ASCI software designed for evaluating key three-dimensional mechanical responses of a re-entry vehicle system to normal flight environments. This initial simulation included three-dimensional weapon geometries with limited mechanics and physics. The focus was on re-entry vehicle launch structural dynamics, separation shock, re-entry random vibration, shock physics, and electromechanical response at contact. This simulation was conducted on ASCI White and utilized approximately 2000 processors for 90 days.

In July 2001, Lawrence Livermore reached the goals of its Level 1 milestone for verifying and validating early-time primary behavior. This milestone demonstrated the current methodology used to assess how well ASCI code capabilities are validated for modeling early primary behavior. It included comparisons of code results with a set of verification test problems that have analytic solutions, as well as with a set of experimental validation data relevant to our current stockpile weapon systems. At that time, these codes had not yet incorporated many of the advanced physics or materials models being developed in the Materials and Physics Modeling program. The quality of code results was quantified by metrics reflecting current design and analysis standards for Legacy codes. The verification tests and results were very thorough and will be featured in the larger picture of primary certification. We now have a useful threedimensional, early primary analysis capability, verified and validated to a quantified degree that can now be credibly applied to our DSW. As ASCI moves into its capability delivery phase, these Verification & Validation (V&V) activities and milestones will become increasingly frequent as a demonstration of the credibility of the simulation products being developed. Figure 6 illustrates how verification can be used to test code capabilities.

In June of 2001, Lawrence Livermore completed the CY00 Three-dimensional Prototype Secondary Burn Simulation Level 1 Milestone, originally due December 31, 2000. The ASCI Burn Code Review Panel determined that this calculation met or exceeded the requirements of the milestone. The simulation used 1504 processors of ASCI White and took nearly 50 days of execution time spread over 73 calendar days. The three-dimensional calculation of the performance of a device secondary in an underground nuclear explosion provided information that compared favorably with nuclear test data.

Additional accomplishments in programs for material science, engineering, and physics modeling continue to improve our understanding of the overall science, design, and diagnostics of weapons. Below are some examples:

- Engineering analysis of the W76 forward mount is shown in Figure 7. Both uncertainty quantification and model validation are done to understand the dynamics of complex mechanical interfaces.
- Radiography is an important diagnostic since it provides images of the interior of dynamic events. A self-consistent simulation capability to generate and analyze synthetic radiographs of dynamically evolving objects has been demonstrated. This tool can be applied to data in Los Alamos' Dual Axis Radiographic Hydrodynamic Test Facility (DARHT-II) four-pulse format. In addition, a new mathematical framework to reconstruct and restore radiographic images of three-dimensional graphics objects has been completed. This new technique works with both noiseless and noisy data.



Figure 6. Comparing simulations to transport models whose solutions are known allows verification as well as an analysis of mesh refinement. In this example with the Noh problem, a shock wave is illustrated (long dashes) by the higher density inside the 0.2-cm wave front and a low density outside. One can see that increasing the resolution by decreasing the grid spacing, Δx , demonstrates convergence of the numerical results to the exact solution.





Figure 7. Model validation and uncertainty quantification for simulating dynamics of complex mechanical interfaces. The W76 forward mount (a) is modeled in detail (b) and then subjected to impulse loading (c). Regions of high stress appear in red. By analyzing experimental data and assessing model responses over a wide range of simulated events, developers refine and validate the model.

- A new void flow model has been developed within the Los Alamos ASCI Telluride project that allows simulation of the filling portion of its die-casting process. The Telluride project also completed porting its code base and capabilities to the initial Compaq system in advance of the ASCI Q installation. This is the first major project to complete such a port. The verification and validation of a mold-filling process is shown in Figure 8.
- Grain-scale simulations on ASCI Blue-Pacific revealed a crucial role of defects in plastic-bonded high explosives (HMX). The cube shown in Figure 9 is 100 micrometers on a side and contains colored grains of HMX and a yellow binder. The high resolution accurately represents the behavior of the small particles. In addition, improvements to the equations-of-state used for the explosive products and improvements to the chemical reaction kinetics models more accurately describe the first, energy-absorbing step in HMX decomposition.



Figure 8. Sigma foundry transparent molds are used to validate the Telluride Mold-Filling code. A

simple Plexiglas box with various injection ports is filled and monitored with high-speed digital video. Two fluid systems are tested—top row: water and air, with a high density ratio and energetic flow with negligible surface tension effects; and bottom row: gallium and water, with a low density ratio, laminar flow with high surface tension effects.



Figure 9. Grain-scale model of high explosives. (a) The individual grains are identified. (b) The voids between the grains are shown. (c) A shock wave propagates through the high explosive, igniting the voids. (d) A model of LX04 high explosive requires a bimodal grain-size distribution.

Some additional results include the development of a chemistry-based, subgrid model for decomposition rates of foams in fire environments. Sub-grid models incorporate the important physical behaviors that occur at much finer resolutions than currently realizable on the ASCI platforms. Grain-scale models including manufacturing voids for shock propagation in lead zirconate titanate (PZT) used in weapon firing sets have also been realized. The program has also developed a new model for spall fracture of metals that will improve our predictive capability for dynamic failure. Material properties of ductile systems can be studied at the atomic scale. In Figure 10, a one-billion atom simulation of copper is shown as it is being pulled apart. This simulation was performed at Lawrence Livermore on ASCI White.



Figure 10. Atomic-scale damage to a block of copper being pulled apart. The block is represented by its outer surfaces. The green sites inside identify locations in the copper that are damaged at the atomic scale. As the block is pulled apart, the damage proliferates. This damage modifies the structural properties of the material. The simulation is a one-billion-atom molecular dynamics simulation performed on ASCI White.

Simulation and Computer Science

To fully utilize the benefits of the advanced computational platforms, a multitude of new infrastructure capabilities are required. The achievements of the Simulation and Computer Science program, which address this issue, focus on obtaining maximum use of our systems.

Problem Solving Environments

In March 2001, the tri-lab Problem Solving Environment (PSE) program met a Level 1 milestone for the extension of initial software development environment on ASCI White. This environment consisted of compilers, libraries, middleware, debuggers, input/output subsystem, and runtime system support. The



extension made ASCI White available and usable for tri-lab code developers, designers, and analysts. The tri-lab PSE team resolved compiler problems, tested new development tools, dealt with machine access issues, verified the reliability and usability of input/output (I/O) and archival systems, and ensured that application codes and tools could function at scale. The ability to generate and run the selected codes was fully demonstrated on ASCI White.

More recently, ASCI applications codes from all three NNSA national laboratories successfully used ASCI White's development and execution environment to complete their 2001 milestones. Some highlights in three areas include:

Security infrastructure

To enable greater access to an integrated tri-lab environment, PSE provided a new, common tri-lab security infrastructure with cross-site authentication and a distributed file system. Additional security efforts enhanced the login utilities on ASCI platforms to support use of one-time passwords.

Application development environment PSE improved and delivered new tools for developing and executing highly scalable applications, including an interactive scalable debugger, high-performance message passing interface (MPI) implementations, and high-performance solver libraries. Moreover, PSE further explored the potential of terascale computing by developing new tools and techniques to analyze the performance of ASCI applications and detect unsafe or incorrect use of parallel communication libraries.

Execution environment

PSE delivered a dramatic improvement in I/O throughput and stability on ASCI White (multiple gigabytes per second data rates) by thorough testing and optimization of file system behavior. Data rates to archival mass storage from ASCI White reached hundreds of megabytes per second, an order of magnitude improvement. Recently released high performance storage system (HPSS) software has increased delivered bandwidth among the three NNSA national laboratories, supporting new high-end tape technologies, and automating tape volume recovery. New releases in 2001 of the resource management software used on ASCI White and other Lawrence Livermore platforms now support automated job pre-emption for rapid job initiation, improved fault tolerance, memory load monitoring and prediction, and real-time resource limits per user.

The Telluride project has developed an innovative algorithm for solving linear and nonlinear sets of equations. These equations describe physical models for fluid flow, phase change, heat transfer, and thermomechanical material response. This speedup was needed because 80 to 90% of the software execution time was being spent in the solution algorithm. With the addition of a new two-level preconditioning scheme, selected applications are now two to ten times faster.

DisCom

Also in March 2001, the tri-lab DisCom program successfully met a Level 1 ASCI milestone by delivering an essential distance-computing environment for use on ASCI White. The DisCom milestone demonstrated the availability of secure, reliable, parallel data communications to satisfy the bandwidth requirements needed to remotely access ASCI White. The demonstration, conducted at Sandia New Mexico, represented a first step towards establishing an integrated ASCI computing environment. Associated achievements included the development of ASCI White remote user support, first deployment of a secure ultra-high-speed (2.4 gigabits per second) wide-area network needed for remote use of the White machine by Los Alamos and Sandia users, and new user grid services including a robust security service.

VIEWS

The Visual Interactive Environment for Weapons Simulation (VIEWS) program element develops and deploys end-to-end scientific data exploration toolsets aimed to allow uniform, distributed data access, management and interactive visualization by all ASCI users.

Visualization

Much of the visualization for milepost simulations was for the first time completed over distance with these tools in 2001. This success was the result of new client-server visualization tools integrated over the highperformance, high-bandwidth, DisCom network. These tools allow simulation data to be displayed to local and remote (Los Alamos or Sandia) desktops, multimillion, pixel-tiled displays and an immersive stereo system to meet user needs.

Data Exploration

Universal data management tools for nearly every major ASCI code, have been deployed at Los Alamos, Lawrence Livermore, and Sandia. These tools allow a user to access and manipulate datasets located on both disks and in tape archives. They include the ability to "mine" and extract relevant data from massive simulation datasets, to ensure that important results do not get lost in the enormous simulation archives.

Visualization Infrastructure

The needed shift to commodity visualization hardware has continued in VIEWS as research visualization clusters are deployed at the three NNSA national laboratories. We have demonstrated aggregate image rendering capacity on these clusters orders of magnitude faster than the current technology. Academic Alliance work continues on Open Source projects in conjunction with (commercial) PathForward contracts to harness this distributed rendering capacity in end-user applications and to enable the deployment of needed next generation commercial displays (e.g., IBM "Bertha" ultra-high-resolution display). VIEWS expanded the horizon of display technologies in 2001 and 2002 with the delivery of ultra-high-resolution flat panels, immersive 3-D displays, and a 64 megapixel tiled display for collaborative use.

At Los Alamos, the Reconfigurable Advanced Visualization Environment (RAVE) facility is now available to support user analysis of weapons simulations. Figure 11 illustrates the RAVE, which is a room 20 feet long by 10 feet wide by 10 feet high, the walls and floor of which are computer display surfaces onto which stereo simulation images are projected.

PathForward

The PathForward program continues to make significant contributions toward constructing future balanced, high-end computing (HEC) systems by scaling and integrating commercially viable building blocks, both hardware and software, to 100 teraOPS and beyond. The PathForward strategy consists of multiple partnerships with U.S. computer hardware and software companies to develop and accelerate





critical technologies and their commercialization needed to meet ASCI requirements. These goals are accomplished by funding projects in key technology areas of interconnect, visualization, storage, file system and runtime system software. Successes of the program include the Compaq Quadrics interconnect project that enabled Compag to bid for and win the ASCI Q procurement and the Sun effort on scalable system software, which allowed it to become a viable bidder on the Q procurement. Similarly, the IBM Federated switch work is expected to be offered in a platform bid in the near future. At the 19th IEEE Mass Storage Conference in April 2002, LOTS Technology demonstrated their 160 megabytes per second LaserTape drive, which reads and writes 1-terabyte cartridges. This is considered a commercial success of PathForward investment in collaboration with the National Security Agency (NSA).

On the software side, the Etnus TotalView debugger has emerged as the premiere parallel debugger in the high-performance computing industry. PathForward is funding MPI Software Technology, Inc., to provide a multivendor message passing interface (MPI) solution on the new and emerging ASCI class platforms, and KAI/Pallas to enhance the scalability and usability of performance tools. This will allow users to measure and analyze the performance of ASCI-scale applications. Users on current ASCI platforms such as White and Q systems are already benefiting from these software efforts.



Figure 11. Reconfigurable Advanced Visualization Environment (RAVE) at Los Alamos.

Integrated Computing Systems

Through collaborations with industry partners (IBM, Compaq, SGI, and Intel) ASCI has developed and fielded many of the largest computers to date.

The current flagship system is IBM's ASCI White, which is capable of more than 12 trillion operations per second (teraOPS). ASCI White covers about 12,000 square feet of floor space—an area greater than that of two NBA basketball courts—and weighs 106 tons. It contains 8192 microprocessors in 512 shared memory nodes interconnected with high-bandwidth, lowlatency interconnect, requiring over 49 miles of cable. Each node contains 16 Power3-II central processing units (CPUs) built with IBM's latest semiconductor technology (silicon-on-insulator and copper interconnects). ASCI White has 8 terabytes of main memory and 160 terabytes of storage space in about 7,000 disk drives.



Figure 12. Former NNSA Administrator General John A. Gordon tells a standingroom-only audience at Lawrence Livermore's ASCI White dedication ceremony that "the foundation of science-based Stockpile Stewardship is to ensure that the nuclear deterrent will continue to be viable in the absence of underground nuclear testing."

By summer 2001, ASCI White was fully utilized by the three NNSA national laboratories and was dedicated in August 2001 by former NNSA Administrator John Gordon (Figure 12). Throughout its first year, ASCI White consistently had full tri-lab usage in the region of 60% to 80%, which is expected for large parallel systems (Figure 13). This success reflects the joint efforts of S&CS and Ongoing Computing. In August 2001, Compaq began to deliver a 30 teraOPS supercomputer known as "Q" to Los Alamos. Initial delivery consisted of 512 fourprocessor, ES-45, Alpha-based nodes interconnected by a Quadrics Elan-3, high-performance communications fabric installed in the Central Computing Facility. By early March 2002, Compaq delivered 768 nodes to the newly constructed Strategic Computing Complex (SCC), providing an additional 6 teraOPS capability.



Figure 13. The range of 60%-80% system utilization, indicated by the color stripe in this figure, is considered to be a fully loaded system when running very large parallel applications. The bars show the sharing of ASCI White between the NNSA national laboratories, as well as the actual utilization during its first year of operation. The lower chart shows how the data archives have increased with a dramatic jump as the White system started operation in 2000. The blue region gives the yearly total while the maroon depicts the cumulative data available in the archive.



Complete system delivery is scheduled for the end of 2002, a slip of two quarters because of technical difficulties discovered on the initial delivery system. When completely installed, Los Alamos will have a 30 teraOPS supercomputer operating in the classified environment, and 2.5 teraOPS in the unclassified arena.

In June 2002, Sandia announced a partnership with Cray, Inc., to develop and deliver the new massively parallel supercomputer Red Storm. In addition to these flagship capability systems, the NNSA national laboratories continue to operate the older ASCI systems (Red, Blue Mountain, and Blue Pacific) to provide capacity production computing. There are also a number of smaller systems that provide support for unclassified research at the NNSA national laboratories as well as capacity for the ASCI Alliances Program. The largest of these systems is the 1.6 teraOPS IBM Frost system at Los Alamos.

University Partnerships: Academic Strategic Alliances Program

In Fall 2001, after reviewing the progress and accomplishments (exemplified in Figures 14–18) of the five Alliance Centers during their first four years of funding, the Alliance Strategy Team and the Tri-Lab Sponsor Team made a recommendation to the ASCI Executives to renew all Alliance Center contracts for an additional five years. This renewal completes ASCI's tenyear commitment to the Centers as envisioned at their inception. Presently, the Centers collectively have access a to as much as 10% of ASCI computers and 10% of the computing resources of the National Science Foundation's (NSF's) National Partnership for Advanced Computational Infrastructure Center at the

Computational Infrastructure Center at the University of California at San Diego. The Alliance Centers are:

- California Institute of Technology: Center for Simulating Dynamic Response of Materials,
- University of Chicago: Center for Astrophysical Thermonuclear Flashes,
- University of Illinois, Urbana-

Champaign: Center for Simulation of Advanced Rockets,

- Stanford University: Center for Integrated Turbulence Simulation, and
- University of Utah: Center for the Simulation of Accident and Fires and Explosions.



Figure 14. The images in this figure demonstrate some recent applications of the Flash code. Clockwise from upper left, these include (a) verification calculations (Orzag-Tang magnetohydrodynamic vortex), (b) validation calculations for laboratory experiments (Rayleigh-Taylor instability), (c) direct numerical simulations of microphysics (cellular nuclear detonation fronts), and (d) supernova calculations. — University of Chicago

Figure 15. Shown in this image is the propagation of a detonation wave onto a metal target that generates a shock wave in the metal target at the end of the cylinder. The calculation, generated by the Virtual Test Facility software of Caltech's ASCI Alliance Center, is noteworthy in that it couples a Eulerian fluid mechanics simulation based on Cartesian meshes and parallel adaptive mesh refinement with a fully Lagrangian solid mechanics algorithm based on tetrahedral meshes. — California Institute of Technology.

During the past year, each Alliance Center demonstrated a significant, integrated simulation in its problem area. Representative results from these demonstrations are highlighted in Figures 14–18. These demonstrations satisfy the milestone requirements established for the Alliances by the ASAP. In the process of meeting their milestones, the Centers added a number of noteworthy accomplishments to their multi-disciplinary efforts. For example: Caltech introduced new engineering models of high explosives that can be easily integrated into the numerical requirements of its virtual test facility; the University of Chicago transitioned to a new version of the FLASH code (version 2.0) and demonstrated excellent scaling on ASCI's Frost supercomputer; the Illinois Center developed an effective hierarchical strategy to couple the complex computational fluid and solid dynamics features that characterize solid rocket motor combustion; the Stanford turbomachinery and combustor modeling groups achieved major algorithmic advances enabling them to simulate the true combustor geometry of the Pratt and Whitney 6000 gas turbine engine; and the Utah team used its computational infrastructure to demonstrate the power and flexibility of the Common Component Architecture (CCA) framework (a DOE standard proposed for high-performance, inter-operable parallel scientific software).

> Figure 16. Simulation of the unsteady compressible flow in the turbine of the Pratt & Whitney 6000 engine revealed important unsteady shock-blade interactions and unsteady ingestion of the blade wakes with the downstream passage flow. — Stanford University.

Figure 17. A volume-rendered image of the temperature in the early evolution of a 10-meter-diameter heptane pool fire. The simulation used 27 million cells, and was performed at Los Alamos on ASCI Nirvana using 1000 processors for 36 hours. – University of Utah.



Because they are well founded in basic science, engineering, computer science and computational science, many of the accomplishments achieved at the Alliance Centers contribute directly to ASCI program goals. In particular, key Alliance contributions to the ASCI program include:

 Scientific collaborations with ASCI projects and personnel at the NNSA national laboratories—leading to a number of joint research publications.

> Figure 18. Cutaway section of fully coupled 3-D simulation of Titan IV Solid Rocket Motor Upgrade booster exhibits flow-induced deformation of propellant that occurred near joint slot in an experimental test firing. — University of Illinois.

- Evaluation and debugging of ASCI supercomputers—including scaling studies and new concepts useful for ASCI code development.
- Development of a healthy pipeline of well-trained graduates in multidisciplinary fields—there have been 90 graduates from the Alliance Centers to date, and twenty-eight of them plus several faculty/staff have been hired by NNSA national laboratories.



PROGRAM ELEMENTS

The ICS and S&CS program elements provide ASCI users with the essential high-performance computing environment for weapons simulations and analysis.

PROGRAM ELEMENTS

This section describes each of the five program elements, followed by the individual top-level strategies that each element is using to contribute to overall ASCI goals. The relative sizes of these program elements are illustrated in Figure 19. The high-level milestones for these program elements are listed and described in Appendix A.

Defense Applications and Modeling

This program develops and maintains all weapons codes at the NNSA national laboratories used to support Stockpile Stewardship needs, including weapon design and assessments, accident analysis, certification issues and manufacturing process studies. The development of the high-fidelity, full-systems codes requires new physics and materials models, improved algorithms, general code development, and a concerted effort in the verification of the codes and their validation against experimental data.

Advanced Applications Development

ASCI is developing the latest highperformance software applications necessary for the simulation tools for the SSP. The key to reaching SSP objectives for initial implementation in 2004 and full implementation in 2010 is in achieving milestones for ASCI's critical applications codes in the intervening years. ASCI will provide simulation tools and capabilities 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 codes; this drives 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 threedimensional capability, finer spatial resolution, and more accurate and robust physics. This will strain the limits of the algorithms used in today's simulation codes. 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. Integrated code teams 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 three-dimensional, high-fidelity physics and geometry.
- Focus on full-system, component, or scenario simulations.
- Focus on coupling of multiple highfidelity physics models (coupled multiphysics) for end-to-end simulations without empirical correlations or designer intervention.



Figure 19. ASCI's integrated development of high-fidelity, three-dimensional weapons simulations requires a diverse collection of program elements. The FY2003 budgets for these elements are shown here.

- Design and implement numerical algorithms to meet the ASCI application requirements.
- Accelerate code performance by developing computational techniques that efficiently exploit the new computer architectures.
- Focus on highest priority applications needed to support DSW.

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. The verification program will evaluate current software engineering practices for application to the ASCI-scale simulations and establish requirements for software projects. The most essential goal of the verification portion of ASCI V&V is to ensure that the models from Advanced Applications give the analytically correct answers when implemented. 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 requires systematic, rigorous V&V methodologies to obtain the level of confidence 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 S&CS activities. The link between V&V activities and the experimental program (i.e., the Campaigns) is crucial to the success of this effort.

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, and compare calculations against, experimental validation data within the SSP.
- 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 (M&PM) In the past, physical properties of materials significant to the nuclear weapons program were often inferred from integral test data. Now, without the ability to conduct such integral tests, there is a premium on the development of advanced capabilities experimental, theoretical, and computational—necessary to predict the physical properties of materials under conditions found in nuclear explosions and stockpileto-target sequences.

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 turbulence, instabilities and mix, spall, hydrodynamics, equations-of-state, and the dynamic properties of materials under conditions of high strain and high-strain rates. Physical processes involving turbulence, friction, and fracture take place at scales at which experimental measurement is difficult. A complete understanding requires knowledge of material properties and responses at vastly different length and time scales as well as the linkage across these scales.

Laboratory experiments conducted by the Defense Science Program, complemented by high-performance simulations using ASCI codes, will provide the basis for the development of predictive models and validated physical data of stockpile materials. Consequently, ultra-scale scientific computing platforms, multiphysics 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 resolved and have led to the partial resolution of longstanding 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 materials models and properties data into the ASCI codes needs to occur in conjunction with the ASCI V&V program for verifying and validating material properties data obtained through the Campaigns. This will provide DSW with the basis to ensure confidence in the performance, safety, and reliability of the stockpile without nuclear testing.

High-performance simulations linking quantum to continuum scales will lead to reliability predictions and lifetime assessment for corrosion, organic degradation, and thermal-mechanical fatigue of weapon electronic subsystems. Similarly, quantum-scale simulations and laserdriven shock compression experiments have validated the equation-of-state of hydrogen up to several megabars, providing valuable insight both into weapons performance and inertial confinement fusion.

Materials and Physics Modeling Strategies

- Determine the multiphase equation-of-state for plutonium and other relevant metals, including melting, solid-solid phase transformations, and dynamic response.
- Develop physics-based models predicting the properties of plutonium under aging due to self-irradiation.
- Develop physics-based models of highexplosives thermal and mechanical properties, including decomposition kinetics, detonation performance, properties of reaction products, and constitutive properties.
- Develop physics-based 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.



Simulation and Computer Science (S&CS)

Simulation and Computer Science develops the infrastructure necessary to make the ASCI platforms available to the users. This infrastructure includes everything from the wide area networks, which allow remote users to securely run applications, to software tools and applications tailored to the supercomputer architectures. The illustration introducing the Program Elements section describes the S&CS environment.

Problem Solving Environment (PSE)

ASCI's unprecedented code development efforts require robust computing and development environments that enable codes to be developed rapidly. Through the PSE program element, ASCI is developing a computational infrastructure to allow applications to execute efficiently on the ASCI supercomputer platforms, to perform effective input/output (I/O) and archival data transfer, and to provide accessibility from the desktops of scientists and engineers. This computational infrastructure encompasses scalable software development tools, run-time libraries, frameworks, solvers, archival storage, high-speed interconnects, scalable I/O, local area networks, distributed computing environments, security, software engineering, and software process improvement.

The DAM program is the main driver for the PSE program requirements and the primary customer for PSE products and services. At the same time, PSE provides software tools and infrastructure that enable the efficient and effective use of DAM's capabilities in support of stockpile stewardship. Thus, PSE is responsible for providing application developers and weapon scientists and engineers with the computational tools they need for the development and execution of applications on ASCI platforms. Furthermore, in collaboration with third-party and platform partners, PSE is responsible for deploying reliable system software on all ASCI platforms.

PSE Strategies

- Create a common, usable, and robust application development and execution environment for ASCI computing platforms and ASCI-scale applications, enabling code developers to quickly meet the computational needs of weapon scientists and engineers.
- Produce an end-to-end, highperformance I/O, networking and storage infrastructure encompassing ASCI platforms and operating systems, largescale simulations, and data-exploration capabilities to enable efficient ASCIscale computational analysis.
- Ensure secure, effective access to "initial delivery" and "general availability" ASCI supercomputers, as well as to other ASCI resources across the three NNSA national laboratories such that ASCI's supercomputers are fully usable for local code development and execution, while being well integrated into the tri-lab distributed computing environment.

Visual Interactive Environment for Weapons Simulation (VIEWS) VIEWS is focused on the problem of "seeing and understanding" the results of multiteraOPS weapons simulations. This involves comparing results across simulations, between simulations and experiments, and exploring and understanding the multi-terabyte simulation datasets. As mathematician R. W. Hamming (best known for his work on errordetecting and error-correcting codes) succinctly stated, "The purpose of computing is insight, not numbers."

The goal of VIEWS is the creation of an infrastructure called Data and Visualization Corridor (DVC) connecting supercomputers to ASCI users in offices and assessment theaters. The corridor is a wide path through which massive quantities of data can flow and through which users can explore data collaboratively.

The corridor concept was defined through a collaboration of weapons scientists and engineers, researchers from academia and industry, and leaders of federal agencies. The VIEWS program will implement the DVC concept within the three NNSA national laboratories.

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 key part of the VIEWS program has targeted research and development to create needed technologies for scientific collaboration, data exploration, visualization, and understanding.

Keys to progress are well-defined technology roadmaps, well-engineered architectures, and a focus on promising technologies that can have direct impacts on ASCI in a two- to four-year timeframe. Once prototype technologies exist, they need to be integrated, tested, and evaluated by users; then deployed in a reliable environment for direct, dayto-day use by ASCI users and applications.

VIEWS Strategies

- Partner with academia, industry, federal agency research and development as needed to focus and leverage technology development.
- Develop needed high-performance DVCs that allow
 - Visual exploration and interactive manipulation of massive, complex data by local and remote users in offices and assessment theaters.
 - Simulation, effective data management, data extraction, and data delivery.
 - Efficient remote and collaborative scientific data exploration.

Distance Computing and Communication (DisCom)

DisCom provides secure, ultra-high-speed remote access to ASCI supercomputers for ASCI users. Distance computing will extend the environments required to support high-end computing to all



Figure 20. The VIEWS Corridor at Sandia National Laboratories, NM, displays its first 60 megapixel image, meeting the VIEWS FY02 Level 1 Milestone.





sites. It will partner with the National Security Agency (NSA) to develop the highspeed encryptors required to interconnect the NNSA national laboratories securely. These solutions will fit seamlessly into the secure ASCI computing environment.

DisCom Strategies

- Extend the environments required to support ASCI computing to the entire Nuclear Weapons Complex.
- Develop and deploy an integrated distributed computing environment.
- Support an enterprise-wide integrated commodity supercomputing architecture for nuclear weapons stockpile stewardship.

PathForward

A key strategy for ASCI to successfully build multi-teraOPS platforms is to construct future high-end computing systems and environments by scaling commercially viable building blocks, both hardware and software. PathForward is the program designed to achieve such goals by collaborating with industry to develop key technologies necessary to accelerate the development of future generations of balanced computer systems. These collaborations develop and accelerate technologies in the vendors' current business plans, which are not necessarily available in either the time frame or the scale required by ASCI. Starting in 1998, PathForward focused on interconnect and data storage technologies, as well as systems software and tools for large-scale computing systems. These technologies were considered the most critical components in the construction of the 30-teraOPS-machine environment in

2001. In the second round of new starts, visualization and run-time system software projects were added to the PathForward portfolio in FY2001. In FY2002, three new projects in the fields of visualization, file system, and optical interconnect technologies were approved.

PathForward Strategies

- Stimulate development of commercially viable building blocks for construction of future ASCI supercomputer systems.
- Focus on opportunities that expand the capabilities, performance, availability, expertise, and products being considered within the normal business plans of the U.S. computer industry.

Open Source Activities

The ASCI program will make a strategic investment in system software that adapts quickly and carries over easily to newer platforms. ASCI will execute a software strategy that leverages Open Source-based systems for system software. We envision that this strategy will be implemented in cooperation with, and with the support of, ASCI platform vendors and the Open Source high-end computing community including other federal high-end computing user agencies (e.g., DOE Office of Science).

An Open Source strategy holds the promise of allowing the ASCI program to move quickly from older to newer platforms while retaining technical innovation, computing environments and program development tools. It will improve the ability to leverage developments from the Open Source community while enabling easier reuse of software developed to meet ASCI programmatic requirements.

Integrated Computing Systems

The platform strategy, procurement and ongoing operation of the ASCI computer systems is directed by the ICS program. Partnerships with industry ensure technology and system development.

Physical Infrastructure and Platforms The three NNSA national laboratories have always been primary customers for new state-ofthe-art, high-performance computers and computing simulation capability. Today, the most powerful computing platforms are needed to achieve the performance, simulation and virtual prototyping applications that the SSP requires. The ASCI program continues to partner with multiple U.S. computer manufacturers to accelerate the development of larger, faster computer systems and software that are required to run these Defense Programs' demanding applications. These systems are located at the three NNSA national laboratories. The largest of these systems is shared among all three laboratories while the older systems provide additional computational capacity.

As of 2002, ASCI is installing a 30-teraOPS Compaq system called ASCI Q at Los Alamos National Laboratory and is placing contracts for the next systems. In a partnership with Cray, the Red Storm system will be installed at Sandia National Laboratories in 2004. The contract for ASCI Purple in 2005 at Lawrence Livermore National Laboratory is also being placed. If ASCI receives the NNSA Five Year National Security Plan (FYNSP) budget, this will be the 100-teraOPS machine.

The ASCI platform strategy calls for the acquisition of "commodity" systems. This has typically resulted in architectures consisting of commodity processors tied together by a communication fabric via a network interface switch. In examining the prospects for future high-end systems, we have recognized that accelerating research into advanced computing architectures is important and could pay off by providing substantial leverage for future ASCI platforms. As a result, we introduced Advanced Architectures, a new program sub-element in 2001, to promote research and development efforts exploring alternative high-performance-computing architectures with implications beyond 2005. Our first, and currently only, programmatic activity in this area is our close collaboration with IBM on their Blue Gene/L architecture.

Platform Strategies

- Accelerate the acquisition of scalable commercial high-end systems.
- Develop partnerships with multiple computer companies to ensure appropriate technology and system development.
- Through Advanced Architectures, stimulate R&D efforts that explore alternative computer designs that promise dramatic improvements in performance, scalability, reliability, packaging or cost.

Ongoing Computing

The Ongoing Computing program element ensures the supply of computing resources needed to support stewardship to the NNSA national laboratories. This element is structured somewhat differently at each of the laboratories, but program-wide it is focused on the operation of each laboratory's computer centers. In general, that effort has two mission elements: (1) to provide ongoing stable production computing services to laboratory programs, and (2) to provide user support for tri-lab customers using the ASCI computational resources.



Ongoing Computing Strategies

- Operate and maintain laboratory computing centers and facilities housing the ASCI computers.
- Deploy the ASCI platforms as they are acquired and support the necessary networks and archives.
- Provide user services and help desks.

University Partnerships

Academic Strategic Alliances Program (ASAP)

The major goals of the ASAP are:

- Solve science and engineering problems of national importance through the use of large-scale, multidisciplinary modeling and simulation.
- Establish and validate large-scale modeling and simulation as viable scientific approaches essential to numerous scientific applications requiring integration across disciplines and complex simulation sequences.
- Enhance overall ASCI effort by engaging academic experts in computer science, computational mathematics, and simulations of science and engineering.
- Leverage relevant research in the academic community, including basic science, high-performance computing systems, and computational environments.
- Strengthen education and research in areas critical to the long-term success of ASCI and the Stockpile Stewardship Program.
- Strengthen ties among the NNSA national laboratories and participating U.S. universities.

Foster computational science as an academic discipline.

Historically, parts of the academic community have always had a close relationship with the three NNSA national laboratories. In fact, the University of California has managed both Los Alamos and Lawrence Livermore for many years. The inception of the ASCI program created new and critical interests in simulation science and highperformance computing that serve as a renewed bridge linking these laboratories and universities.

The success of ASCI depends on the ability to demonstrate that high-fidelity numerical simulations can be used credibly as a means of ensuring stockpile confidence. Universities also have a strong interest in improving the ability of simulations to reflect reality since such simulations have already contributed to the development and exploration of new scientific ideas. Thus, ASCI's efforts to revitalize the historic relationship between the NNSA 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 NNSA national laboratories. The need to develop an unprecedented level of simulation capability requires strategic alliances with leading research organizations. In the broadest terms, 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 along with the associated supporting technology for highperformance computer modeling and simulation. These alliances play a key role in supporting the development and credible validation of this simulation capability.

ASCI also works with the entire computing community to develop and apply commercially acceptable standards. Moreover, ASCI fosters exchange programs to bring top researchers directly into the project while allowing laboratory personnel to expand their experience base in external projects. The ASAP, in particular, is helping develop the next generation of scientists needed for ongoing and new national security programs at the NNSA national laboratories.

Strategic Alliances

Five major centers are engaged in long-term, large-scale, unclassified, integrated multidisciplinary simulation and supporting science and computational mathematics representing ASCIclass problems. The centers are finishing their first five-year funding commitment (due to end 9/30/02). And the decision has been made to renew this funding for an additional five years. Currently, these centers collectively have access to approximately 10% of the ASCI-class computing resources at the three NNSA national laboratories and 10% of the computing resources of the National Science Foundation's National Partnership for Advanced Computational Infrastructure Center at the University of California in San Diego. The centers are:

- California Institute of Technology: Center for Simulating Dynamic Response of Materials,
- Stanford University: Center for Integrated Turbulence Simulation,
- University of Chicago: Center for Astrophysical Thermonuclear Flashes,
- University of Illinois, Urbana-Champaign: Center for Simulation of Advanced Rockets,
- University of Utah: Center for Simulation of Accident and Fire Environments.

ASCI Institutes

In addition to the ASAP, ASCI's academic collaborations include the ASCI Institutes, which were initiated in FY2000. The Institutes are located at each of the three NNSA national laboratories, and their charter 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 SSP. These collaborations are conducted through a variety of mechanisms, ranging from one-day seminars to multi-month sabbaticals at the laboratories. The focus of the collaborative efforts at each of the institutes differs somewhat, depending on laboratory needs; however, they all coordinate and leverage their activities to ensure the maximum benefit to ASCI. Hiring qualified and experienced computer and computational scientists has proven to be an extremely challenging activity at the laboratories. For this reason, one of the objectives of the ASCI Institutes is to enhance the laboratories' ability to attract top-notch academicians to the SSP.

Alliances/Institutes Strategies

- Encourage strategic alliances and collaboration.
- Leverage other national initiatives.



- Collaborate with the best R&D programs of other departmental offices, other agencies, universities, and industry.
- Attract top researchers in 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 narrowly focused problems, such as fluid turbulence.
- Expose students and postdocs to career opportunities at the NNSA national laboratories.

ASCI Integration

One Program—Three Laboratories

The problems that ASCI will solve for the SSP span the activities and responsibilities of the three NNSA national laboratories. Cooperation among them 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 laboratories. ASCI will be implemented by project leaders at each of the laboratories guided by NNSA's Office of Research, Development, and Simulation through its Office of Advanced Simulation and Computing, under the Deputy Administrator for Defense Programs. The 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, threelaboratory program activity with seamless management and execution across the laboratories.
- Sponsor annual principal investigator meetings.
- Encourage collaboration on development and share hardware and software resources.
- External workshops and meetings.



ASCI FACILITIES

View from a meeting room, of the floor of the Nicholas C. Metropolis Center for Modeling and Simulation, prior to the installation of the ASCI Q platform.

ASCI FACILITIES

The unprecedented reliance put upon numerical simulation by the SSP and the resulting demands on ASCI are forcing a transformation in the way computing is viewed, employed, and advanced. Simulation environments are needed to smoothly coalesce both the generation and the assimilation of data at the terascale level. The simulations being developed by ASCI today promise a level of physical and numerical accuracy that will provide a credible substitute for largescale experiments. To this end, four unique new facilities are planned to create the simulation environments that will go beyond traditional computer centers.

Strategic Computing Complex (SCC)



Figure 21. The new Strategic Computing Complex (SCC) — Nicholas C. Metropolis Center for Modeling and Simulation at Los Alamos National Laboratory.

The SCC (located in Technical Area 3— TA-3) is a three-story structure (Figure 21) with approximately 302,000 gross square feet that will initially house the ASCI Q machine in a specially designed 43,500 net square-foot computer room. Electrical and mechanical rooms occupying over 60,000 square feet will support the computer room. The SCC can be upgraded to accommodate a 100-teraOPS-class system. The SCC and its associated infrastructure of high-speed networks, workstations, visualization centers, interactive data-analysis tools, and collaborative laboratories will support the SSP through simulations of complex phenomena of national importance.

The SCC will provide a dynamic environment for approximately 300 nuclear weapons designers, computer scientists, and code developers who will work together, with support personnel, in simulation laboratories.

The SCC's construction was finished on January 9, 2002, and the building is now occupied. The installation of the Q machine began in the first week in February. The fiber communications system is undergoing security testing and approval. The building was dedicated as the Nicholas C. Metropolis Center on May 17th, 2002.

Terascale Simulation Facility (TSF)



Figure 22. The TSF at Lawrence Livermore National Laboratory.

The Terascale Simulation Facility (TSF) (Figure 22) at Lawrence Livermore is being constructed to provide power and space that is capable of accommodating two simultaneous 100-teraOPS-class system operations and assessment areas and networking control areas necessary for direction and assimilation of data. A four-story office structure will provide staff space to manage and utilize the simulation environment.

The TSF will provide a uniquely capable simulation environment to generate and to assess the petabytes of data, which will emerge from ASCI 3-D weapons science codes. The DOE/NNSA will use this capability to simulate nuclear weapons tests—an essential element of our nation's Stockpile Stewardship effort.

Within its total of 253,000 square feet, the TSF features two 23,000 square foot machine rooms, which allow for simultaneous siting and stabilization of a new system while an existing system

continues to provide user access. Rated at 15 MW of power and equivalent cooling, the TSF will provide a facility platform with flexibility in future operations for generations of advanced systems. This flexible capability and high power/cooling density are unique in computer operation center design.

The Advanced Simulation Laboratory within the TSF will function more as an experimental facility than as an operational computer center. It will support uninterrupted collaboration between ASCI staff and analysts. The TSF will also house a consolidated Networking Operations Center, providing for the scalable system area networks and permitting smooth functioning of remote data access and visualization assessment theater operation.

The TSF will provide a first computer floor occupancy for system sitting in June 2004 and for full facility completion in 2006.

Joint Computational Engineering Laboratory (JCEL)

Figure 23. The JCEL at Sandia National Laboratories in Albuquerque, NM.

The JCEL (Figure 23) is a critical element for Sandia to achieve validated, full-physics, high-fidelity computa-

tional analyses for nuclear weapons. The need for the JCEL lies with our ASCI requirement to provide computational analyses from concept through design through above-ground component and subsystem testing to achieve safety, reliability, and security of the nuclear stockpile. The JCEL will house equipment and activities associated with ASCI high-performance computing, communications, and computer-



aided design and engineering. The JCEL will promote rapid development and application of modeling and simulation tools needed to support science-based stockpile stewardship and stockpile management. The facility will meet top-secret restricted data (TSRD) classification requirements. The JCEL is currently under construction. The facility is scheduled for completion in the fall of 2003.

Distributed Information Systems Laboratory (DISL)

Figure 24. The DISL at Sandia National Laboratories in Livermore, CA.



The DISL (Figure 24) will be used to provide technologies that will enable seamless, secure, and reliable access to information, allowing integration and preservation of that information throughout the nuclear weapons complex. Activities in the DISL will focus on integration of PSE, VIEWS, and DisCom capabilities, secure networking, and collaborative environments technologies, and on implementation and use of those technologies by engineering teams. The DISL will pro-

vide the facilities to enable development of a distributed information systems infrastructure that will be deployed across the Nuclear Weapons Complex (NWC) for collaborative design and manufacturing utilizing ASCI-scale computational capabilities. The facility will meet TSRD classification requirements. The DISL design was completed in December 2001, and construction began in June 2002. The facility is scheduled for completion in the fall of 2003.



PROGRAM MANAGEMENT

The Executive Committee quarterly meetings and biweekly teleconferences are critical to our integrated tri-lab management of the program. Shown here are the attendees of the March 2002 meeting in Washington, D.C.

PROGRAM MANAGEMENT

Program Management Objectives

ASCI program management has two important objectives:

 Provide leadership. ASCI is developing 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 NNSA national 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 laboratories, 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 be incorporated into laboratory capabilities that will replace nuclear testing.

Facilitate the interactions among the laboratories. ASCI is breaking new ground in the degree of collaboration among the laboratories. The ASCI management structure strives to understand and eliminate barriers that could inhibit collaboration.

Program Management Planning Process

ASCI program management uses the following planning process:

- ASCI Program Plan. The Program Plan (this document) 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 Plan. This plan is prepared annually and describes the work planned at each laboratory to support the overall ASCI objectives. The program element management teams ensure that the work at each laboratory is interconnected and is reflected in the individual implementation plans. The implementation planning effort begins in April and includes a coordination meeting in July in anticipation of the beginning of the fiscal year on October 1.
- Program Milestones. ASCI milestones are established using a tiered approach and consist of Level 1, 2, and 3 milestones. Level 1 milestones demonstrate the completion of a major new capability by the program and are structured to provide integration across ASCI. The descriptions of the Level 1 milestones are given in Appendix A. The Executive Committee reviews the schedule and content of the Level 1 milestones at least annually to ensure alignment with the needs of DSW and the other Campaigns. As part of its review, the Executive Committee solicits feedback from the external peer review panel assigned to each Level 1 milestone. The Executive Committee must approve changes to Level 1 milestones before inclusion in the Program Plan. A formal external peer review is required for a

Level 1 milestone to determine whether the milestone was completed satisfactorily.

Level 2 milestones demonstrate the completion of advanced capabilities by the program. These milestones directly support the completion of a Level 1 ASCI milestone, a major Campaign milestone, or a DSW deliverable. The cognizant program-element management team establishes Level 2 milestones. The Level 2 milestones are reviewed annually and revised as part of the development of the annual Implementation Plan. Descriptions of the Level 2 milestones are included in the Implementation Plan. Appropriate internal or external review of the Level 2 milestones is encouraged, but formal review is not required. Level 3 milestones demonstrate the completion of important capabilities within a program element and measure technical progress at the subprogram level. Typically, Level 3 milestones directly contribute to Level 2 milestones. Subprogram leaders working closely with the program element managers establish Level 3 milestones. These milestones are updated periodically and are documented in the internal laboratory plans.

Progress on Level 1 and 2 milestones, as listed in the published Implementation Plan, is reported quarterly.

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 ASCI Headquarters. The Executive Committee sets overall policy for ASCI, develops programmatic budgets, and provides oversight for the execution of the program.

 Program Element Management Teams. These teams are responsible for the planning and execution of the implementation plans for each of the program elements: Applications, V&V, Materials and Physics Modeling, Problem-Solving Environment, DisCom, PathForward, VIEWS, Physical Infrastructure and Platforms, Ongoing Computing, Advanced Architectures, Alliances, Institutes, and One Program— Three Laboratories. The program element management teams consist of two representatives—a primary and alternate from each laboratory, and the corresponding program area manager from ASCI Headquarters.

ASCI Headquarters Team. This team consists of NNSA federal employees supported by representatives from the NNSA national laboratories and production facilities. The ASCI Headquarters team is responsible for ensuring that the program supports the overall SSP. The ASCI Headquarters team facilitates the program's interactions with other government agencies, the computer industry, and universities. In addition, the team sets programmatic requirements for the laboratories and reviews management and operating contractor performance.



Program Collaboration Meetings

ASCI holds 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 are held annually and provide a forum for ASCI's scientists and engineers (principal investigators) to meet and discuss progress on their research areas. These meetings 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 include participants from out-
- side the NNSA national laboratories) also serve a peer-review function. These meetings provide an annual technical review for the ASCI HQ team.
- Executive Committee Meetings. Every two weeks, the ASCI Executive Committee conducts a teleconference to discuss important issues. At these teleconferences relevant issues are identified, discussed, and resolved in a timely manner. The biweekly teleconferences are supplemented with quarterly meetings.

Program Reviews

ASCI regularly conducts external technical reviews of the program. These reviews add immense value by providing critical insights into the technical progress of the program. An external peer review panel has been formed for each major technical element of the program. These panels consist of experts from academia, industry, and the NNSA national laboratories in the technical fields relevant for each Level 1 milestone. The principal role of these panels is to assess the completion of Level 1 milestones.



APPENDIX A: LEVEL 1 MILESTONES

APPENDIX A: LEVEL 1 MILESTONES

ASCI Level 1 milestones are first listed in this section by an identification label, the quarter in which they are to be completed, and a title. Following that list, a brief description is provided of each milestone. The identification label identifies the milestone in the following way: milestone "NA-3.1" is the first (".1") milestone to be completed in the area of Nuclear Applications ("NA") in the fiscal year 2003 ("3").

Nuclear Applications

NA-3.1	FY2003 Q1	Enhanced primary physics initial capability
NA-3.2	FY2003 Q1	Focused secondary physics capability at LLNL
NA-4.1	FY2004 Q1	High fidelity physics three-dimensional primary burn initial capability
NA-5.1	FY2005 Q1	High fidelity physics 2-D/3-D physics secondary burn initial capability
NA-6.1	FY2006 Q1	Advanced weapons physics simulation
NA-8.1	FY2008 Q1	High fidelity physics full system initial capability

Nuclear Safety

NS-3.1	FY2003 Q2	Nuclear safety simulation of a complex abnormal explosive
		initiation scenario

Nonnuclear Applications

NN-2.1	FY2002 Q4	Stockpile-to-Target Sequence abnormal environment
		prototype simulation for crash and burn events
NN-3.1	FY2003 Q4	Stockpile-to-Target Sequence hostile environment simulation
		for cable SGEMP and electrical response to x-rays
NN-5.1	FY2005 Q4	Stockpile-to-Target Sequence normal environment simulation
		for spin motor performance, slap-down, and earth penetration
NN-7.1	FY2007 Q4	Stockpile-to-Target Sequence normal environment simulation
		for spin-up flight dynamics, lay-down, and electrical system
		performance
NN-8.1	FY2008 Q4	Coupled Stockpile-to-Target Sequence abnormal environment
		simulation of weapon thermal response to a fire environment

Verification and Validation

VV-4.1	FY2004 Q2	Initial validation of Stockpile-to-Target Sequence abnormal environment
VV-4.2	FY2004 Q2	Initial validation of focused secondary capability (Campaign-4 focus)
VV-4.3	FY2004 Q4	Initial validation of focused enhanced primary and nuclear safety simulation capability
VV-5.1	FY2005 Q1	Initial validation of Stockpile-to-Target Sequence hostile environment blast and impulse simulation
VV-5.2	FY2005 Q3	Initial focused validation of high-fidelity physics primary burn capability
VV-5.3	FY2005 Q4	Initial validation of Stockpile-to-Target Sequence normal – lay-down and nose crush
VV-6.1	FY2006 Q3	Initial focused validation of high fidelity physics secondary burn
VV-7.1	FY2007 Q3	Initial focused validation of advanced weapons physics simulation
VV-7.2	FY2007 Q4	Initial validation of Stockpile-to-Target Sequence normal – penetration

Simulation and Computer Science

SC-3.1	FY2003 Q4	User environment for the Q platform at LANL
SC-5.1	FY2005 Q4	User environment for the Red Storm platform at SNL
SC-6.1	FY2006 Q2	User environment for the 100T platform at LLNL
SC-8.1	FY2008 Q2	User environment for the 200T platform at LANL

Physical Infrastructure and Platforms

PP-4.1	FY2004 Q4	Red Storm at SNL, final delivery and checkout
PP-5.1	FY2005 Q2	100-teraOPS system at LLNL, final delivery and checkout
PP-7.1	FY2007 Q2	200-teraOPS system at LANL, final delivery and checkout

NUCLEAR APPLICATIONS

NA-3.1 FY2003 Q1 Enhanced primary physics initial capability

By December 31, 2002, ASCI will demonstrate an initial enhanced primary capability on the path to a high fidelity physics calculation of the explosion (milestone NA-4.1) of a primary system with three-dimensional features. The simulation will produce relevant information that will be compared to experimental data for primary behavior.

NA-3.2 FY2003 Q1 Focused secondary physics capability at LLNL

By December 31, 2002, ASCI will demonstrate the capability to perform secondary calculations capable of studying specific issues identified in Campaign 4.

NA-4.1 FY2004 Q1 High fidelity physics three-dimensional primary burn initial capability

By December 31, 2003, ASCI will make a high-fidelity-physics calculation of the explosion of a primary system with three-dimensional features. The simulation will produce relevant information, including the primary yield that will be compared to a nuclear test.

NA-5.1 FY2005 Q1 High fidelity physics 2-D/3-D physics secondary burn initial capability

By December 31, 2004, ASCI will make a high-fidelity-physics calculation of the explosion of a secondary system with three-dimensional features. The simulation will produce relevant information, including the secondary yield that will be compared to a nuclear test.

NA-6.1 FY2006 Q1 Advanced weapons physics simulation

By December 31, 2005, ASCI will make series of a high fidelity physics simulations of a weapons system either that addresses a stockpile or campaign issue or baselines a stockpile weapons system. The simulations will produce information that is intended to be part of the certification of a weapons system.

NA-8.1 FY2008 Q1 High fidelity physics full system initial capability

By December 31, 2007, ASCI will make a high-fidelity-physics calculation of the explosion of a full weapon system (primary+secondary) with three-dimensional features. The simulation will produce relevant information, including primary and secondary yields that will be compared to a nuclear test.

NUCLEAR SAFETY

NS-3.1 FY2003 Q2 Nuclear safety simulation of a complex abnormal explosiveinitiation scenario

By March 31, 2003, ASCI will complete a calculation of a nuclear-safety related nuclear test that has more simulation complexity than any previous similar calculation. The complexity may come from the problem geometry or initial conditions, such as more complex abnormal initiation of the explosive than in previous simulations, or from the complexity of the physical models required to represent essential phenomena. Results presented to fulfill this milestone will include a description of the test being simulated, the aspects that characterize the complexity, and comparisons between the simulation and relevant nuclear and non-nuclear test data. The laboratory program leaders will have a leading role in the selection of problem and feature sets for the milestone simulations to ensure they will contribute to meeting DSW and/or Campaign needs.

NONNUCLEAR APPLICATIONS

NN-2.1 FY2002 Q4 Stockpile-to-Target Sequence abnormal environment prototype simulation for crash and burn events

By September 30, 2002, ASCI will complete a set of three 3D analyses for an STS abnormal environment crash and burn accident involving a nuclear weapon. Simulation will include 3D system and component geometry.

NN-3.1 FY2003 Q4 Stockpile-to-Target Sequence hostile environment simulation for cable SGEMP and electrical response to x-rays

By September 30, 2003, ASCI will complete a demonstration of ASCI software to compute the electrical response of a weapon system in hostile (nuclear) environments. The application will demonstrate capabilities for cable SGEMP and transient x-ray response of weapon representative electrical components.

NN-5.1 FY2005 Q4 Stockpile-to-Target Sequence normal environment simulation for spin motor performance, slap-down, and earth penetration

By September 30, 2005, ASCI will simulate the coupled 3D mechanical response of bomb lay-down and penetration systems to normal flight environments. Simulations will include 3D weapon system and component geometry along with key sub-grid physics models. The simulations will include spin motor performance, fin dynamics, nose-crush through slap-down conditions, and penetration under a wide variety of impact conditions.

NN-7.1 FY2007 Q4 Stockpile-to-Target Sequence normal environment simulation for spin-up flight dynamics, lay-down, and electrical system performance

By September 30, 2007, ASCI will demonstrate simulations of mechanical and electrical limits for bombs during normal flight and impact. Simulation will include aeroelasticity of flight dynamics, adaptive coupling of internal, external, and structural components during impact, and full electrical system models with temperature effects.

NN-8.1 FY2008 Q4 Coupled Stockpile-to-Target Sequence abnormal environment simulation of weapon thermal response to a fire environment

By September 30, 2008, ASCI will demonstrate 3D coupled physics analyses for an STS environment crash and burn accident. The simulation will investigate safety issues related to the stockpile, expanding the accuracy of previous analyses by incorporating full system models and combined environments (fire coupled with thermal and quasi-statics).

NONNUCLEAR APPLICATIONS

VV-4.1 FY2004 Q2 Initial validation of Stockpile-to-Target Sequence abnormal environment

By March 31, 2004, the accuracy of the thermal response model will be assessed through an integrated experimental and analysis program. Comparisons between experimental and analytical results will include consideration of uncertainties in measurements and predictions. Sensitivity studies will be preformed to identify dominant phenomena and model parameters.

VV-4.2 FY2004 Q2 Initial validation of focused secondary capability (Campaign-4 focus)

By March 31, 2004, ASCI will complete a focused quantitative verification and validation assessment of the physics models and simulation capability used to complete a simulation for a campaign 4 milestone.

VV-4.3 FY2004 Q4 Initial validation of focused enhanced primary and nuclear safety simulation capability

By September 30, 2004, ASCI will complete a focused quantitative verification and validation assessment of the physics models and simulation capability used to complete the simulation for the NA-3.1 enhanced primary physics initial capability ASCI Level 1 milestone and the NS-3.1 Nuclear safety simulation of a complex abnormal explosive initial scenario ASCI Level 1 milestone.

VV-5.1 FY2005 Q1 Initial validation of Stockpile-to-Target Sequence hostile environment blast and impulse simulation

By December 31, 2004, current state-of-the-art validation techniques, which account for uncertainties present in both experimental data and computational predictions, will be applied to full-body models to characterize the transient response of an AF&F assembly. Sensitivity studies will be performed to identify relationships between the dominant physical phenomena and model parameters.

VV-5.2 FY2005 Q3 Initial focused validation of high-fidelity physics primary burn capability

By June 30, 2005, ASCI will complete a focused quantitative verification and validation assessment of the high-fidelity physics models and simulation capability used to complete the simulation for the NA-4.1 high fidelity physics primary burn initial capability ASCI Level 1 Milestone.

VV-5.3 FY2005 Q4 Initial validation of Stockpile-to-Target Sequence normal lay-down and nose crush

By September 30, 2005, ASCI will use current state-of-the-art validation techniques, which account for uncertainties present in both experimental data and computational predictions, and apply them to finite element simulations of bomb lay-down events for both initial impact and secondary tail slap. Simulations will compare acceleration time histories, and other relevant physical phenomena such as buckling, fracture, and crushing.

VV-6.1 FY2006 Q3 Initial focused validation of high fidelity physics secondary burn

By June 30, 2006, ASCI will complete a focused quantitative verification and validation assessment of the high-fidelity physics models and simulation capability used to complete the simulation for the NA-5.1 high-fidelity physics secondary burn initial capability ASCI Level 1 Milestone.

VV-7.1 FY2007 Q3 Initial focused validation of advanced weapons physics simulation

By June 30, 2007, ASCI will complete a focused quantitative verification and validation assessment of the high-fidelity physics models and simulation capability used to complete the simulation for the NA-6.1 Advanced weapons physics simulation ASCI Level 1 Milestone.

VV-7.2 FY2007 Q4 Initial validation of Stockpile-to-Target Sequence normal—penetration

By September 30, 2007, ASCI will complete a validation study of penetration into hard targets with new emphasis on validation analysis methods to plan testing programs, understand the total weapon response, and predict weapon responses into different targets with varying impact conditions.

SIMULATION AND COMPUTER SCIENCE

SC-3.1 FY2003 Q4 User environment for the Q platform at LANL

By September 30, 2003, ASCI will demonstrate a user environment that provides application development and execution, data analysis and visualization, and distance computing in accordance with ASCI Q and application requirements.

SC-5.1 FY2005 Q4 User environment for the Red Storm platform at SNL

By September 30, 2005, ASCI will demonstrate a user environment that provides application development and execution, data analysis and visualization, and distance computing in accordance with ASCI Red Storm and application requirements

SC-6.1 FY2006 Q2 User environment for the 100T platform at LLNL

By March 31, 2006, ASCI will demonstrate a user environment which provides application development and execution, data analysis and visualization, and distance computing in accordance with ASCI 100T and application requirements

SC-8.1 FY2008 Q2 User environment for the 200T platform at LANL

By March 31, 2008, ASCI will demonstrate a user environment that provides application development and execution, data analysis and visualization, and distance computing in accordance with ASCI 200T and application requirements

PHYSICAL INFRASTRUCTURE AND PLATFORMS

PP-4.1 FY2004 Q4 Red Storm at SNL, final delivery and checkout

By September 30, 2004, the Red Storm computer platform will be located at SNL for final assembly and checkout.

PP-5.1 FY2005 Q2 100-teraOPS system at LLNL, final delivery and checkout

By March 31, 2005, a 100-teraOps computer platform will be located at LLNL for final assembly and checkout.

PP-7.1 FY2007 Q2 200-teraOPS system at LANL, final delivery and checkout

By March 31, 2007, a 200-teraOps computer platform will be located at LANL for final assembly and checkout.

APPENDIX B: GLOSSARY

A P P E N D I X B: G L O S S A R Y

Advanced Architectures—An ASCI program element that is focused on development of more effective architectures for high-end simulation and computing.

ASAP—Academic Strategic Alliances Program, a program element within the University Partnerships category of ASCI.

ASC—Advanced Simulation and Computing. ASC is the program element of the Stockpile Stewardship Program that is developing the advanced simulation capabilities needed to analyze and predict the performance, safety, and reliability of nuclear weapons and certify their functionality. For historical reasons, ASC is more commonly known as ASCI.

ASCI—Accelerated Strategic Computing Initiative. ASCI is the name initially given to the Stockpile Stewardship Program element that is now called Advanced Simulation and Computing.

ASCI Blue Mountain—A Silicon Graphics system located at Los Alamos National Laboratory. In 1998, ASCI Blue Mountain was installed as a 3.072-teraOPS computer system.

ASCI Blue Pacific—An IBM system located at Lawrence Livermore National Laboratory. In 1998, ASCI Blue Pacific was installed as a 3.89-teraOPS computer system.

ASCI Frost—An IBM system located at Lawrence Livermore National Laboratory. This is a smaller (1.6 teraOPS) version of ASCI White used to support unclassified computing.

ASCI Heartland—An SGI system located at the Kansas City Plant. Heartland is currently operating at about 0.1 teraOPS and will be upgraded to about 0.2 teraOPS.

ASCI Manhattan—An SGI system located at Y-12. Manhattan is currently operating at about 0.1 teraOPS.

ASCI Purple—The next ASCI system to be located at Lawrence Livermore National Laboratory in 2005.

ASCI Red—An Intel system located at Sandia National Laboratories (NM). ASCI Red was the first teraOPS platform in the world when it was installed in 1998 (1.872 teraOPS). Processor and memory upgrades in 1999 converted ASCI Red to a 3.15-teraOPS platform.

ASCI Red Storm—A Cray system to be located at Sandia National Laboratories (NM), scheduled for delivery in FY2004, Quarter 4.

ASCI Q—A Compaq system located at Los Alamos National Laboratory. ASCI Q is a 30-teraOPS-computer system and is scheduled for delivery in 2002.

ASCI White—An IBM system located at Lawrence Livermore National Laboratory. In 2000, ASCI White was installed as a 12.3-teraOPS supercomputer system.

burn code—A computer code used to simulate the behavior of a weapon that involves significant energy released by thermonuclear reactions.

Bertha—The IBM 22.2-inch LCD computer display, which has 204 pixels per inch. It has a resolution of 3,840-by-2,400 pixels, which allows display of 12 times as much data as a common 1,024-by-768 pixel display.

Campaigns—An organization of the SSP activities that are focused on the scientific and engineering aspects that address critical capabilities, tools, computations, and experiments needed to achieve weapons stockpile certification, manufacturing, and refurbishment now and in the future, in the absence of nuclear testing.

capability/capacity systems—terminology used to distinguish between systems that can run the most demanding single problems versus systems that manage aggregate throughput for many simultaneous smaller problems.

CPlantTM—The Computational Plant project at Sandia National Laboratories is developing a largescale, massively parallel computing resource from a cluster of commodity computing and networking components.

CPU—Central Processing Unit.

DAM—Defense Applications and Modeling, the ASCI program component focusing on development of three dimensional, physics-model based codes that are formally verified and validated.

DARHT—The Dual Axis Radiographic Hydrodynamic Test Facility will examine implosions from two different axes.

DisCom—Distance Computing and Communication, a program element within ASCI focused on computing at a distant location, data communications between geographically distant locations.

DISL—The Distributed Information Systems Laboratory, a computing and communications facility scheduled for Sandia National Laboratories (CA).

DoD—U.S. Department of Defense.

DOE—U.S. Department of Energy.

DP-Defense Programs, one of the three major programmatic elements in NNSA.

DSW—Directed Stockpile Work, those SSP activities that directly support the day-to-day work associated with the refurbishment and certification of specific weapons in the nuclear stockpile.

DVC—Data and visualization corridors provide the capabilities to allow visualization and manipulation of massive scientific datasets.

FY—Fiscal year. The U.S. Government's fiscal year runs from October 1 through September 30.

FYNSP—Future Years Nuclear Security Plan, the multiple-year planning process used by NNSA.

Gigabyte—2³⁰ bytes; 1,024 megabytes.

HMX—Plastic-bonded high explosives.



HPSS—High performance storage system.

ICS—Integrated Computer Systems, the program component that provides the computing platforms and centers.

JCEL—The Joint Computational Engineering Laboratory, a computing and communications facility scheduled for Sandia National Laboratories (NM).

Lawrence Livermore—Lawrence Livermore National Laboratory, a prime contractor for NNSA located in Livermore, California, and operated by the University of California.

Los Alamos—Los Alamos National Laboratory, a prime contractor for NNSA located in Los Alamos, New Mexico, and operated by the University of California.

MESA—The Microsystems and Engineering Sciences Application facility, scheduled for construction at Sandia National Laboratories (NM), will provide the design environment for nonnuclear components of a nuclear weapon.

MPI—Message passing interface.

NIF—National Ignition Facility

NNSA—National Nuclear Security Administration, a semi-autonomous agency within DOE.

NPR—Nuclear Posture Review

NSA—National Security Agency

NSF—National Science Foundation

NTS—Nevada Test Site, the primary site of past U.S. underground nuclear tests and the site for ongoing subcritical and large-scale nonnuclear tests.

PathForward—ASCI program element that partners with industrial partners to accelerate the development of critical technology leading to commercial products needed by ASCI.

Petabyte—10¹⁵bytes; 1,024 terabytes.

PSE—Problem Solving Environment, an ASCI program element focused on the development of an infrastructure that provides effective software development tools, production computing environments, and archival storage.

PZT—Lead zirconate titanate.

Sandia—Sandia National Laboratories, a prime contractor for NNSA with locations primarily in Albuquerque, New Mexico, and Livermore, California, and operated by Lockheed Martin Corporation.

SCC—The Strategic Computing Complex, a combination computer facility and office complex under construction at Los Alamos.

S&CS—Simulation & Computer Science, the program element that provided the infrastructure necessary to connect the applications and platforms into integrated systems. science-based—Indicates the effort to increase understanding of the basic phenomena associated with nuclear weapons, to provide better predictive understanding of the safety and reliability of weapons, and to ensure a strong scientific and technical basis for future United States nuclear weapons policy objectives—compare with "test-based."

SFI—Significant Finding Investigation. An SFI results from discovery of some apparent anomaly with the enduring stockpile. DSW Surveillance generally initiates an SFI. For complex SFIs, resolution comes from the Assessment & Certification element of DSW, often in partnership with ASCI capability.

SIERRA—A code development framework being developed by Sandia.

SLEP—The Stockpile Life Extension Program. SLEP is the Defense Programs element responsible for planning and execution of component and weapon refurbishments.

SSP—The Stockpile Stewardship Program, Defense Programs' response to its responsibility to ensure the safety, performance, and reliability of the U.S. nuclear stockpile.

STS—Stockpile-to-Target Sequence, a complete description of the electrical, mechanical, and thermal environment in which a weapon must operate, from storage through delivery to a target.

terabyte—Trillions of bytes, abbreviated TB, often used to designate the memory or disk capacity of ASCI supercomputers. A byte is eight bits (binary digit, 0 or 1) and holds one ASCII character. (ASCII—the American Standard Code for Information Interchange.) For comparison, the book collection of the Library of Congress has been estimated to contain about 20 terabytes of information.

teraOPS—Trillions of floating-point operations per second.

test-based—The traditional approach used for the development of nuclear weapons based on full-scale nuclear tests—compare with "science-based."

Tri-lab—Referencing Lawrence Livermore National Laboratory, Los Alamos National Laboratory, and Sandia National Laboratories.

TSF—Terascale Simulation Facility, a computer and office facility scheduled for construction at Lawrence Livermore.

V&V—Verification and Validation. Verification is the process of confirming that a computer code correctly implements the algorithms that were intended. Validation is the process of confirming that the predictions of a code adequately represent measured physical phenomena.

VIEWS—Visual Interactive Environment for Weapons Simulation. VIEWS is the ASCI program element that provides the capability for scientists and engineers to "see and understand" the results of a simulation.













