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# FY 2005–2006 IMPLEMENTATION PLAN

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National Nuclear Security Administration

Los Alamos
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Sandia National
Laboratories

University of California
Lawrence Livermre
National Laboratory

# Advanced Simulation and Computing

# FY05–06 IMPLEMENTATION PLAN
## Volume 2

**July 30, 2004**

**Approved by:**

| | | |
|---|---|---|
| *Dimitri Kusnezov,* NNSA ASC Project Manager | Signature | *7/21/04* Date |
| *Michael Vahle,* SNL ASC Executive | Signature | *7/21/04* Date |
| *Michel McCoy,* LLNL ASC Executive | Signature | *7/21/04* Date |
| *James Peery,* LANL ASC Executive | *Signature not available* Signature | Date |


**ASC Focal Point**

*Dimitri Kusnezov*
NA 114.1
Tele.: 202-586-1800
FAX: 202-586-0405
dimitri.kusnezov@nnsa.doe.gov

**IP Focal Point**

*Njema Frazier*
NA 114.1
Tele.: 202-586-5789
FAX: 202-586-7754
njema.frazier@nnsa.doe.gov

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# Contents

# I. Executive Summary

The Stockpile Stewardship Program (SSP) is a single, highly integrated technical program for maintaining the safety and reliability of the U.S. nuclear stockpile. The SSP uses past nuclear test data along with future nonnuclear test data, computational modeling and simulation, and experimental facilities to advance understanding of nuclear weapons. It includes stockpile surveillance, experimental research, development and engineering programs, and an appropriately scaled production capability to support stockpile requirements. This integrated national program will require the continued use of current facilities and programs along with new experimental facilities and computational enhancements to support these programs.

The Advanced Simulation and Computing program (ASC)[1] is a cornerstone of the SSP, providing simulation capabilities and computational resources to support the annual stockpile assessment and certification, to study advanced nuclear weapon design and manufacturing processes, to analyze accident scenarios and weapons aging, and to provide the tools to enable stockpile life extension programs and the resolution of significant finding investigations (SFIs). This requires a balanced system of technical staff, hardware, simulation software, and computer science solutions.

The first decade of the ASC strategy was focused on demonstrating simulation capabilities of unprecedented scale in three spatial dimensions. The next decade will focus on increasing the ASC predictive capabilities in a three-dimensional simulation environment while maintaining the support to stockpile stewardship. To achieve these goals, three objectives must continue to be met by ASC:

- Objective 1: Robust Tools

  Develop robust models, codes, and computational techniques to support stockpile needs such as refurbishments, SFIs, life extensions programs (LEPs), annual assessments, and evolving future requirements.

- Objective 2: Simulation as a Predictive Tool

  Deliver validated physics and engineering tools to enable simulations of nuclear weapons performances in a variety of operational environments and physical regimes, and to enable risk informed decisions about the safety and reliability of the stockpile.

- Objective 3: Balanced Operational Infrastructure

  Implement a balanced computing platform acquisition strategy and operational infrastructure to meet directed stockpile work (DSW) and SSP needs for capacity and high-end capability simulations.

[1] The Advanced Simulation and Computing (ASC) program evolved from the Advanced Strategic Computing Initiative (ASCI).

# II. Introduction

The predecessor to ASC, namely the Accelerated Strategic Computing Initiative or ASCI, was established in 1996 as an essential element of the SSP to provide nuclear weapons simulation and modeling capabilities. Prior to the start of the nuclear testing moratorium in October 1992, the nuclear weapons stockpile was maintained through (1) underground nuclear testing and surveillance activities, and (2) "modernization" (such as, development of new weapons systems). A consequence of the nuclear test ban is that the safety, performance, and reliability of U.S nuclear weapons must be ensured by other means for systems far beyond the lifetime originally envisioned when the weapons were designed. The National Nuclear Security Administration (NNSA) was established in 2000 to carry out the national security responsibilities of the Department of Energy (DOE), including maintenance of a safe, secure, and reliable stockpile of nuclear weapons and associated materials capabilities and technologies.

NNSA will carry out its responsibilities through the twenty-first century in accordance with the current administration vision and the Nuclear Posture Review (NPR) guidance. NNSA Administrator Ambassador Brooks summarized the NNSA objectives for SSP in a May 2004 presentation to the Heritage Foundation, as follows, "…We will continue to lead the way to a safer world through the deep reductions in nuclear forces codified by the Moscow Treaty, through Nunn-Lugar and other cooperative threat reduction efforts, and through other actions. At the same time, although conventional forces will assume a larger share of the deterrent role, we will maintain an effective, reliable, and capable—though smaller—nuclear force as a hedge against a future that is uncertain and in a world in which substantial nuclear arsenals remain. Our ongoing efforts to reduce the current stockpile to the minimum consistent with national security requirements, to address options for transformation of this smaller stockpile, and to create a responsive nuclear weapons infrastructure are key elements of the Administration's national security strategy…."

A truly responsive infrastructure will allow us to address and resolve any stockpile problems that may be uncovered in our surveillance program; to adapt weapons (achieve a capability to modify or repackage existing warheads within 18 months of a decision to enter engineering development); to be able to design, develop and initially produce a new warhead within 3–4 years of a decision to do so[2]; to restore production capacity to produce new warheads in sufficient quantities to meet any defense needs that arise without disrupting ongoing refurbishments; to ensure that services such as warhead transportation, tritium support, and other on-going support efforts are capable of being carried out on a time scale consistent with the Department of Defense's (DoD's) ability to deploy weapons; and to improve test readiness (an 18-month test readiness posture) in order to be able to diagnose a problem and design a test that could confirm the problem or certify the solution (without assuming any resumption of nuclear testing).

Additionally, the NPR guidance has directed that NNSA maintain a research and development and manufacturing base that ensures the long-term effectiveness of the nation's stockpile; and to begin a modest effort to examine concepts (for example, advanced concepts initiatives to include the Robust Nuclear Earth Penetrator) that could

[2] While there are no current plans to develop new weapons, gaining the capability is an important pre-requisite to deep reductions in the nuclear stockpile

be deployed to further enhance the deterrent capabilities of the stockpile in response to the national security challenges of the twenty-first century.

The ASC program plays a vital role in the NNSA infrastructure and its ability to respond to the NPR guidance. The program focuses on the development of modern simulation tools that can provide insights into stockpile problems, and provides tools with which designers and analysts can certify nuclear weapons and guide any necessary modifications in nuclear warheads and the underpinning manufacturing processes. Additionally, ASC is enhancing the predictive capability necessary to evaluate weapon effects, design experiments, and ensure test readiness.

ASC continues to improve its unique tools to solve progressively more difficult stockpile problems, with a focus on sufficient resolution, dimensionality, and scientific details, to resolve the increasingly difficult analyses needed for the stockpile stewardship. ASC is pushing the envelope in leading-edge technology in high-performance computing and predictive simulation to meet the short and long term SSP needs (to include the annual assessments and certifications, LEPs, and SFI. The following list summarizes past, present, and planned future ASC contributions to these needs.

## Advanced Simulation and Computing Contributions to the Stockpile Stewardship Program

- In FY96, ASCI Red was delivered. Red, the world's first teraops supercomputer, has since been upgraded to over three teraops.
- In FY98, ASCI Blue Pacific and ASCI Blue Mountain were delivered. These platforms were the first 3-teraops systems in the world.
- In FY00, ASCI successfully demonstrated the first-ever, 3D simulation of a nuclear weapon primary explosion and the visualization capability to analyze the results; ASCI successfully demonstrated the first-ever, 3D hostile-environment simulation; and ASCI accepted delivery of ASCI White, a 12.3-teraops supercomputer.
- In FY01, ASCI successfully demonstrated simulation of a 3D nuclear weapon secondary explosion; ASCI delivered a fully functional problem solving environment for ASCI White; ASCI demonstrated high bandwidth distance computing between the three national laboratories; and ASCI demonstrated the initial validation methodology for early primary behavior. Lastly, ASCI completed the 3D analysis for a stockpile-to-target sequence (STS) for normal environments.
- In FY02, ASCI demonstrated 3D system simulation of a full-system (primary and secondary) thermonuclear weapon explosion; and ASCI completed the 3D analysis for a STS abnormal environment crash and burn accident involving a nuclear weapon.
- In FY03, ASCI delivered a nuclear safety simulation of a complex, abnormal, explosive initiation scenario; ASCI demonstrated the capability of computing electrical responses of a weapon system in a hostile (nuclear) environment; and ASCI delivered an operational 20-teraops platform on ASCI Q machine.
- In FY04, ASC provided simulation codes with focused model validation to support the annual certification of the stockpile and to assess manufacturing options. These efforts will continue beyond FY09. ASC supported the life extension refurbishments of the W76 and W80, in addition to the W88 pit certification. In addition, ASC provided the simulation capabilities to design various non-nuclear experiments and diagnostics.

- In FY05, ASC will identify and document SSP requirements to move beyond a 100-teraops computing platform to a petaops-class systems; ASC will deliver metallurgical structural model for aging to support pit lifetime estimations, including spiked-plutonium alloy. In addition, ASC will provide the necessary simulation codes to support test readiness as part of the NNSA national priorities.
- By FY06, ASC will develop, implement, and validate an initial physics and engineering capability in advanced ASC simulations for the W76 and W80 benchmarked against legacy codes and experiments; ASC will support the completion of B61 and W80-3 warhead certifications, using quantified design margins and uncertainties; and ASC will provide a basic 100-teraops platform user environment supporting the SSP requirements. ASC will provide data for model development and verification and validation to support hydro test activities, as defined in the *National Hydro Test Plan*; ASC will provide the integrated codes to assess manufacturing options and impacts to support the CD-1 approval of the modern pit facility. In addition, ASC will support the life extension refurbishment of the first production unit for the W80-3.
- By FY07, ASC will support the completion of the W76-1 warhead certification using quantified design margins and uncertainties; ASC will also provide a robust 100-teraops-platform production environment supporting DSW and Campaign simulation requirements. In addition, a capability platform will be sited at LANL.
- By FY08, ASC will deliver the codes for experiment and diagnostic design to support the CD-4 approval on the National Ignition Facility (NIF).
- By FY09, a modern baseline of all enduring stockpile systems, using ASC codes, will be completed.
- In FY13 and beyond, ASC will continue to deliver codes for experiment and diagnostic design to support the indirect-drive ignition experiments on the NIF.

**MISSION: Provide leading edge, high-end simulation capabilities needed to meet weapons assessment and certification requirements**

To meet the above mission and enhance the ability of the SSP to respond to stockpile needs in FY 2005–2010, ASC will:

- Continue supporting the immediate stockpile needs, including the annual assessments and certifications, LEPs, and SFIs
- Advance the development of ASC codes to provide the increased predictive capability necessary to understand aging phenomena that pushes our current science-based tools outside tested regimes
- Stimulate the U.S. computer manufacturing industry to create the powerful high-end computing capability required by the SSP
- Expand computational infrastructure and operating environment to enable better accessibility and usability of ASC capabilities
- Enhance integration with the science campaigns, to develop and incorporate improved, validated physics and materials models into the ASC codes

**VISION: Predict, with confidence, the behavior of nuclear weapons, through comprehensive, science-based simulations**

ASC will further enhance both the science and technology necessary to accomplish the above vision, by integrating with science campaigns and DSW to develop better science models; incorporating enhanced physics models into the simulation codes; delivering robust codes with enhanced computational techniques; applying verification and validation methodologies early into the modern code development process; and providing leading edge technology in the platforms and operating environments necessary for executing complex science-based simulations.

# III. Accomplishments

## Simulation and Computer Science

The Simulation and Computer Science (S&CS) program successfully completed all level 1 and level 2 program milestones.

### Capability Platforms

- **Q user environment** externally reviewed level 1 milestone

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

  There were several layers to the milestone set out through meetings of the review committee chaired by Paul Woodward of the University of Minnesota:

  - 20 teraops full-system application run QA/QB capability test
  - "Breadth" tests of integrated system performance, functionality, and usability
  - "Depth" tests of narrowly defined system capabilities and functionality

  The review committee concluded, "The panel believes that the ASC S&CS team has met all aspects of the milestone. We feel that this process has helped to focus efforts by the S&CS team toward making the Q system serve its user community well. The combination of breadth and depth tests seems to have worked well in addressing the functionality and performance of the system as well as its usability. The panel congratulates the S&CS team on a job well done."

- **Deploy Initial Software Environment for Early Purple Deliveries** level 2 milestone

  All the hardware has been delivered/installed/accepted for first 128-node system (March 31, 2004). All the hardware has been delivered/installed/accepted for second 128-node system (June 9, 2004). The first user on the system, Steve Langer, was very pleased that the machine "just worked." The first system, UM, went into limited availability in the Secure Computing Facility on June 15, 2004.

### Capacity Platforms

- **Usable linux-based software environment deployed on secure capacity platform** level 2 milestone

  This milepost demonstrated that key ASC application code teams can make effective use of a linux-based software environment on a secure capacity-computing platform, and included capabilities for secure access, data movement on and off the machine, scalable parallel file system, robust code development, flexible job scheduling and resource management, and high bandwidth access to archival storage.

### Data Management and Visualization

- **Commodity Visualization Deployment** level 2 milestone

  At LANL, a cluster-based rendering system was built to drive the 31-million-pixel PowerWall in the Strategic Computing Complex. Driving this PowerWall from commodity-based clusters with production visualization software, rearchitected to use the distributed environment, is a first step in driving all visualization devices at LANL (desktops, PowerWalls, and Immersive spaces).

At LLNL, a transition to a new architecture targeted toward clusters was completed through release of a new software stack, including new releases of DMX, Chromium, MIDAS, and Telepath. Together, these packages provide a dynamic environment capable of scaling with dataset size, display size, and desired levels of performance using commodity clusters.

At SNL, Chromium, DMX, and an internal ParaView release are in use, where aggressive deployment and use of commodity-based data/visualization clusters continued in FY04 to support the emerging Red Storm environment and PowerWall visualization facilities.

- **UDM I/O infrastructure to support Shavano project to Eolus project linkage and additional linkage to EnSight** visualization level 2 milestone

  In FY04, the unified data model was delivered to provide important data management functionality for Los Alamos code projects. Through a multi-group collaborative effort, unified data model now provides efficient parallel input/output for code projects running on high performance computing platforms.

- **Next Generation Data Management and Analysis Environment** level 2 milestone

  SimTracker capabilities were integrated on commodity clusters. Users now can launch VisIt's front-end on their local desktop and automatically launch VisIt's back-end on the host where the data resides. Hopper 1.1 was released, including incorporation of persistent parallel file transfer capabilities. A contour spectrum generation tool was released including support for topological based data summaries and scaling to the largest datasets. A new TeraScale browser was released with a redesigned graphical user interface for initiation and control of remote data preparation jobs.

- The PathForward program successfully completed the Cray application-specific integrated circuit chip, Etnus Totalview Debugger, KAI Performance Analysis Tool, MSTI message passing interface (MPI) technology, Red Hat Open Source Visualization Software, and Hewlett Packard Scalable Rendering projects, and started a major new open source software initiative.

## University Partnerships

### Sandia Computer Science Research Institute

- During the past year, the Sandia Computer Science Research Institute (CSRI) has hosted over 125 short-term visitors and over 60 summer students and faculty representing over 17 man-years of onsite research. The CSRI has also hosted five large workshops with over 150 external attendees in key technical areas for ASC modeling.
- A previous CSRI workshop in the area of electrical modeling and simulation has resulted in significant advances during the current year. This workshop identified algorithmic solutions to several problems that resulted in more robust and scalable convergence in the most recently released version of Xyce. The workshop also resulted in several long-term collaborations. One of these has resulted in the multi-time partial differential equation algorithm that recently demonstrated an algorithmic speedup of over 100 times for some problems. Another research

collaboration resulting from this workshop has resulted in a package of improved direct solvers included in the latest release of the Trilinos solver framework.

- New SAND (simultaneous analysis and design) algorithms and sensitivity analyses were included in the PREMO code.
- Improved finite element discretizations resulted in more accurate answers and better scalability (10 times improvement for large problems) in the ALEGRA modeling code.
- Hypergraph partitioning algorithms for Zoltan (dynamic load balancing) have improved the performance of Xyce, Trilinos, and others.
- New algorithms for mesh refinement and adaptivity that are included in the Sierra framework and used in codes such as CALORE.

### Lawrence Livermore ASC Institute for Terascale Simulation

- This past year, new linear solver developments enabled the largest-ever structural dynamics simulations in ASC's Arbitrary Lagrangian-Eulerian (ALE) 3D code. These simulations are now being done on meshes with 610 million degrees of freedom on 4032 processors of ASC White—100 times larger than the simulations of only three years ago, with 10 times the number of processors.
- We also developed a unique coupled radiation-hydrodynamics solver that combines dynamic AMR techniques with ALE methods for hydrodynamics. As part of this work, new nonlinear multigrid methods for radiation diffusion were also developed. In addition, a new multi-block mesh capability was developed to support adaptive ALE calculations, and the parallel performance of our adaptive mesh refinement (AMR) software technology was demonstrated for adaptive calculations on up to 1024 processors.
- During the 2003 summer program, 20 students and 4 faculty members visited for two to three months (a larger summer program is in progress in 2004).
- The Institute for Terascale Simulation (ITS) lecture series hosted five distinguished speakers.
- The ITS held one workshop on multiscale methods, which about 50 researchers attended to discuss topics in this new and important area.
- The ITS supported conferences, including the International Conference on Preconditioning Techniques for Large Sparse Matrix Problems in Scientific and Industrial Applications and the Copper Mountain Conference on Iterative Methods.

### Los Alamos Computer Science Institute

A striking indicator of The Los Alamos Computer Science Institute's (LACSI's) widespread impact and technology transfer is that 25 percent of all SuperComputing 2004 tutorials will be presented by groups that have received LACSI support. Specific recent accomplishments that support ASC missions include:

- Software component technology collaboration with the ASC Marmot project.
- Optimization of ATLAS BLAS linear algebra software generation for Opteron and Itanium
- Generalization of ATLAS tuning technology to more complex mathematical libraries
- OpenMPI project building the premier MPI library and deploying on ASC platforms

- Co-Array Fortran compiler and optimizations for ASC clusters and applications
- High-speed adaptive cluster communication over internet protocol
- Clustermatic software stack enhancements for ASC platforms
- Automatic software differentiation for ASC verification and validation analyses
- HPCtoolkit release, deployments on ASC platforms, and optimizations
- Modeling ASC platform/application combinations for systematic performance improvement
- Improved performance application program interface capabilities to gather performance counter data on ASC platforms
- Community interactions via the LACSI Symposium, specialized meetings, High Performance Computer Science Program

# IV. Goals

**Deliver increasingly accurate simulation and modeling tools, supported by necessary computing resources, to sustain the stockpile**

Development and implementation of comprehensive methods and tools for certification, to include simulations, is one of the top Defense Programs (DP) priorities that will meet the SSP vision:

> *To be an integrated nuclear security enterprise, consisting of research and development, tests, and production facilities that operates a responsive, efficient, secure, and safe nuclear weapons complex and that is recognized as preeminent in personnel, technical leadership, planning, and program management.*

To assure its ability to respond to stockpile needs and deliver accurate simulation and modeling tools, ASC has three major objectives to address both the short- and long-term components of the SSP:

- Objective 1: Robust Tools

  Develop robust models, codes and computational techniques to support stockpile needs such as refurbishments, SFIs, LEPs, annual assessments, and evolving future requirements.

- Objective 2: Simulation as a Predictive Tool

  Deliver validated physics and engineering tools to enable simulations of nuclear weapons performances in a variety of operational environments and physical regimes, and to enable risk informed decisions about the safety and reliability of the stockpile.

- Objective 3: Balanced Operational Infrastructure

  Implement a balanced computing platform acquisition strategy and operational infrastructure to meet SSP needs for capacity and high-end capability simulations.

# V. Activity Descriptions

## SECTION 2: SIMULATION AND COMPUTER SCIENCE

The ASC S&CS program is composed of the Problem Solving Environment (PSE), Distance Computing (DisCom), Path Forward, and Data and Visualization Sciences (DVS) program elements with an aggregate mission to maximize the productivity of ASC computational environment users through research, development, and deployment of the infrastructure needed for code development, large scale simulation execution, data analysis and management, and distance computing. To that end, S&CS partners closely with the ASC Defense Applications and Modeling program to understand and quantify requirements, and the ASC Integrated Computing Systems (ICS) program to identify and bridge the technical gaps between what is provided through platform procurements and capabilities needed to meet terascale user requirements. As the ASC platform program moves to the more cost-effective, open source commodity-based strategy for capacity and capability computing, the role of S&CS takes on added significance with increased responsibility for integration of the software environment.

## *2A: Simulation and Computer Science Activities*

### 2.1 Problem Solving Environment

The ASC PSE program is responsible for deploying the system software infrastructure necessary to enable application users to make productive use of ASC platforms for capability and capacity computing. PSE activities are focused on the near term deployment of software technology needed to “stand up” emerging platforms, as well as the longer term research and development necessary to deploy the demanding technology required by next generation peta-scale platforms. PSE is a component of the larger integrated S&CS program, whose goal is to maximize the productivity of ASC computing environment users through the deployment of common environments across the tri-lab composed of a minimal set of highly capable tools that meet user requirements.

To facilitate the deployment of common software environment on ASC platforms, PSE maintains a strong tri-lab working arrangement at all levels of development. Common thrust areas are identified and regular communications and meetings take place. PSE is loosely organized around these three project research and development areas—ASC simulation development environment, data transfer and storage, and computer systems infrastructure—but the efforts covered by these projects do not mirror organizational lines at any of the laboratories.

#### 2.1.0 Tri-Lab Problem Solving Environment Activities

PSE activities in support of ASC capability platforms fall into three general categories: a relatively small level of effort to complete deployment activities against platforms already in production status, a primary focus involving work to deploy the system software infrastructure required to “stand up” emerging platforms, and research to develop out-year technology anticipated to be required by the next generation of peta-scale platforms. In this context, over the FY05–06 time frame, PSE will complete deployment of the production environment in support of the White and Q platforms, engage in a major effort to deploy initial software infrastructure required by the SNL Red Storm platform, begin efforts to deploy the initial software environment for the LLNL Purple system, and engage in research and development and coordinate related activities directed to develop the next generation "peta-scale" software environment.

PSE is additionally engaged in activities to deploy the open source Linux-based software environment in support of commodity hardware capacity platforms. These systems provide a new level of price performance for the program. The software work in support of these systems will likely be leveraged to support the next generation of capability platforms. Platforms supported here include the LLNL ASC Linux cluster (ALC), the Intel Pentium 4 Xeon processor (x) early development technology vehicle (EDTV) and LANL Lightning systems.

PSE activities are focused on the following general thrust areas:

- Code Development. Develop, as necessary, and deploy the software tools (for example, compilers, debuggers, and performance analysis tools) needed to efficiently develop quality, scalable ASC application codes
- Code execution. Develop and deploy system software (for example, job schedulers, resource management, data management, archival storage, and data analysis) required by end-user designers to utilize simulation codes as tools to carry out the ASC programmatic mission
- Infrastructure. Develop and deploy the software infrastructure (for example, security, operating system, and networking) required that underpins usable platforms

As PSE is a tri-lab managed program, all activities are described in this section. PSE products are either jointly developed (for example, high-performance storage system (HPSS)), deployed on multiple platforms (for example, TotalView), or used by tri-lab application users (for example, LSF, a platform computing resource management product). To enhance user productivity, PSE is striving to deploy a common software environment across the tri-lab computing environment.

### *PSE Major Activities in FY05 and FY06*

The major activities for FY05 and FY06 follow:

- Pursue development of high-performance, open source, Linux-based computing environments, with initial deployment targeting capacity computing. Work in areas including system administration, resource management, parallel file systems, and development tools and libraries. Establish features of a common core application environment across the three defense laboratories. Identify and improve areas of the Linux-based applications environment to approach the standards of ASC capability systems.
- Develop and deployment of the Lustre file system required for several new ASC platforms. Continue evaluating alternative file systems as required. PSE also will be involved in testing the file systems delivered with capability platforms during this period and planning for integration with these systems and archives. An architecture for tighter integration of global file systems and HPSS archives will be pursued, prototyped, and deployed.
- Work to develop and deploy a major new HPSS release will continue, both to remove the dependence on distributed computing environment software mentioned

below, along with integration of site-specific non-distributed computing environment (DCE) infrastructure solutions. In addition, the unique non-DCE platform architectures deployed will require differing approaches to archive integration. The HPSS project will develop and enhance strategies to support the extreme archival requirements of each machine.

- Make security capabilities generally available for local site use, in preparation of the deployment of a new ASC tri-lab security infrastructure (a quarter three of FY06 level 2 milestone). These capabilities include a Kerberos-based authentication service, lightweight directory access protocol-based directory services to be used for storing authorization data and administrative tools and services to support the infrastructure. Tasks include deployment of services and integration with account management processes to facilitate the transition from the DCE infrastructure. There is continued effort to remove the dependency on DCE software from the ASC security infrastructure. Work in this area includes supporting the development and migration efforts of existing DCE-based applications (for example, HPSS and scientific data management (SDM)) and pursuing Network File System, version four, as a replacement wide-area distributed file system. Additionally, the focus for deploying the new ASC tri-lab security infrastructure involves coordination between sites for interoperability and consistency in behavior for the user.
- Deploy a Red Storm user environment that supports application development, execution, and data analysis as defined in the Red Storm usage model, based on the initial user software environment provided in FY04. This integrated Red Storm environment will lead to a milestone demonstration of the Red Storm environment in late FY05, which includes remote access and applications testing from LANL and LLNL. A performance evaluation of the system, including performance prediction based on the early hardware and software environment, will be performed by LANL in collaboration with SNL.
- Deploy and test the Purple system in late FY05, including tracking of performance of MPI, the federation switch, and the extension of network file systems to access the new Terascale Simulation Facility (TSF) housing Purple. This will be followed by a demonstration of Purple for limited availability in FY06, with a formal level 1 milestone associated with Purple general availability in FY07.
- Test and deploy components of the BlueGene/L system as they are delivered in FY05, with formal release for limited availability use in FY06. Specifically, this includes a wide variety of activities: testing the functionality and performance of the system software delivered by IBM, especially the quality of their compilers and MPI-2 implementation; testing the compute and input/output (I/O) node kernels and function shipping between them; development of job launch and system administration services; testing of overall reliability; monitoring the Etnus contract for BlueGene/L Totalview; porting performance analysis tools based on the performance application program interface; porting and tuning (with academic collaborators) basic scientific libraries (Fast Fourier Transform routines, BLAS, ScaLAPACK), continuing to help developers of high-level scientific libraries and applications, within the tri-labs and ASC Alliance centers, to port their codes, obtain performance information, and tune for better performance on BlueGene/L.
- Encompass hardware, applications, and system software in performance-related activities. Perform interconnect studies. Performance analyses will be performed for the Linux software stacks and Linux capacity platforms deployed. A set of tri-lab applications will be established to represent the ASC computational workload. Implement a database to track the changes in performance of these and other ASC applications with changes in the hardware and software environment, and advances

in the application development. Through benchmarking and performance modeling, carry out architectural studies to maximize the performance and throughput of the ASC platforms, including usage of these performance methodologies throughout the procurement process of the new capability machine at LANL. Assist the applications teams with benchmarking and performance optimization.

- Plan and prepare for future systems. Evaluate new interconnect technologies. Procurement activities for the next ASC flagship system at LANL will begin; predictive performance modeling of applications representative of the ASC workload will play a prominent role.
- Continue work on a high performance, fault tolerant, thread safe MPI-2, and run-time system. The work will transition from the LA-MPI code base to the new open MPI code base. The open MPI effort is a national collaboration including LANL, SNL, Indiana University, University of Tennessee, and Ohio State University. LA-MPI is currently the production MPI on LANL's Linux platforms, and it is being used heavily at SNL on certain testbed machines.
- Monitor new open source contracts placed to develop the Valgrind memory tool, a performance measurement package, and InfiniBand for the current capacity systems and future Linux-based capability systems. Test and deploy delivery results from these contracts as they are available. Participate in design decisions as appropriate.
- Provide tools enhancements required for ASC applications development teams, deploy tools, and assist applications teams with the use of tools so they receive the full benefit of the their capabilities.
- Continued development and deployment by SNL of problem setup tools (such as SIMBA, CUBIT, and WISDM) to create an integrated design-through-analysis environment for analysts and designers.
- Continue to develop mathematical software at LLNL to be deployed by ASC code teams. The Hypre effort will migrate users to the version translated into the Babel intermediate language for cross language, giving more native language interfaces. Hypre performance issues at the large scale on Purple and BlueGene/L will be addressed with new algorithms. In the nonlinear solver area, coupling within preconditioners for nonlinear transport is being done in collaboration with researchers in LLNL's AX Division. Different nonlinear solvers for CVODE are being addressed, and the SUNDIALS package (CVODE, KINSOL IDA, COVDES, and IDAS) continues to be supported. The SAMRAI project is adding functionality for scripting and steering interfaces to be used in LLNL Defense and Nuclear Technologies Directorate codes such as CALE, and SAMRAI is also developing new algorithms for scaling adaptive computations and dynamically changing grids for systems such as BlueGene/L (tens of thousands of processors).
- Support application customers, as required, on all ASC systems.

## 2.2 Distance Computing

DisCom's programmatic goal is to provide secure, very high-speed remote access to tri-lab users of ASC supercomputers to create a computing environment appearing as if it were local to the remote user, to the extent possible.

### 2.2.0 Tri-Lab Distance Computing Activities

Secure computing at a distance is necessary for the three laboratories to access all ASC supercomputing platforms, as required. This distance capability involves the creation of a high-speed, parallel, secure infrastructure architecture (both hardware and software), development and implementation of monitoring and testing capabilities, development of service applications, user support, and partnering with the PSE and DVS elements, to integrate services and security functions necessary for efficient remote access. In addition, DisCom aims to enable high-performance ASC computing at both the Y-12 and Kansas City plants.

### *Distance Computing's Goals*

Elements of the strategy for DisCom include:

- Develop and maintain a wide-area infrastructure (links and services) that enables distant users to operate on remote computing resources as if they were local (to the extent possible)
- Provide a reliable, available, secure (RAS) environment for distance computing through system monitoring and analysis, modeling and simulation, and technology infusion
- Develop and implement user support services that complement the Computational Systems and Simulation Support program element activities in support of distance users through user acceptance testing, user guides, Web-accessible information about the computing environments, and Web-accessible system status
- Enable remote access to ASC applications, data, and computing resources to support computational needs at the plants

### *Distance Computing Organization*

Because distance computing among the NNSA laboratories is critical to meeting ASC and DSW milestones, DisCom maintains a strong tri-lab working arrangement at all levels of development and implementation. Common projects are identified and weekly communication and coordination telecoms and quarterly review meetings take place.

### *Distance Computing in FY05*

DisCom provides remote access to current major ASC platforms (Red, Blue Mountain, White, and Q). In FY05, DisCom intends to deliver additional key computing and communications technologies to efficiently integrate the ASC platforms of Red Storm, Purple, and beyond. As the Red Storm environment comes on line, the wide area network (WAN) is expecting increased utilization with higher expectations on availability and better quality of service. DisCom will be deploying tools in support of more reliable and persistent file-transfer mechanisms over the WAN. DisCom's major thrusts in FY05 include:

- Provide operational support for the WAN through continued management of the Qwest and AT&T contracts for the WAN, operational support of the WAN environments, tri-lab coordination of the distance computing environments, and continued security integration support.
- Enhance WAN capacity and capability through planning and preparation for rapid WAN bandwidth enhancements to support changing user requirements, creation of traffic-engineering models to predict future throughput demands, evaluation of load sharing and fail over techniques for encryptors, and evaluation of routing SecureNet traffic over the WAN to take advantage of the WAN's higher bandwidth.
- Enhance end-to-end throughput through advanced development of modeling and simulation capabilities to evaluate network usage issues, evaluate new network technologies to improve WAN utilization and prepare for future application needs,

and ensure local site infrastructure for new ASC computing platforms meet DisCom requirements.

- Continue to support Q and support the ASC distance-computing environment for new platforms such as Red Storm and EDTV/Purple. Actively support machine area network development and deployment, and participate in writing the test plan and usage model document for incorporating Red Storm into the ASC distance computing environment.
- Enhance WAN services for the ASC distance-computing environment by developing techniques and providing tools for persistent and reliable file transfer over the WAN (included in this is the Grid file transfer protocol application being developed for DisCom by Argonne National Laboratory).
- Provide operational and development support for SecureNet. DisCom is responsible for the distance-computing environment for ASC. To provide this environment, it relies on SecureNet for network interconnections among the laboratories, Y-12, and the Kansas City Plant. In this effort, DisCom provides operational support for SecureNet. In addition, it is important for DisCom to support development activities at the plants and in deployment of new technologies (for example, encryptors) to support DisCom's distance computing needs.
- Implement and integrate enhanced status and monitoring capability at the laboratories.
- Provide the ASC Red Storm distance-computing environment for limited availability.
- Deliver communications technologies to efficiently integrate the ASC Purple platform and beyond.
- Support increased utilization and availability and better quality of service as Red Storm reaches general availability.

### *Planned Efforts for FY06*

DisCom provides remote access to current major ASC platforms (Blue Mountain, White, Q, and, in FY05, Red Storm). In FY06, DisCom intends to complete production level support for Red Storm and shift focus for new service required for the ASC Purple machine at LLNL that will be coming into production in FY06.

### *Distance Computing Partners*

DisCom leverages its efforts in the following manner:

- Supports contracts and teaming with industry, other government organizations, and academia as appropriate to ensure technologies are available when needed to support the distance environment
- Partners with other S&CS program elements and ICS to support the development, deployment, and operation of services needed within the computational environments
- Leverages other laboratory-specific programs and projects to enhance ASC capabilities and manage cost

## 2.3 PathForward

PathForward is an essential element of the integrated S&CS program (PF, PSE, Discom, and DVS) focused on strategic targeted investments with vendor partners designed to accelerate the development of hardware and software technology needed to ensure that complete balanced systems for capability and capacity computing are available in the marketplace for out-year procurements by the program. These investments need to be made early enough, generally one to three-plus years ahead of system procurements, to ensure the technologies required are available, mature, and usable when the ASC systems are procured. Path Forward focuses on technologies that are essential for the successful deployment of platforms, such as interconnects, file systems, and the system software stack. Partner vendors are chosen where there is alignment between ASC program needs and the vendor business interests.

Initiated in FY04, the S&CS program is developing a software strategy to support commodity capacity and capability platforms that is based on open source software. ASC is pursuing this strategy to ensure consistency, control, and sustainability of the software base across systems that are expected to be procured from many vendors. Investments made in open source software carry forward across platforms, provide a consistent user and applications development environment, provide for continuous improvement of the ASC platform software base, and allow ASC technical staff to add value in areas critical to our mission such as security, performance at scale, reliability, and improved manageability. PathForward, working with other S&CS program elements, is focused on making investments in targeted critical open source projects where acceleration is required or capabilities are lacking, such as the software stack to support the interconnect and scalable file system.

## 2.3.0 Tri-Lab PathForward Activities

All PathForward activities are tri-lab. As such, each sub-project's technical team is composed of members from all three laboratories. These team members have dual responsibilities and work on projects for both PathForward and other program elements such as Platforms, PSE, and DVS.

Below are high-level details of current projects. More technical details of these efforts can be obtained from their Statements of Work upon request.

### *Current Work Scope*

**IBM/Corning optical switch**: Addresses the development of an optical interconnect for possible application on these future ASC platforms. Planned future ASC platforms are expected be a variation of a clustered symmetric multiprocessor (SMP) architecture. The purpose of the project is to design, build, and deliver a prototype 64-port, vendor-neutral computer-to-computer interconnect switch. The switch will be designed for minimal latency, maximum bandwidth, and high availability.

**Etnus memory correctness and usage tool**: Addresses ASC memory debugging requirements by adding functionality to the existing Etnus TotalView tool environment, which is already supported on all ASC platforms via extending heap allocation

**Silicon Graphics International open-source performance tools**: ASC requires a software tool or suite of integrated tools with a common look and feel, that will provide a collection of basic measurements to give insight into the performance of parallel programs. This project is an open source development effort to produce a parallel performance measurement package, aimed at the needs of high-performance technical computing community in general and ASC's parallel capacity computing systems specifically.

**Hewlett Packard/Cluster File Systems scalable global secure file system**: Focuses on the Lustre file system technology, which introduces an innovative object storage stack that enables modular development of client/target networking, storage management, and file system modules. Lustre envisages a networked environment with three types of systems: (1) clients that have access to the file system (thousands of them), (2) object storage targets that control persistent storage but have extensive capabilities for "on-controller-processing," and (3) cluster-control nodes that handle metadata updates and arbitrate file system security.

**Spray cooling**: Focuses on 3D chip spray cooling technology.

### *Planned Efforts*

Among many new start proposals planned for FY05 and beyond, the technical areas below represent the most promising:

- Open-source visualization software: At the time of the July 2004 *ASC Implementation Plan* submission date, the contract with the selected vendor was going through the approval process. Further information will be provided in the FY05 *ASC Implementation Plan* addendum.
- Interconnect technologies: Provides the necessary interconnects for ASC's next-generation platforms.
- Open-source software development: Provides additional software tools and technologies in areas such as interconnect, compilers, visualization, and resource management.

## 2.4 Data and Visualization Sciences

The DVS mission is to create and deliver high-performance data analysis and visualization environments where massive quantities of data easily flow to user desktops and collaborative workspaces, and through which scientists and engineers can absorb and exploit such data. DVS focuses on "consolidating, visualizing, and comprehending" the results of multi-teraops physics simulations and comparing results across simulations, and between simulation and experiment to improve the predictive capabilities of ASC applications and models. DVS tasks include research and development, testing and evaluation, and production deployment.

### 2.4.0 Tri-Lab Data and Visualization Sciences Activities

DVS strategies are to:

- Develop and deploy high-performance tools and technologies to support interactive exploration of massive, complex data; effective data management, extraction, delivery and archiving; and efficient remote or collaborative data exploitation.
- Develop and deploy scalable data manipulation and rendering systems that leverage inexpensive, high-performance commodity graphics hardware.
- Develop and deploy high-capability office display access to data by leveraging high-bandwidth networks and low-cost, high-capability commodity desktop computers.
- Collaborate closely with academia and industry to focus and leverage technology development with an emphasis on scalable technologies.
- Provide direct user training, hands-on classes, and tool documentation to support designers, analysts and code developers.

DVS has two primary groups of customers and works closely with each. DVS provides "production-quality" hardware and software "see and understand" tools to ASC designers and analysts, and develops and deploys customized infrastructure for office and shared space access to high-performance data and visualization resources. Training and support also are required to enable designers and analysts to rapidly learn and use the tool and infrastructure environment. DVS also interacts closely with the ASC code teams to anticipate, support, track, and meet their specific code development and execution requirements. Working with code teams and with other parts of S&CS, DVS has developed usage models, requirements documents and lab-specific deployment plan documentation to help drive project efforts.

DVS requirements are also derived from and driven by ASC platform decisions and environments. With ASC platform deployment teams, DVS participates in planning for new platforms and systems. DVS (in cooperation with ICS and other SCS elements) helps develop and deploy the archive, data processing, visualization, office delivery, and high-performance networking infrastructures to meet requirements to use the platform. To meet requirement challenges of future platforms, the S&CS roadmaps process (including specific roadmaps for visualization and scientific data management) helps anticipate future user needs.

DVS supports the current major ASC systems (Red, Blue, White, Q) and continues groundwork and planning to ensure that timely solutions are available for ASC platforms expected in FY05 (Red Storm, Purple, and BlueGene/L). DVS also addresses the shift to capacity computing Linux clusters by designing and deploying environments that support both the major ASC platforms and the needs of newer clusters.

In FY05, DVS efforts target the following Level 2 S&CS and ICS milestones:

- Deploy Limited Availability Red Storm User Environment (ID #0018)
- Initial Productization of Design-Through-Analysis Environment (ID #0019)
- Provide Visualization for Capability Calculations on Red Storm (ID #1313)
- Terascale Simulation Facility Activation (ID #1348)
- Immersive Visualization Environment Deployed for ASC Users (ID #1352)

The tri-labs jointly support a number of academic contracts for scientific data management/exploration and visualization research. The major academic partners are: University of South Florida, University of California—Irvine, University of Minnesota, The Ohio State University, Brown University, University of Utah, University of North Carolina at Chapel Hill, University of California—Davis, Princeton, Stanford University, Georgia Tech, and the University of Virginia.

DVS historically leverages results from PathForward and other commercial contracts to further develop critical parts of the infrastructure—especially for scalable visualization, data formats, and data model technology development. Current partners for visualization include Computational Engineering International (CEI), Kitware, and Tungsten Graphics. Funding is planned to continue for contracts with the University of Illinois for HDF-5 and with Limit Point Systems for libSheaf, both of which relate to scientific data formats and data models.

#### *2.4.0.1 Scientific Visualization*

This project supports existing and new ASC simulation platforms with a complete visualization software environment, from system level components through end-user tools to support tri-lab local and distributed visualization post-processing models. A major challenge is continuing to exploit previous investments in open source software, commercial tools, and scalable, distributed component infrastructures now used for visualization, while at the same time adjusting plans to face the ever-changing nature of user requirements and a strategic move from costly, monolithic visualization servers to commodity clusters. An additional long-term challenge is defining the directions that visualization research must take in upcoming years to support next-generation deliverables in areas such as object and topology-based data representation and complex dataset reduction.

Scientific Visualization goals for FY05 include:

- *Develop and deploy end-user visualization and data analysis tools to address user and system requirements*: develop and release a version of the TeraScale browser with distributed rendering capabilities (LLNL); develop end-user tools for the interactive exploration of multi-resolution topological data representations (LLNL); identify and develop custom data transformation and visualization tools for unique problems (LLNL, SNL, LANL); Develop and release a distributed memory client version of the CEI EnSight visualization tool (LANL); develop and deploy prototype comparative visualization tool (LANL); deploy prototype cluster-based volume rendering tool (LANL); support and extend local legacy visualization tools (PoP (post processor) and GMV (general mesh viewer)); (LANL); and targeted end-user tool development based on gathered analyst-driven requirements for improving the design through analysis cycle (SNL).
- Deploy new data manipulation and rendering scalable infrastructures based on Linux and client-server application models to support new ASC computational platforms (for example, Red Storm, Purple, and BlueGene/L), focusing on providing scalable infrastructures: enhance and deploy cluster-based rendering infrastructure components to improve scalability and exploit forthcoming graphics processing unit capabilities in conjunction with Red Storm, Purple, and BlueGene/L support (LLNL, SNL, LANL); new releases of the MIDAS remote image delivery system and the Telepath interactive session management tools (LLNL); explore revolutionary or novel hardware architectures (for example, cell-based approaches) for longer-term future visualization and rendering platforms (LLNL, SNL, LANL); and provide solutions for run-time visualization simulation results (SNL)
- Continued investment in visualization and data research to support increasingly large, complex datasets generated by the ASC platforms: research and prototype view dependent remote data services systems and end-user tools for hierarchical topological representations of data (LLNL); research into data layouts and mechanisms for optimal out-of-core mesh streaming (LLNL); research and develop new techniques for non-mesh-based simulation results (such as radiation transport) (SNL); research and develop tools/techniques in support of verification and validation activities (SNL); and research and develop large data streaming algorithms and techniques with the visualization toolkit and ParaView infrastructure (LANL, SNL).
- *Direct end-user support, including both production support for common data pipelines and the development of specialized, custom codes for specific applications*: provide ongoing end-user support for visualization facilities and infrastructure, and software tools and infrastructure components across the breadth of ASC systems (LLNL, SNL, LANL); provide expert visualization and analysis assistance for ASC users, including investigation of new techniques to understand phenomenon of interest to ASC scientists (LANL, LLNL, SNL); and expanded production support to include both commercial (CEI/EnSight) and visualization toolkit-based (ParaView) end-user tools (SNL).

### *2.4.0.2 Scientific Data Management*

This project supports user tools and system infrastructure to help generate, organize, search, access, extract, compare, track, transform, manipulate, and archive large-scale scientific data. Three thematic aspects of SDM within DVS are: (1) metadata infrastructures and applications for enhancing data access and organization; (2) data query and data discovery techniques and tools to represent, explore, and extract pertinent information; and (3) data models and data formats to facilitate efficient parallel I/O and data interchange between applications. Long-term SDM research and development challenges exist in scalable data access methods, smart comparison of simulation data, legacy information integration, interactive example-based discovery, and capabilities for unstructured mesh transformations.

SDM goals for FY05 include:

- *Enhance data access and organization through continued tri-lab development and deployment of the metadata infrastructure and applications*: facilitate integrated simulation data management environment via integration of SimTracker metadata and provision of needed metadata production and consumption capabilities (SNL); develop Alexandria project to enable tracking of all aspects of the simulation system environment for validation and historic analysis (LANL); incorporate advanced comparison operators into the simulation comparison framework, enabling a wide range of approaches for comparing datasets and runs (LLNL); extend Hopper file management application to provide automated data transfer optimization and to support additional tri-lab protocols (LLNL)
- *Continue research in data query and data discovery techniques, with an emphasis on object tracking, smart comparisons, and handling massive datasets*: Provide scalable pattern recognition for massive mesh-oriented data (SNL); implement example-based discover and efficient tracking of objects in 3D simulation data on a regular mesh (LLNL); enable smarter comparisons of simulation datasets, including comparing non-equivalent meshes (SNL, LLNL); extend ad hoc query capability against both unprocessed mesh data and optimized models of the original data based on user feedback (LLNL); deliver an integrated set of scalable tools to support query, extraction, and manipulation of simulation data (SNL); and deploy a data service for high performance, automated archiving of large data in the Red Storm environment (SNL).
- *Provide ongoing enhancement of and support for data models and formats*: develop new capabilities necessary for I/O, mesh data structures, material properties, and visualization (LANL); develop support for mesh transformations from non-uniform structured to uniform structured meshes (LANL); and continued integration and support of libSheaf data model capabilities (LLNL).

### *2.4.0.3 Infrastructure and Facilities*

This project supports the development, deployment, testing, evaluation, and support of DVS hardware infrastructure, including user office displays, collaborative end-user facilities, immersive environments, data manipulation and rendering clusters, advanced data delivery networking, and data archiving facilities. A major focus is the deployment of scalable, easily administered, cluster-based visualization hardware in support of user desktops and collaborative spaces. Commercial off-the-shelf graphics hardware is successfully being adapted by DVS for use in highly scalable visualization clusters, but a long-term challenge is how best to utilize new advances in digital networking, compression techniques, and resource orchestration capabilities to replace existing analog video delivery with next-generation, high-bandwidth digital image delivery.

Infrastructure and Facilities goals for FY05 include:

- *Deploy DVS systems in the laboratories' new computer facilities*: complete classified theater (TSF Advanced Simulation Laboratory) and deploy initial user "drop-in" facilities (LLNL); design and deploy Microsystems and Engineering Sciences Applications (MESA) Microlab Design & Education Center. ASC-developed expertise and visualization technologies will be leveraged to provide a facility for micro-design visualization, review, and training in the SNL MESA complex. (Note: Equipment funding to be provided by the MESA program.) (SNL).
- *Deploy new production visualization and display capabilities for user community*: deploy new projection systems with stereo for Building 111 Visualization Work Center, and deploy new visualization system for Building 111 Poseidon Room (LLNL); deploy a new high-resolution stereo immersive CAVE® system in the Metropolis Center (LANL); deploy a new Silicon Graphics International (SGI) 3900 rendering system to support offices, collaboratory PowerWalls, and the new Metropolis immersive system, and adapt key software and hardware (LANL); and extend the analog matrix switch software as needed for use in the LANL visualization infrastructure (LANL).
- *Continue/complete transition to new production visualization servers*: deploy new unclassified Linux graphics cluster to support unclassified data visualization requirements (LLNL); deploy classified server machine for driving the four-by-two-tiled projector PowerWall in Building 453 (LLNL); retire SGI Onyx machines and reconfigure image delivery capabilities for new Linux-based clusters (LLNL); procure and deploy DVS Red Storm platform nodes (nodes on the Red Storm platform that are provided for data and visualization processing (SNL); extend data analysis and visualization cluster-server infrastructure; procure any additional hardware and deploy limited availability production Red Storm environment clusters, for both classified and unclassified (SNL); and begin deployment of a next-generation (InfiniBand, PCI-Express) visualization cluster to support a broader set of end-users (LANL).
- *Prototype new visualization technologies*: deploy next-generation (for example, InfiniBand and PCI-Express) visualization server as a prototype for BlueGene/L, visualization, and support for software research and development of future systems (LLNL, LANL); evaluate newer display technologies such as volumetric and high-performance projectors, and networked and point-to-point video delivery equipment (LLNL)
- *Archival infrastructure in support of end-to-end environments*: procure and deploy HPSS archive storage hardware infrastructure in support of Red Storm and initial BlueGene/L and Purple platform deliveries (SNL, LLNL); and move existing archive hardware and media into the TSF in a minimally disruptive manner (LLNL)

#### 2.4.0.4 FY06 Goals and Activities

Scientific Visualization goals for FY06 include:

- *Continue visualization and analysis tool development to meet user requirements:* Provide end-user support for the ASC visualization toolset (LLNL, LANL, SNL); Integrate solutions to new and continuing end-user requirements to the scalable visualization toolset (LLNL, LANL, SNL); enhance tools to aid in quantitative analysis of simulations, comparison of simulation results with experimental results, and comparison with analytical solutions (LANL); continued development and delivery in support of improved design through analysis (SNL).

- *Investigate and deploy new data manipulation and rendering platforms to support new ASC computational platforms (Purple and BlueGene/L), and new visualization systems to take advantage of new visual data presentation and interaction technologies*: Deploy systems to support use of Purple and BlueGene/L (LLNL); Investigate systems to support the next-generation Los Alamos compute platform (LANL); develop and deploy new interaction paradigms for collaborative spaces (LLNL, LANL); evaluate new tiled and stereo display technologies and develop frameworks for their seamless integration into the ASC simulation post-processing environment (LLNL).
- *Continue research into next generation visualization platforms and data representations:* Research run-time programmable systems to exploit advances in commercial off-the-shelf graphics hardware in third generation visualization platforms for both visualization and higher-level data processing (LLNL, LANL, SNL); integrate aspects of alternative data representations and access mechanisms into production end-user tools (LLNL).

Scientific Data Management goals for FY06 include:

- *Extend metadata infrastructure and applications, including integration of legacy information:* Extend web-based simulation-tracking tool to support millions of simulation records per user by using relational and XML database technologies (LLNL, SNL).
- *Continue research and development in areas of data discovery and data query:* Enable interactive, example-based discovery in unstructured simulation datasets, thus allowing a user to specify an object or event of interest, and the system would find other similar examples on the fly (SNL); provide feature extraction and analysis capabilities simultaneous with the simulation, thus permitting the steering of a simulation by humans or other computational processes (SNL); implement example-based discovery and tracking of objects, in 2D AMR and unstructured meshes (LLNL).
- *Expand capabilities of libraries supporting advanced data models and formats:* Extend transformation capability to cover transformation from unstructured mesh to structured mesh (LANL); provide a cross-processor file comparison, enabling the detection of differences between two simulations with different processor configurations (LANL).

Infrastructure and Facilities goals for FY06 include:

- *Upgrade and complete existing visualization facilities:* Upgrade Building 132 Data Assessment Theater to stereo projection (LLNL); deploy production visualization cluster for multi-teraop visualization of BlueGene/L simulations (LLNL); extended deployment of cluster rendering capabilities targeted to multiple facilities and user desktops (LANL); deploy a usable remote digital video distribution system (LANL).
- *Deploy DVS systems in the laboratories' new computer facilities:* Design and deploy visualization laboratory(ies) for the MESA Weapons Integration Facility (equipment funding to be provided by the MESA program) (SNL); deploy new high performance display capability(ies) in the TSF's small-scale collaborative workspaces (LLNL).
- *Other infrastructure in support of end-to-end environment:* Procure and deploy additional HPSS archival hardware infrastructure in support of production Purple and full BlueGene/L platform use (LLNL); design and deploy visualization laboratory(ies) and office capabilities for users in the new National Security Sciences Building (LANL).

## 2B: Simulation and Computer Science Integration

The S&CS program area interacts closely with numerous organizations that are internal and external to ASC. The four S&CS elements (PSE, DISCOM, PathForward, and DVS) depend on and thus tightly interact with one another on tri-lab and technical issues to provide to the ASC users a secure, local and distance computing environment that includes a scalable, high-performance problem-solving environment, visualization, archival, and storage capabilities. Furthermore, S&CS works with the ASC Defense Applications and Modeling code development teams to support, anticipate, track, and meet their requirements. With the ASC platform deployment teams, S&CS participates in the planning for new platforms and systems and via the S&CS roadmap process, S&CS can plan for the new challenges it will face in standing up to the user environments for the coming systems.

External to the ASC program, S&CS supports all Campaigns and DSW activities that, as customers of the ASC program, utilize ASC applications and platform resources. Other S&CS interactions with external groups include participation on the review teams of the five Level 1 alliance centers and the technical management teams of the various PathForward projects. For longer-horizon research activities, the S&CS program is coordinated with the ASC Institutes program and other laboratory research activities such as individual laboratory directed research and development projects, SNL's CSRI, LLNL's ITS, and LANL's Los Alamos Computer Science Institute (LACSI).

## 2C: Simulation and Computer Science Risk Assessment

The following table summarizes top risks and mitigation approaches for S&CS:

**Table 2C-1. Top Risks for S&CS**

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| 1 | Significant changes in target platform architecture and bundled vendor capabilities impacts S&CS research and development. | Very High | High | High | Control: Promote standard solutions to accommodate changes; communications to anticipate delays. |
| 2 | Community support for open source software solutions erodes. | Moderate | High | Medium | Control: Promote standard solutions; have secondary sources. Understand stability of open source business models. |
| 3 | Independent software vendor partners may have changes in business plan or organization that impact deliverables or discontinue service. | Moderate | High | Medium | Control: Promote standard solutions; have secondary sources; promote open source products. Understand stability of business models. |

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | **Consequence** | **Likelihood** | **Risk Exposure** | |
| 4 | Delivered hardware or software may be unstable or not perform as expected. | Moderate | High | Medium | Control: Close involvement with supplier/partner. Promote source code availability for faster diagnosis and fix; research and development in fault tolerance; early deliveries where possible for new kinds of hardware to identify problems. |
| 5 | Resource constraints may impact needed investment in S&CS-related research areas. | Moderate | Moderate | Medium | Control: Work with other agencies to try to find outside coverage for lost funds. Lower expectations and stretch out deliverables that require research. |
| 6 | Difficulty hiring and attrition may lead to wrong skill mix. | Moderate | Moderate | Medium | Control: Deliverables or research efforts may be delayed or cancelled. |

# SECTION 3: INTEGRATED COMPUTING SYSTEMS

Meeting ASC's program requirements for developing advanced applications requires not only large, complex application codes that drive the scale of computing machinery, but also the infrastructure that supports these large systems and simulations. The goal of Integrated Computing Systems (ICS) is to develop and provide these computing resources and infrastructure and ensure that applications run satisfactorily on the most appropriate machines, at any given time, end-to-end, from input to data analysis and visualization to archiving the results. The ICS architecture continues to evolve as platforms, networks, archival storage, and visualization facilities change or are replaced. The strategy for integration is to maximize the use of standard tools, common system structures, and code portability to enable inter-laboratory collaborations. The ICS program area comprises Physical Infrastructure and Platforms (PI&P), Computational Systems, Simulation Support, and Advanced Architectures.

To accommodate the paradigm shift taking place through the Defense Applications and Modeling strategy, ICS acquires powerful ASC platforms in partnership with U.S. industry and operates computing centers necessary to run the codes. The adequacy of this strategy will be assessed with the following performance indicators:

- Total capacity of ASC production platforms with regards to procurements and system retirements
- Amount of capability of ASC production platforms

## *3A: Integrated Computing Systems Activities*

### 3.1 Physical Infrastructure and Platforms

The PI&P program element acquires computational platforms to support the SSP. The 20-teraops ASC Q platform was deployed in FY03 at Los Alamos. The Red Storm system at SNL will be completed in FY05. The 100-teraops ASC Purple platform is scheduled for full delivery and installation at LLNL in FY05, with an early technology demonstration system in FY04 and buildup of the major system in FY05. PI&P strategies include:

- Accelerate the acquisition of scalable, commercial, high-end systems
- Develop partnerships with multiple computer companies to ensure appropriate technology and system development
- Stimulate research and development efforts, through advanced architectures, that explore alternative computer designs, promising dramatic improvements in performance, scalability, reliability, packaging, or cost

#### 3.1.1 Sandia Platforms

The purpose of the Platforms program element at SNL is to provide capability computing for the Nuclear Weapons Program. The capability computing systems deployed are shared resources for the NNSA tri-lab and are intended to be used primarily for large capability jobs.

#### 3.1.1.1 Red Storm

The Red Storm computer system will be the next ASC capability machine to come on-line in the NNSA tri-lab environment. The first quarter of the system will be installed in September 2004 with installation of the full machine is expected to be completed in November 2004. The contract to build Red Storm was awarded to Cray, Inc., in FY02 after a competitive procurement process. The Red Storm contract continues for five years after delivery of the machine to SNL and provides full maintenance and support during this period.

Red Storm is a tightly coupled massively parallel processor with a little over 40 teraops of peak processing capability. The machine uses Advance Micro Devices Opteron processors and a custom, very high performance 3D mesh communication network. Red Storm has a total of nearly 11,000 Opteron micro-processors. In its initial form, Red Storm will have over 11 terabytes of memory and over 240 terabytes of high-performance local disk.

The Red Storm computer system was designed to provide for a relatively easy upgrade path. The 3D mesh can be expanded to 32,000 processors by simply adding additional cabinets and communication cables. The Opteron processors are high volume commodity parts that can be replaced with higher performance processors as simply as in an upgrade to a personal computer. The memory is high volume commodity double data rate dual inline memory modules that could be increased to 8 gigabytes per processor with currently available memory dual inline memory modules.

Red Storm has several unique features among which are its RAS system, its red/black switching capability, and its partitioned system software functionality. In effect, Red Storm has a separate parallel computer system to manage and monitor the main system. This system has its own network and processors and its own operating system. All major components (including RAS system components) in the system are monitored by the RAS system. All errors, recoverable and non-recoverable, are logged by the RAS system.

Red Storm's unique red/black switching capability makes it possible for the machine to be used as both a classified and unclassified computing resource. The machine has 10,368 compute nodes each with 1.0 gigabytes of double data rate memory and 512 service and I/O nodes, each with 4 gigabytes of double data rate memory. (Compute node memory will be expanded to at least 2.0 gigabytes shortly after Red Storm is installed.) The 512 service and I/O nodes are equally divided between classified and unclassified use. Through the red/black switching capability, the compute nodes can be either all classified or all unclassified, approximately 25 percent classified and approximately 75 percent unclassified, or approximately 75 percent classified and approximately 25 percent unclassified.

Partitioning of the Red Storm system software functionality provides a full LINUX operating system on the service and I/O nodes and a lightweight kernel operating system on the compute nodes. The lightweight kernel operating system provides a substantial performance advantage on the compute nodes while the full LINUX provides the full set of features that users expect to see on logging in. The LINUX operating system used on the service and I/O nodes is being enhanced to provide users and system administrators a single system view.

**Red Storm Work Scope**

Red Storm development continued throughout FY03 and FY04. The focus of the development was on the Seastar communication application-specific integrated circuit (ASIC), system cabinet design, service and I/O node and compute node board design, and system software development. The Seastar ASIC was released to manufacturing in December 2004. The first prototype chips were returned from fabrication and packaging in February 2004. Cray began hardware testing of these chips immediately. Two significant problems and a couple of minor problems were discovered in testing these chips. The first major problem resulted in a failure of the Seastar hyper-transport link to communicate with the Opteron hyper-transport link. This problem was traced to an error in some Seastar hyper-transport test logic. The problem was fixed through an engineering change order for the Seastar metal layer. Modified chips have been built and tested and are working correctly. This metal layer change is designated version 1.1.

The second major problem involved a clock being out of phase in the receive side of the SERDES (serialization de-serialization component) in the router part of the Seastar chip. Because of this problem, the SERDES would only run correctly at about half of the planned speed. This problem has also been fixed through an engineering change order for the Seastar metal layer, version 1.2. Prototype test chips will be returned in late June 2004. The Seastar chip has now been through a full set of hardware tests, and Cray is confident that this problem has been fixed and all of the hardware problems that can be found through testing at a small scale have been found. As a result Cray has released several thousand chips to manufacturing. These chips will be available in the middle of July 2004 and will become part of the production system.

Cray will receive about 200 Seastar chips (version 1.1) in early June of 2004. These chips will be used to build a small prototype system (Red II) for hardware and system software testing. Because these chips are Seastar version 1.1, they will not provide the full communication bandwidth, however, they will allow significant testing.

Prototype cabinets, service and I/O boards, and compute boards have all been built and tested. The production bill of materials for the final system is nearly complete and is expected to be finished in June of 2004. Production version Red/Black switches have been built. Cray will begin building production cabinets in June of 2004. Manufacturing of the production service and I/O boards and compute boards will begin in as soon as the Seastar chips become available.

System software development for Red Storm was carried out on small cluster systems, both IA32 (the instruction set for 32-bit processors standardized by Intel) and Opteron systems, during FY03. This work has continued in FY04. Also in FY04, the Red Storm system software was ported to ASC Red hardware so that it could be tested at a much larger scale. This port was completed in May 2004 and testing at scale was begun at the end of May. In May, software testing moved to prototype boards with Seastar chips. When the hardware testing of the Red II system is completed, software testing will move to Red II.

The first large scale Red Storm system (about one-quarter of the final system) will be assembled in early August 2004. This system will be used to demonstrate that the hardware works at scale and for system software development and testing, including large-scale file system testing. Red Storm system software development is a joint project between Cray and SNL. Cray has overall responsibility and responsibility for the service and I/O node operating system, compilers, math libraries, debugger, and performance monitoring tools. SNL has primary responsibility for the compute node operating system and run-time environment.

The Red Storm project is about four months behind schedule. The schedule slip resulted from problems with the Seastar chip. From the beginning of the Red Storm project, it was recognized that Seastar chip development was the critical path development for the project. Most of the schedule uncertainty associated with Seastar has now been resolved since the chips have been released for production. However, there is still some schedule uncertainty associated with the system software since it cannot be fully tested without a large Red Storm system. Once a large scale Red Storm system becomes available, the system software will become the critical path item.

## 3.1.2 Lawrence Livermore Platforms

The major goals for FY05–06 in PI&P are the delivery and installation of the 100-teraops ASC Purple platform and BlueGene/L.

**Charter**

The LLNL PI&P program element develops and acquires the capability and capacity computing platforms needed by the other elements of ASC and SSP. In addition, LLNL PI&P actively partners with their LANL and SNL counterparts to develop tri-lab platform strategies and aid in the PI&P efforts at the other labs.

**Products/Capabilities**

The current capability platform at LLNL in the classified partition is ASC White (12.3 teraops peak). In the unclassified partition, capability platforms that have been purchased with multiprogrammatic and institutional computing funds with some ASC co-investment include Multiprogrammatic Capability Cluster (MCR) (11.1 teraops peak) and Thunder (22.9 teraops peak).

Current multi-teraops parallel capacity platforms at LLNL in the classified partition are Lilac (9.2 teraops peak, xEDTV), Violet and Magenta (2 times 6.1 teraops peak, IBM Power 4+ processor (p) EDTV), and Adelie and Emperor (2 times 1.4 teraops peak). In the unclassified partition, ALC (9.2 teraops peak) and Frost (1.6 teraops) provide parallel capacity.

### *3.1.2.1 ASC Purple*

ASC Purple, a collaboration of the tri-lab community led by LLNL, represents the technology for delivering a 100-teraops capability to the SSP in 2005. This delivery has been a goal of the ASC Program since 1995, when it was envisioned as the minimum entry-level computational resource needed to support working, high-fidelity, 3D simulation codes for SSP simulations.

**Recent Accomplishments for ASC Purple**

EDTV platforms have been successfully demonstrated at LLNL in FY04. The pEDTV (IBM Power 4+ processor early development technology vehicle) systems have demonstrated IBM POWER4+ p655 servers operating with IBM's new Federation switch technology, new system administration software, and new, full 64-bit code development software. xEDTV has used to evaluate Linux clusters for ASC applications. ALC has successfully been utilized to develop and scale the Lustre parallel file system, demonstrating shared use across multiple clusters.

**Planned Efforts for ASC Purple**

The major architectural components of Purple consist of a computational cluster, a high-performance network infrastructure, and a cluster-wide storage subsystem. The heart of the ASC Purple cluster is IBM's new pSeries POWER5 based SMPs. The pSeries POWER5-based SMP is IBM's latest offering in the scalable POWERparallel (SP) family of scalable, parallel computing solutions. The high-performance network infrastructure is IBM's Federation 4-gigabyte switch, an evolutionary step in network data transfers using technology based on the proven architecture of SP Switch and SP Switch2. The cluster-wide storage subsystem is based on IBM's Global Parallel File System (GPFS) parallel file system running over 2 gigabytes per second Fibre Channel. Access to the storage system from outside Purple will be accomplished using parallel file transfer protocol over 1- and 10-gigabytes per second ethernet.

Initial nodes of Purple are planned for power-on in early FY05 at IBM's manufacturing facility. As part of this activity, selected user applications will be run on the initial Purple nodes.

Purple is currently scheduled for delivery to LLNL in two portions. The first 256-node piece, called Purpura, will be delivered in mid-FY05, with acceptance in the third quarter of FY05. The remaining approximately 1280-node portion of Purple is expected to be demonstrated in the fourth quarter of FY05. The two systems will be combined by about the second quarter of FY06 and enter limited availability status—selected users have access to the system. Soon thereafter, probably in the third quarter of FY06, Purple will enter general availability—any user with a valid account can access the system. Purple is planned to have a five-year lifespan, with the likely end of life in FY10.

**Expected Deliverables for ASC Purple**

LLNL's proposed delivery schedule for Purple is still under discussion with our vendor partner. The following represents our current plan, which may be modified during negotiations.

| | |
|---|---|
| FY05Q3 | Demonstrate a 256-node portion of Purple (about a one-sixth) called Purpura. Purpura will provide an early demonstration of the full three-stage Federation switch needed for Purple. After successful demonstration, Purpura will be moved into the classified partition. |
| FY05Q4 | Demonstrate the remaining nodes of Purple (about five-sixths) in the unclassified partition. Acceptance will likely occur in the following quarter. |
| FY06Q2 | Combine the two portions of Purple into a single system in the classified partition and move full-system status to limited availability. |
| FY06Q3 | General availability status for Purple is obtained. |
| FY10Q4 | End of life; Purple is decommissioned. |

### *3.1.2.2 BlueGene/L*

BlueGene/L, a next-generation massively parallel computing system, is focused on SSP science applications for broad application classes of interest to the program. With a peak compute capability of about 350 teraops, BlueGene/L is designed to address some of the most important issues facing high-end systems today: cost of platforms and facilities, single-node performance, and network performance. As a result, BlueGene/L may represent a viable approach to affordably achieve peak speeds of 1,000 teraops (petaops) and beyond. BlueGene/L is also a computational research vehicle that will allow for scaling applications to high processor counts, expected to be required for petaops-scale applications.

**Recent Accomplishments for BlueGene/L**

DD-1.0 (first generation) compute-node and link ASICs have been fabricated. Multiple prototype systems through systems with 2048 nodes have been built. Multiple applications and benchmarks have been successfully run on these prototype systems. Results of these early runs were presented at a BlueGene/L workshop in Reno in October 2003. Multiple organizations have been running applications on the prototype systems. LANL has published benchmark results for SAGE and SWEEP3D, with very encouraging projections for runs scaling to the full 65,536-node system. DD-2.0 (second generation) ASICs have been successfully fabricated and prototype systems are being built. It is likely that a 128-node system will be loaned to LLNL for application and system software development in FY04.

**Planned Efforts for BlueGene/L**

BlueGene/L is a next-generation massively parallel computing system designed for research and development in computational science targeted at selected applications of interest to the ASC tri-lab community and its University Alliance partners. A select but broad set of science-application areas have been identified as an initial focus for execution on BlueGene/L.

A critical step in deploying BlueGene/L is development of a cluster-wide parallel file system. We are currently planning on deploying the Lustre file system and efforts are under way to port the client to the BlueGene/L I/O nodes.

A phased build of the full 65,536-node system is planned, starting with the first delivery to LLNL of 16 racks (16 times 1024-nodes, one-fourth the full system), followed by a second delivery of 16 racks, completed by a final delivery of 32 racks. See the expected deliverables below for the expected delivery dates.

It is likely that BlueGene/L will undergo acceptance testing in late FY05 or early FY06, including full-system runs of Linpack. Full-system science runs will begin after acceptance is complete.

LLNL is actively involved with the wider community, participating in Argonne National Laboratory's efforts to form a BlueGene/L consortium of owners and users. In the past, LLNL has invited review of the project from a broad collection of high-end computing experts from outside the labs. LLNL has organized workshops that are open to a wide class of participants, and we anticipate holding one or more workshops each year.

**Expected Deliverables for BlueGene/L**

The following represents our optimistic plan for delivery of BlueGene/L to LLNL:

| | |
|---|---|
| FY05Q2 | 16 racks (16 times 1024 nodes) of BlueGene/L are delivered to LLNL. In aggregate, this represents one-fourth of the complete system. |
| FY05Q3 | An additional 16 racks (16 times 1024 nodes) are delivered to LLNL. In aggregate, this represents half of the complete system. |
| FY05Q4 | The final 32 racks (32 times 1024 nodes) are delivered to LLNL. In aggregate this represents all of the complete system. |
| FY06Q2 | Version 2.0 of the BlueGene/L operating system is delivered and installed. |
| FY08Q3 | End of life; BlueGene/L is decommissioned. |

### 3.1.3 Los Alamos Platforms

The platforms portion of the ASC program provides computational engines that enable the predictive simulation and virtual prototyping capabilities of the advanced weapon codes. The ASC platforms initiative has and will continue to accelerate development of high-performance computing far beyond what might be achieved in the absence of a focused initiative. This has been accomplished through multi-laboratory phased procurements that address the program needs for capability and capacity computing.

The major goal of the Platforms program element is to provide the weapons program with a computational resource to satisfy its critical national security requirements. The Platforms program element addresses this goal by first understanding the computing requirements and then developing partnerships with U.S. computer manufacturers to develop larger, faster computer systems to meet those requirements. The program also explores alternative high-performance computing architectures.

Capability computing always has been at the core of the ASC program because of the focus on developing and applying high-resolution, 3D techniques to difficult weapons issues. The ASC program recognizes that capacity computing is also critical (that is, using smaller computer systems dedicated to running the smaller 1D and 2D jobs so that the large capability computers can be dedicated to running the very large 3D jobs). The most recent installation of a capability machine is the 20-teraops Q machine at LANL, which took place in October 2002. This system, called ASC Q, has become a multi-laboratory resource.

At LANL, Q was complemented in FY03 by a Linux cluster and additional Compaq clusters aimed at addressing capacity computing needs. Linux-based systems are of interest to the program because of their relatively low cost for the same performance and because they promise a more constant systems environment as we move to future installations. The Linux system (called Lightning) is currently being beta tested and will be available to the user community in October 2004. The Compaq clusters are currently being fully utilized by capacity users from the weapons community.

A 100-teraops-scale computer system is scheduled for FY06. Our goals for that procurement are to:

- Focus on productivity platform rather than peak performance
- Provide tight coupling with application requirements
- Use prototype applications for modeling system performance
- Minimize time between award of contract and system availability
- Take advantage of price/performance trends

We are planning for a 100-teraops-class capability supercomputing platform to be delivered by the third quarter of 2006 and integrated into the tri-lab secure production computing environment by the third quarter of FY07. We will implement early delivery technology systems in the unclassified and secure environments to allow sufficient time for system integration as well as appropriate scaling work to facilitate the integration of the 100-teraops-class system.

## 3.2 Computational Systems

Computational Systems provides computational and data storage systems and their networking infrastructure at the three defense laboratories, including systems management personnel, maintenance contracts, and capital operating equipment for these systems. Efforts in FY05 will emphasize different phases of major platform deliveries in progress. LANL will provide tri-lab computational support on the Q machine. At SNL, Red Storm delivery and integration will occur. LLNL will emphasize integration and early use of the initial delivery system for the Purple contract and preparation for delivery of the full Purple system in FY05.

Computational Systems strategies include the following:

- Deploy ASC platforms as they are acquired

- Provide system management of the laboratory ASC computers
- Deploy and support the necessary networks and archives for laboratory ASC computers

### 3.2.1 Sandia Computational Systems

This activity encompasses all scientific production computing efforts at SNL for the two central computing facilities, one each in New Mexico and California. The work is encompassed in three projects as detailed below. This work element provides operating funds for system administration of large scientific computing platforms, including the ASC capability platforms, hardware and software maintenance and licensing, and infrastructure needs of these high-performance computers in terms of networking and hierarchical storage. Some capital equipment budget is allocated to purchases of mid-range systems, network switching equipment, high performance disk, tape silos, and peripherals.

The primary focus of this activity in FY05 will be the integration of the Red Storm computer system within the new supercomputer annex and transition of the system to limited availability supporting classified and unclassified processing.

As in FY04, the quarterly status will be reported by means of metrics, including usage of major ASC computing platforms and data storage, power consumption of the facility, and deferred replacement of systems. This utilization information is combined with the new consolidated milestone reporting tool in use throughout the nuclear weapons complex.

FY05 activities will focus on initial deployment work for Red Storm and concurrent support for ASC Red. System maintenance activity for ASC Red will be reduced to subsistence levels (such as, only critical bug fixes and no new features). We anticipate retiring ASC Red as soon as Red Storm has demonstrated stability and the scalability features expected of the system. Capacity computing systems represented by Cplant™ and other commercial platforms will continue in operation or be upgraded with new technology as appropriate.

#### *3.2.1.1 Production Systems*

This project administers and maintains high-performance scientific computing platforms in three categories: ASC capability level systems such as ASC Red and Red Storm; scalable cluster systems represented by Cplant™; and commercial systems such as SGI Origin and Onyx systems, Sun servers, IBM R/S 6000 servers, and Hewlett Packard SIERRA clusters. Some incremental investments in disk storage subsystems and network enhancements will be applied to these existing systems. Final construction of the high-performance computing network should be complete in FY05, including gigabit Ethernet to most nuclear weapons analyst and developer offices.

#### *3.2.1.2 Networks and Related Services*

This project support high-performance network research, design and development, deployment, operation, and maintenance for scientific computing systems. It coordinates phased purchases of network equipment with Platforms and DVS program elements to enable initial deployment of new capability systems and support full performance of systems as they enter general availability status. It also supports network-based file servers such as Network Appliance and BlueArc systems, and infrastructure services such as domain name servers, security servers (also known as Kerberos), and coordinates activities with corporate network providers and cyber security department. Finally, this project investigates high-speed interconnect technologies and applications such as extending the machine interconnect fabric into a machine area network configuration designed to support high performance file system use by multiple supercomputer platforms, visualization systems, and archive storage services.

#### *3.2.1.3 Storage*

This project supports operation of hierarchical storage systems comprised of disk cache and long-term tape storage systems. Currently, SNL utilizes the HPSS as the data management and high performance file transfer system. Disk cache systems in California transfer files to tape systems in New Mexico. Storage systems support computing needs on classified and restricted networks. Plans are to acquire additional resources to support future platforms, principally Red Storm. By the end of FY05, we will have symmetric storage systems serving both the classified and the unclassified networks and customers of Red Storm.

### 3.2.2 Lawrence Livermore Computational Systems

LLNL provides a world-class, high-performance scientific computing capability consisting of computers, storage, networks, and associated development environments and services that enable scientists to perform leading-edge research and scientific discovery. This project is responsible for maintaining and integrating the deliverables from Computational Systems, Simulation Support, DVS, DisCom, PSE, and PathForward into a reliable scientific computing environment and fostering their evolution into a production terascale simulation environment.

Classified and unclassified computing services are provided 24 hours a day, 7 days a week for stockpile stewardship customers computing locally and remotely from ASC-funded sites. The production scientific computing environment includes large SMP clusters, massively parallel systems (in particular, classified and unclassified ASC terascale computers), supporting servers, terabyte storage archives, data assessment theaters for visualizing huge data sets, and an interconnected, integrated networking infrastructure. Two scientific computing environments are maintained by the Livermore Computing (LC) program, served largely by expertise within the Integrated Computing and Communications Department (ICCD)—the Secure Computing Facility (SCF), a classified environment, and the Open Computing Facility (OCF), an unclassified environment.

Responsibility for the development, integration, and support efforts to maintain and advance LLNL's scientific computing environment are provided by the High Performance Systems Division (HPSD), Services and Development Division (SDD), and Networks and Services Division (NSD). These three divisions of LLNL's ICCD report to the ICCD department head and the ICCD deputy department head. The ICCD divisions most closely aligned with the Computational Systems program element are HPSD and NSD.

The HPSD mission is to develop, integrate, and support ICCD's high-performance scientific computing environment. This environment consists of world-class supercomputers, production computing resources, archival storage facilities, and other services that support and provide a secure computing environment. The HPSD consists of the following five groups:

- The Computer Systems Group is responsible for the integration, administration, and support of the ASC production and visualization platforms, network attached storage services, and other infrastructure components of the scientific computing environment.

- The Production Linux Group is responsible for the integration, administration, and support of large-scale production Linux clusters and the development and support of LLNL's Linux distribution (CHAOS) and other Linux-based support tools.
- The Data Storage Group is responsible for the integration, development, and support of the production archival storage systems necessary for a balanced scientific computing environment.
- The Security Technologies Group is responsible for the development, deployment, and support of security technologies and software to ensure secure computing. The Security Technologies Group also monitors the scientific computing environment for security incidents and vulnerabilities.
- The Operations Group is responsible for round-the-clock monitoring of all components of the scientific computing environment and responding to problems and service interruptions.

NSD's mission is to provide secure, reliable, effective access to information and computing resources from the desktop by delivering networks, centralized system administration services, and centralized enterprise services. The NSD consists of the following four groups:

- The Network Services Group architects and provides lifecycle support for enterprise-wide services in support of the chief information officer mission and vision. Presently, the suite of enterprise services includes e-mail services, calendaring, Entrust encryption, remote access services (for example, virtual private network (VPN) and integrated services digital network (ISDN), and modems), perimeter firewalls, directory services and various network services such as domain name service, and Internet access.
- The Application Services Group researches, develops, deploys, and supports a set of just-in-time technology services in response to customer needs and driven by operational requirements. Services focus on enterprise identity management, authentication, authorization, remote access management and control, network registration, and computer security program database services. The scope of services spans from the directorate level down to the end-user. Most offerings use redundancy for improved quality of service as well as geographical distribution for high availability.
- The System Management Solutions Group enables LLNL employees to effectively use the computer software and hardware they need to perform their jobs, and enables efficient and secure management of the desktop and server systems on LLNL networks.
- The Network Group is responsible for the design, maintenance, support, and monitoring of the classified and unclassified networks for ICCD, and classified and unclassified backbone networks for LLNL. This group provides classified connectivity to other DOE facilities via SecureNet and the DisCom WAN. They also maintains the associated NNSA-approved encryptors required for SecureNet and the DisCom WAN.

#### *3.2.2.1 Production Systems*

This project includes activities related to the integration and support of all computational systems operated by the LLNL center for developing and running user codes. Included are the development of selected system software components and kernel enhancements. Thrust areas consist of:

- Deploying new platforms as they are acquired

- Monitoring of production servers and daily system administration
- Monitoring systems for security events
- Analyzing and improving performance of key subsystems
- Developing scripts and tools to aid in administration
- Upgrading and patching operating systems as required for new functionality and fixing bugs, particularly in Linux environments
- Scaling and debugging of Linux clusters, including development work on various system software components to enable efficient use of these clusters in a high-performance computing environment
- Continuing development and enhancement of Linux cluster tools
- Maintaining hardware and software and supporting all computation, infrastructure, and storage-related platforms and equipment

#### *3.2.2.2 Networks and Related Services*

This project includes all network-related components for LLNL center's backbone and high-performance systems area network, including all network, infrastructure, and network-attached storage services. Thrust areas consist of:

- Designing, developing, acquiring, deploying, and supporting classified and unclassified network hardware and services, including high-performance large area network and WAN technologies
- Daily administering, problem resolving, monitoring, and improving SCF and OCF network services such as name and time servers, backup systems, e-mail services, and security components (for example, intrusion detection systems), and integrating new hardware and software to support the various network services
- Deploying and supporting a robust network-attached storage facility for use by the computation systems
- Investigating anomalies flagged by various intrusion detection tools and responding to incidents referred by others

#### *3.2.2.3 Storage*

This project includes all archival-related storage components and their support. At LLNL, PSE funds most HPSS software development, and DVS funds most hardware acquisitions. Computational Systems funds some development, most ongoing support efforts, and some hardware acquisitions. Thrust areas consist of:

- Daily data archive systems and security administration and monitoring
- Parallel file transfer protocol/file transfer protocol/network file system administration, updates, and deployment
- Archive media tracking and reporting
- Archive statistics tracking and reporting
- ASC platform to archive performance tuning
- Visualization platform to archive performance tuning
- Tri-lab inter-site archive data transfer performance tuning

### 3.2.3 Los Alamos Computational Systems

Computational Systems consists of the hardware platforms and system software infrastructure, the network, and data storage. These include personnel assigned to provide these services as well as all other associated infrastructure costs to run the services, for example, hardware and software maintenance, contractor support, and equipment purchases. Quarterly status will be reported by means of metrics, including usage of major ASC computing platforms and data storage, power consumption of the facility, and deferred replacement of systems.

Production Computing provides and supports the classified and unclassified LANL high-performance computing and data storage resources for local and remote tri-lab computing at LANL. Primary requirements are to provide computing cycles and data storage capabilities for the code development and simulation runs supporting many ASC level 2 milestones and DSW deliverables. Computing resources also support level 1 milestones such as the annual weapon system assessments and significant finding resolution for the LANL stockpile weapons, various safety studies, certification with quantified design margins and uncertainties, feasibility concept studies, as well as weapon engineering analysis. Primary customers for the completion of the level 1 and level 2 milestones described above include the Applied Physics and Engineering Sciences and Applications Divisions and their tri-lab counterparts. Production computing is required to provide both the capability computing to allow for the huge size of problems needed for this work as well as the capacity computing to provide for daily work of all users in accomplishing these tasks. Project Production Systems will maintain a close collaboration with systems software research and development being undertaken in the Computer and Computational Sciences (CCS) Division to ensure that the production computing requirements of our user base are delivered for future systems. Unclassified computing systems and infrastructure support the unclassified ASC Alliances as well as all unclassified computing needs for weapons physics.

#### *3.2.3.1 Production Systems*

This project includes all services for computational systems operated by the center for the purpose of developing and running user codes. These services include platform integration, system configurations, computer security, resource management, system administration, and customer-driven system software development. The project is key in the integration of major new capability platforms and also for installing and integrating additional capacity resources to meet user demand. The project works with users to troubleshoot problems experienced with running their applications on new systems, and also works with users to plan and carry out transitions off of older platforms. This project is also required to provide production support of visualization servers.

This project is also required to collaborate with systems research and development efforts in the Computational Systems program element and in CCS Division to usher new technology into production. A requirement is to ensure that system research and development is directed toward the development of systems that will support the production requirements of our users. This effort will also establish new technology on actual emerging production systems and help to test and stabilize the new technology. Current efforts are directed toward collaboration with the CCS Division to refine the science appliance system software for a high-performance computing (HPC) Linux production environment. The project also collaborates with the DVS program element to establish new hardware solutions for visualization servers.

Additionally, this project is also required to provide statistical support to ascertain the reliability of ASC clusters. Group D-1 is responsible for gathering data and reporting it to this project in a timely manner. Thrust areas consist of:

- Computer system support. Conduct daily system administration and monitoring of production systems, infrastructure servers, and desktop systems. Install operating system patches and other software. Monitor systems for security events. Analyze and improve performance of key subsystems, including file systems. Develop scripts and tools to aid in administration. Design and deploy new infrastructure architectures and services.
- Scheduling environment daily management. Provide daily administration, monitoring, and problem resolution of software subsystems used in resource scheduling, including accounting data generation.
- RAS. Continuously improve the end-to-end level of service as seen by the users. Ongoing study and improvements in the stability of large, integrated systems, including the development of improved diagnostic and monitoring capabilities.

#### *3.2.3.2 Networks and Related Services*

The network aspect of Production Computing provides the network technical support to high-end production computing and data storage services for the use of ASC computing. Near-term commitments include ASC Q and HPSS and access to the DisCom WAN through which LANL users can access White at Livermore, Red Storm at SNL, and Purple at Livermore when those systems are available. Network services in the classified partition are required to maintain an environment that is acceptable to users in order to complete their assignments. Increased availability and security require a more automatic network monitoring and intrusion detection in the classified network. Increased network backbone bandwidth within the LANL campus is being planned to support growth in HPSS storage from local and remote ASC computing. Thrust areas consist of:

- Network support. Designing, developing, acquiring, deploying, and supporting classified network hardware and services to support Computational Systems. This includes operating and maintaining the new services such as e-mail, authentication, and Web servers, plus operating and managing the high-performance network backbone, services networks, local paths to ESNet, SecureNet and the DisCom WAN, and the high-performance parallel interface/gigabit systems networks.
- Network intrusion detection monitoring. Monitor and investigate anomalies using the Network Anomaly Detector and Intrusion Report system. Follow up on all suspicious findings. Continue regularly scheduled network scanning of secure systems for potential vulnerabilities.

#### *3.2.3.3 Storage*

Storage provides and supports the LANL data resources needed by the various components of the nuclear weapons program for local and remote tri-lab archiving of data at LANL. Primary requirements are to provide data storage capabilities for the code development and simulation runs supporting many of the ASC level 2 milestones and DSW, as tracked through many of the NNSA level 1 and level 2 milestones. Thrust areas consist of:

- Data archive support. Provide a highly scalable, reliable, and available archive storage service that meets user requirements for preserving their data from ASC computing platforms. Ensure sufficient archive storage bandwidth is available and storage capacity exists to meet user requirements. Provide the tools that enable remote data transfers to/from the LANL archive. Ensure current and future storage components are capable of leveraging parallel technologies and capabilities within the data path.

- Tactical planning: Planning local-site implementation of upgrades and improvements to HPSS configuration to meet archival storage demands of ASC platform users for each successively larger ASC system.
- Remote archival storage support. Troubleshooting network and storage configurations for remote stores to archival storage, either ASC White to LANL HPSS or ASC Q to LLNL HPSS.

## 3.3 Simulation Support

Simulation Support provides support services for computing, data storage, networking, and users, including facilities and operations of the computer centers (including electrical power costs), user Help Desk services, training, and software environment development that supports the usability, accessibility, and reliable operation of high-performance and institutional computing resources at the three laboratories. The following activities define Simulation Support:

- Operate and maintain laboratory facilities that house ASC computers
- Operate laboratory ASC computers and support integration of new systems
- Provide analysis and software environment development and support for laboratory ASC computers
- Provide user services and help desks for laboratory ASC computers

### 3.2.1 Sandia Simulation Support

This element provides funding for personnel engaged in support of analysts and developers that utilize ASC codes and platforms in the performance of their milestone and stockpile support tasks. Training, problem solving, and consulting services aimed at the local capability platforms (ASC Red and Red Storm) as well as general computing assistance in the tri-lab environment are being deployed this year at SNL in concert with the availability of Red Storm. System analysis and programming support for platforms users, including consulting and assistance with applying scaleable I/O in practice, as well as operating system research and development and some integration activities for cluster systems are provided. Infrastructure support costs, such as space and electricity, in addition to security plans and evaluation of security needs on platforms, are supported here as well.

FY05 will present major challenges as new platforms are moved into production, and existing platforms must continue to supply critical cycles to directed stockpile work and ASC projects. Porting of large application codes and improving performance and stability of new systems will occupy a majority of staff time during FY05. Close cooperation with Cray, Inc., (the system provider for Red Storm) will be enhanced by the presence of several Cray support personnel on site at SNL. Immediate feedback to corporate support will be provided by these onsite representatives.

#### *3.2.1.1 User Support and Consulting*

This project provides user assistance and consulting, training and problem identification, analysis and correction for applications and operating systems as needed for capability platforms and other scientific computing resources. It coordinates account management activities within SNL and among tri-lab users. It continues deployment of the Web-based synchronized account request automated process (SARAPE) into the nuclear weapons complex. This project supports early access customers for Red Storm in code conversion activities and tuning and conduct scaling analysis and characterization studies of Red Storm using SNL applications beyond the 7x performance suite used for platform acceptance. ("7x" is the requirement for Red Storm to provide at least a seven-fold improvement in performance over that is provided by ASC Red.) It manages early demonstration runs of applications on Red Storm. It prepares and presents appropriate training sessions and documentation for tri-lab customers. It establishes a customer assistance hotline and coordinates access schedules for system integration, infrastructure development, and Red Storm acceptance testing. Finally, it assists in preparation of Red Storm for limited availability.

#### *3.2.1.2 Analysis and Software Development*

This project provides operating system support for the ASC Red teraops operation system and Cougar on an as-needed basis, effectively keeping the system functioning but not adding features. It continues development and deployment activities for operating systems, run-time systems, system management and RAS subsystems for capacity computing systems and future capability platforms. Coordinate activities and advise on operational aspects of operating systems and file systems issues related to Red Storm limited availability. Add to the existing effort to characterize and improve ASC code central processing unit utilization and efficiencies by including LANL and LLNL codes in the process.

#### *3.2.1.3 Infrastructure Support*

This project funds space and power needs for all scientific computing platforms. It provides facility management personnel supporting continuous 24-hours-a-day, seven-days-a-week operations. It supports maintenance activities of Grid/Globus systems. It coordinates with and supports facilities needs (including some capital equipment expenditures) for future supercomputer installations. Finally, this project supports the level 2 milestone roadmap to a petaops study.

### 3.3.2 Lawrence Livermore Simulation Support

LLNL provides a world-class, high-performance scientific computing capability consisting of computers, storage, networks, and associated development environments and services that enable scientists to perform leading-edge research and scientific discovery. This project is responsible for maintaining and integrating deliverables from Computational Systems, DVS, DisCom, PSE, and PathForward into a reliable scientific computing environment and fostering evolution into a production terascale simulation environment.

Classified and unclassified computing services are provided 24 hours a day, 7 days a week for stockpile stewardship customers computing locally and remotely from ASC-funded sites. The production scientific computing environment includes large SMP clusters, massively parallel systems (in particular classified and unclassified ASC terascale computers), supporting servers, terabyte storage archives, data assessment theaters for visualizing huge data sets, and an interconnected, integrated networking infrastructure. Two scientific computing environments are maintained by the Livermore Computing Program, served largely by expertise within the ICCD; the SCF, a classified environment; and the OCF, an unclassified environment.

Responsibility for the development, integration, and support efforts to maintain and advance LLNL's scientific computing environment are provided by the HPSD, SDD, and NSD. These three divisions of LLNL's ICCD report to the ICCD department head and the ICCD deputy department head. The ICCD division most closely aligned with the Simulation Support Program Element is SDD.

The SDD develops tools, system software, and an application infrastructure that enable efficient and effective use of LLNL's high-performance and institutional computing resources. SDD provides extensive ongoing interaction, coordination, and collaboration with the ASC user community to ensure they have access to and achieve optimum performance from the ASC platforms. SDD also provides user services, training, documentation, and consulting to support the usability, accessibility, and reliable operation of high-performance and institutional computing resources. The SDD consists of the following four groups:

- The Customer Services Group supports users from the multi-lab community and the ASC Alliances by providing a central point-of-contact for help with computer system problems and questions. This group includes the institutional help desk, account management, the HPC hotline, and extensive documentation services.
- The Development Environment Group supports and maintains a large variety of vendor-supplied and locally developed tools (including compilers, debuggers, and libraries) for developing parallel scientific applications. Training and consulting services assist customers in the effective use of these tools.
- The Integrated Computational Resource Management Group is responsible for resource monitoring, workload scheduling, and resource accounting across a computational grid. This includes development and support of the Livermore Computing resource manager and the Simple Linux Utility for Resource Management.
- The Information Management and Graphics Group provides graphics consulting and development support, and designs and develops tools that assist scientists in managing, visualizing, and exploring scientific data and information. The group also operates visualization laboratory facilities, and provides Web and database development and consulting support.

#### *3.3.2.1 User Support and Consulting*

This project includes help desk and hotline centers, user services, training, documentation, and consulting that support the usability, accessibility, and reliable operation of high-performance, institutional, and desktop computing resources. Thrust areas consist of:

- Providing daily technical consulting and user support services
- Responding to customer calls to resolve questions about systems use or status
- Providing account management activities and system event scheduling including technical bulletin publishing
- Administering and maintaining the Remedy HelpDesk system for users' problem reporting and tracking
- Developing and maintaining ICCD Web pages; FY05-specific activity will be to create documentation and training for Purple and BlueGene/L initial systems
- Providing round-the-clock monitoring of all components of the scientific computing environment and responding to problems and service interruptions

#### *3.3.2.2 Analysis and Software Development*

This project includes analysis and software development to enable efficient and effective use of high performance and institutional computing resources. Thrust areas consist of:

- Graphics consulting and development. Provide daily graphics support to the LC user community on all of the production platforms, including debugging graphics-related code, interacting with users, installing new software, and creating prototype front ends.
- Video production, audiovisual, and power-wall support. Provide video production service for the classified and unclassified LC environments. Services include presentations, editing, modeling, and animation as well as providing color output service. Provide support for power walls on the classified and unclassified sides, including coordination of demos and support for managers and scientists presenting work on power walls. FY05-specific activity will be to help users create science run videos of capability runs during the early limited availability period on Purple and BlueGene/L.
- Application development support. Technical consulting and collaborations with customers on issues related to the application code development environment on production systems, including documentation and training. Support a common, usable, and robust application development and execution environment for ASC computing platforms and ASC-scale applications, enabling code developers to more readily meet the computational needs of weapon scientists and engineers.
- Provide integration support for "initial delivery" and "general availability" ASC supercomputers at LLNL. Support other ASC resources across the three defense laboratories so ASC's supercomputers are fully usable for local code development and execution while being well integrated into the tri-lab distributed computing environment. FY05-specific activities will be to help application code developers port and optimize their codes and libraries for Purple.
- Benchmarking. Conduct systems, file systems, and network performance benchmarking studies. Be aware of trends in commercial technology and benchmark these technologies with our current systems.
- Scheduling environment daily management. Daily administration, monitoring, and problem resolution of distributed production control system, LoadLeveler, rotating mass storage, and other software subsystems in resource scheduling. Includes accounting report generation. Responsible for resource monitoring, workload scheduling, and resource accounting across a computational grid. This includes the development and support of the distributed production control system, which provides this functionality within LLNL, and Globus-based grid services, which provides a subset of this functionality on a tri-lab basis. FY05-specific activity will be to port LCRM to Purple and BlueGene/L initial systems.

#### *3.3.2.3 Infrastructure Support*

This project involves continual monitoring and support of the production and infrastructure systems, as well as facilities operated by the center. Thrust areas consist of:

- Maintenance of real property and installed equipment to ensure safe and reliable operation in individual facilities. This can include facilities management; administration and clerical; custodial support; environment, safety, and health team support; supplies and expenses; building operations; and upkeep.
- Facility revitalization for alteration of existing facilities to make space more effectively adapted or utilized for designated purposes, as well as enhancements to improve energy efficiency.

- Support of institutional infrastructure through indirect charges for preventive maintenance, repairs, replacements in-kind, non-cap improvements, and maintenance management activities for roads, electrical utility lines (low voltage) and mechanical utility services at the LLNL site.
- Electricity power supply for offices and computer rooms.

### 3.3.3 Los Alamos Simulation Support

Simulation Support includes all supporting infrastructure for computational services, including Help Desk support, facilities and operations, and analysis and software development of the user environment. All these services directly support nuclear and non-nuclear applications, nuclear safety simulations, verification and validation efforts, and materials and physics modeling, and provide both classified and unclassified resources. This project includes all supporting services for computing and data storage and their users, as well as facilities and operations of the computer centers, user Help Desk services, and software environment development and support.

#### *3.3.3.1 User Support and Consulting*

This project is comprised of three teams: the Integrated Computing Network (ICN) consulting office, responsible for direct customer service to local and remote users of LANL HPC resources, the training and documentation team, responsible for the development and delivery of documentation and training materials for LANL HPC resources, and the external computing support team, responsible for usage statistics and the administrative interface for external HPC users such as tri-lab ASC and ASC Alliances. This project will involve staffing efforts in the ICN consulting office, the external computing support team, and the training and documentation team as well as establishing a baseline customer satisfaction survey. Thrust areas consist of:

- User support services. Daily technical consulting and user support services. The ICN consulting office provides direct customer service to local and remote users of the LANL HPC resources in support of ongoing computing and the ASC program. Respond to customer calls to resolve questions about systems use or status. Conduct account management activities and system event scheduling. Provide administration and maintenance of user problem reporting and tracking systems.
- Web page development and support. Develop and maintain web pages at LANL in support of ASC.
- Operational metrics for HPC environment. Collect additional data regarding machine usage, machine availability, and mean-time-to-failure as needed by various interested parties and make that data more accessible.
- Documentation and training. Will continue to be developed.
- Specific work planned. Provides excellent on-demand support to customers and will be establishing ongoing customer satisfaction surveys to quickly identify and deal with any future shortcomings.

#### *3.3.3.2 Analysis and Software Development*

This project establishes and maintains reliable, available, and scalable capabilities in commercial and custom software development tools for the production ASC clusters. The focus is on established tools and working through issues with their use. This project Works with users to apply these capabilities to solve problems in developing, debugging, and measuring and improving the performance of the applications. It studies and benchmarks performance of the Q machine and other upcoming clusters. It recommends tuning adjustments to the systems and applications for efficient use. Thrust areas consist of:

- Application development support. Technical consulting and collaborations with customers on issues related to the application code development environment on production systems. Support and maintain tools and products needed by users to develop, debug, and optimize their codes. Develop and maintain documentation and arrange training classes upon request.
- User Assistance. Assist users in applying tools to their production and institutional problems. Arrange for training where necessary. Much work in this area is done with TotalView and to a lesser extent with profiling, code coverage, and memory debugging. Tool use assistance is expected to be a higher effort as more people use Lightning, and Lightning grows and moves from a 32-bit to a 64-bit operation.
- Integration and Testing. Integrate and test tools for production resources. This year will see the transition to a 64-bit operation. The unique characteristics of the Bproc environment and the use of the LANL-developed Los Alamos MPI (LA-MPI) will require efforts with vendors to address issues that arise using their products in this environment. Products being enhanced through PSE and PathForward projects will require efforts to make them usable in a production environment.
- Benchmarking. Conduct systems, file systems, and network performance benchmark studies for LANL clusters versus available commercial technologies. Make recommendations on the tuning and use of these technologies to improve application performance on all clusters.
- Third-Party Software. Run the procedures for managing requests for and installations of third-party software on the production systems. Keep up-to-date software inventories. Track the expenditures for software and allows evaluation of the effectiveness of products as support contract renewals come due.
- Production MPI support. Ensure MPI communications are functioning properly on production clusters, especially as changes occur in the production clusters. Support risk mitigation capabilities by working with the science appliance team, Myricom, and Panasas to ensure that MPI Chameleon (MPICH) functions correctly in the BProc environment. Additionally, work continues with Hewlett Packard to ensure both the thread-safe Alaska and MPICH-based MPIs work correctly on Q.
- Support the data transfer and storage archive (HPSS) project. This active project is creating a redundant array of independent tapes and archive alternative capabilities and will continue into 2005. Part of this work is managing the University of Minnesota contract for object archive. This work indirectly supports the LANL remote disaster recovery milestone through its support of HPSS.
- Support underlying communications infrastructure needs for file systems. Assist with study to determine optimal gigabyte per second Ethernet network for Lightning. Identify what the performance of the Q machine should be for studied applications and provide recommendations on how to tune Q to maximize the level of performance for all studied applications. Perform the same activity for Lightning and future platforms.

#### *3.3.3.3 Infrastructure Support*

LANL has structured its infrastructure support into four projects: Operations, Strategic Computing Complex (SCC), Laboratory Data Communications Center (LDCC), and Central Computing Facility (CCF).

The operations project requires staff to provide around-the-clock operations of the LANL's scientific computing resources including high-performance computers such as ASC Q and Lightning and data storage and retrieval systems such as the HPSS. This work is in direct support of the tri-lab's compute resource needs for meeting their ASC milestones for stockpile stewardship. The primary customer is the production systems team, which is responsible for providing computer resources necessary for stockpile stewardship. Customers also include the entire tri-lab user community including LANL, SNL National Laboratory, and LLNL. The staff supports the entire computing environment (classified and unclassified) located in three major computing facilities (the SCC, LDCC, and the CCF).

The CCF, LDCC, and SCC projects require staff to operate and maintain mission-critical equipment (electrical and mechanical systems) that supports high-performance computing systems located in the three computing facilities. The project covers the cost of running the SCC facility including labor, materials and supplies, equipment and installation upgrades, electrical power, and all maintenance contracts associated with critical equipment. It also covers the cost of running the programmatic portion (for example, labor, materials and supplies, and maintenance contracts) of the other two facilities, the LDCC and the CCF. The project provides support for infrastructure design upgrades and computer site preparation for all three facilities. This work is in direct support of the tri-lab compute resource needs for meeting their ASC milestones for stockpile stewardship. The tri-lab community requires the systems to be operational at all times. The main customer is the production systems team, which is responsible for providing compute resources necessary for stockpile stewardship. This project provides the utility support for the high-performance computer systems by striving to ensure continuous and uninterruptible computing to the tri-lab community. Thrust areas consist of:

- Operations support. Provide round-the-clock attendance of computing facilities by the operations team. Monitor all operations and respond to problems. Interface with systems support personnel and hardware engineers.
- Facilities. The Simulation Support budget funds the computing facilities, including the CCF, the LDCC, and the SCC, along with ongoing charges for space and power for the systems. In FY05, we will be completing phase two and three of the SCC utilities infrastructure upgrade. This will provide an additional 3.6 megawatts of power, a 1200-ton chiller, and two cooling towers resulting in total power availability for the main computer room in the SCC of 7.2 megawatts. It is necessary to complete this work to support future platforms brought into the center.

## *3B: Integrated Computing Systems Integration*

### Lawrence Livermore Integration

#### LLNL Platforms

Coordinated contributions from other ASC program elements are required to enable ASC Purple and BlueGene/L to operate as ICS, delivering useful work for ASC and the SSP.

Concurrent deployment of the I/O infrastructure for these systems require integration efforts between Ongoing Computing, PI&P, PSE, and DVS program elements at LLNL. Success will depend on the combined effort of these ASC program elements along with collaboration with IBM platform and archive personnel as well as 10-gigabit ethernet vendors.

The operating system, system libraries, code development and performance analysis tools, math and graphics libraries need to be developed, installed, and stabilized for access by a general user community. To achieve this state, close integration of efforts from PSE is required to assure that the computing environment is available and functional on the system. Ongoing Computing must complete training of system and network administrations, operators, maintenance personnel, and user support personnel.

### LLNL Computational Systems

Security measures are coordinated with SNL and LANL and other groups within LLNL. We work closely with the Simulation Support, DisCom, PI&P, and Advanced Architectures major technical elements.

Each year production computing pays IBM to maintain the HPSS code base and to provide HPSS support. The level of funding from LLNL is between $200,000 and $250,000 per year.

Computational Systems funds a consulting contract with Gleicher Enterprises, L.L.C., for performance analysis and improvement, and interface development and debugging for LC archives.

### LLNL Simulation Support

We strive towards a common code development and execution environment for all production systems coordinated with SNL and LANL. We participate in integration of new platforms and supply benchmarking support and analysis. We have close and active collaboration with Computational Systems, PSE, DVS, DisCom, PathForward, PI&P, and Advanced Architecture major technical elements to meet the needs of our users and to integrate products and services.

Extensive ongoing interaction, coordination, and collaboration with major science and ASC users to ensure they can access and achieve optimum performance from the ASC platforms. We collaborate with the application teams, the weapons designers, and the LLNL ASC Defense Application and Modeling leads at LLNL and at the other two defense laboratories. We also support DSW by enabling efficient access to and effective utilization of our systems and services.

## Los Alamos Integration

PSE, DVS, Platforms, Computational Systems, and Simulation Support work together to provide the computing needed to achieve nuclear weapons program goals, including:

- Research, design, and development of new technology
- Managed introduction into production
- Acquisition and integration of major new platforms

We also collaborate with integrated weapons applications, Verification and Validation (V&V), and Materials and Physics Modeling (M&PM) to establish requirements for the production computing environment and to ensure that major applications will perform as expected on new platforms.

### Sandia Integration

The operation of major computing platforms at Sandia requires substantial additional infrastructure in the form of machine room and WANs, archival storage and data services, visualization, and space, power, and cooling. Support services for operation and maintenance of the large computing platforms are required. Also, a substantial effort is required to provide the users with direct support for using the machines and with indirect support to make the machines more useable.

The machine room and WANs that provide access to Red Storm are provided through a combination of the ASC ongoing computing program, DisCom, and some internal funding.

Archival storage and data services and visualization are provided through the ASC DVS program. The DVS program supplies hardware and software. It also provides direct user support for using the resources that it provides.

The majority of the day-to-day operation and maintenance of Red Storm is provided through the contract with Cray for the machine. Additional support is provided through the ASC ongoing computing program.

The Platforms program element is closely coordinated with the ASC Applications program and with the need to make sure that priority stockpile stewardship and directed stockpile work are completed in a timely manner.

Computational Systems coordinates capital equipment purchases with the DVS and DisCom programs to ensure infrastructure investments match the schedule and capabilities of computational platforms and user environment needs. Simulation Support engages in regular meetings with user support groups at LANL and LLNL and participates in the weekly expedited priority request telecoms, which set priority for capability systems user requests. In addition, the SARAPE Web-based account request system provides a common method for all remote customers to request computer accounts at SNL, both ASC-related and for additional nuclear weapons complex applications. This system was introduced to the user support groups at several nuclear weapons complex locations and is in use by the ASC Alliance Universities for requesting accounts. The DisCom program leads our interactions with the nuclear weapons complex for common access methods and authentication for remote users. The Simulation Support project implements these authentication methods on the computational platforms, while the Computational Systems administrators maintain current access lists and password files including remote authorized users. Coordination with the Sandia password control organization provides a timely method for addition and removal of active accounts on all scientific computing platforms.

## *3C: Integrated Computing Systems Risk Assessment*

The following table summarizes top risks and mitigation approaches for ICS:

**Table 3C-1. Top Risks for Integrated Computing Systems**

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| **Physical Infrastructure and Platforms** | | | | | |
| **Sandia Red Storm** | | | | | |
| 1 | Seastar ASIC fails to meet performance requirements | High | Moderate | Medium | Control: Red Storm will be operated with the reduced interconnect performance provided by the initial Seastar ASIC until respin of chip can provide full performance. |
| 2 | Seastar ASIC delivery is delayed sufficiently to impact Red Storm delivery schedule | High | Moderate | Medium | Control: There is no fall back for late delivery of the Seastar ASIC. The Seastar ASIC is about four months behind schedule, however, it has been released for production and as a result no further delays associated with the Seastar chip development are expected. |
| 3 | System software fails to meet functional and/or performance requirements at time of Red Storm delivery | Moderate | High | Low | Control/Assumption: System Software development will continue after delivery of Red Storm to SNL. In addition, SNL has experience maintaining system software for a system similar in size to Red Storm and is prepared to actively work on improving the Red Storm system software if necessary. |
| **Lawrence Livermore ASC Purple** | | | | | |
| 1 | New node – POWER5 SMP node is a new node not previously used for ASC simulations | Moderate | Low | Low | Assumption: The node will not be available in time to incorporate it in the EDTV system. However, this node will see widespread commercial service and will general availability as part of IBM's product line in CY04Q1, three quarters before being delivered with Purple. |

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| 2 | New high-speed interconnect – the Federation switch and software will be new with Purple. | Moderate | Moderate | Medium | Control: EDTV system will demonstrate operation and scalability of this critical technology. |
| 3 | New high-speed adapter – the Federation switch adapter and multiple switch planes will be new to Purple. | High | Moderate | Low | Control: This technology will be tested on the EDTV system with two planes of interconnect; we are relying on IBM for extensive testing in simulation. Early 1280-node portion of Purple will demonstrate full 3-stage switch. |
| 4 | New system administration software (cluster system management). | Low | Low | Low | Control: EDTV system will demonstrate operation of this critical technology. |
| 5 | New file-system software – GPFS over fiber channel. | Moderate | High | Medium | Control: EDTV system will demonstrate operation of this critical technology; will demonstrate with 1 petabyte disk of disk (half of Purple scale) at throughput of 50 GB/s, ramping to full scale after demonstration of Purple. |
| 6 | Schedule risk – system is late | High | Low | Low | Control: Early shipment of 256-node Purpura system will provide advanced warning of significant schedule risk. |
| 7 | Scalability risk – system software and hardware doesn't scale | High | Moderate | Low | Control: EDTV and Purpura systems provide intermediate scaling platforms on way to full system. |
| **Lawrence Livermore BlueGene/L** | | | | | |
| 1 | Large node count – 65,000 nodes | Moderate | Moderate | Medium | Control: Extensive R&D effort. 512-way prototype system. 128-node apps development loaner to LLNL in FY04. Phased build gives early access to increasingly larger systems. |

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| 2 | New file system | High | Moderate | Medium | Control: 128-node apps development loaner to LLNL in FY04. Phased build gives early access to increasingly larger systems. |
| 3 | New system management software | Moderate | Moderate | Medium | Control: Additional funding has been obtained to improve system management software. |
| **Computational Systems** | | | | | |
| **Sandia** | | | | | |
| 1 | Lustre file system fails to support Red Storm scaling needs | High | Low | Medium | Avoidance: Continue low-level support of parallel virtual file system Version 2 development/ deployment in the cluster computing regime. Use multiple Unix file systems as temporary fallback. |
| 2 | Hardware and/or software problems accelerate the demise of ASC Red before Red Storm is in general availability | Moderate | Low | Low | Assumption: Reduce overall hardware components as devices fail. Put operating system into stasis with no new features. Upgrade capacity platforms to absorb ASC Red workload. Defer scaling work to Red Storm. |
| **Lawrence Livermore** | | | | | |
| 1 | Platform plans change or deliveries delayed. | High | High | High | Control: Promote standard solutions to accommodate changes; encourage communications to anticipate impacts. |
| 2 | Delivered hardware or software may be unstable or not perform as expected. | Moderate | High | Medium | Control: Promote source availability for faster diagnosis and fix; encourage early initial hardware deliveries when possible to identify problems early. |
| 3 | Difficulty hiring and attrition may lead to wrong skill mix. | Moderate | Moderate | Medium | Control: Train existing staff when possible; shuffle staff to highest priority efforts. |

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| 4 | Commercial platform or ISV partners may have changes in business plan or organization that impact deliverables or discontinue service. | Moderate | Low | Medium | Control: Promote standard solutions; have secondary sources; promote open source products. |
| 5 | Security rules may change impacting security software infrastructure. | Low | Low | Low | Assumption: Promote standard solutions to accommodate changes; encourage communications to anticipate impacts. |
| **Los Alamos** | | | | | |
| 1 | Availability/ reliability of power (Institutional issues). | High | Moderate | Medium | Control: 3rd power line for LANL, investigating power backup options for SCC. |
| 2 | Availability of trained, cleared staff. | Moderate | High | Medium | Control: |
| 3 | Shortage of computing resources for program deliverables. | High | High | High | Control: Increase capacity computing, leverage low cost systems. |
| 4 | Global file system for Linux clusters of scale. | Moderate | Low | Medium | Control: Lustre, Panasas projects. |
| 5 | Escalation of operational costs as systems and infrastructure grows. | High | Moderate | Medium | Control: Consolidation of systems and facilities, phasing out older systems, transition to systems software enabling more efficient management, staff training and improvement. |
| 6 | Inadequate resources for development and support of open source system software | High | Low | Medium | Control: Coordinate system software for large Linux clusters as far as possible across tri-lab computing community and leverage development and support efforts. |

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| **Simulation Support** | | | | | |
| **Sandia** | | | | | |
| 1 | Each lab's cyber security mechanism for two factor authentication control is different and are not interoperable. | Moderate | High | Medium | Risk Transfer: A common exchange standard for authentication credentials must be developed and maintained if the current DCE cross-cell trust relationship is to be retained. The conversion routines for each lab's system to the common format must be supported indefinitely. |
| **Lawrence Livermore** | | | | | |
| 1 | Platform plans change or deliveries delayed. | Moderate | High | Medium | Control: Promote standard solutions to accommodate changes; encourage communications to anticipate impacts. |
| 2 | Delivered hardware or software may be unstable or not perform as expected. | Moderate | High | Medium | Control: Promote source availability for faster diagnosis and fix; encourage early initial hardware deliveries when possible to identify problems early. |
| 3 | Difficulty hiring and attrition may lead to wrong skill mix. | Moderate | Moderate | Medium | Control: Train existing staff when possible; shuffle staff to highest priority efforts. |
| 4 | Commercial platform or ISV partners may have changes in business plan or organization that impact deliverables or discontinue service. | Moderate | Low | Medium | Control: Promote standard solutions; have secondary sources; promote open source products. |
| 5 | Security Rules may change, impacting security software infrastructure. | Low | Low | Low | Assumption: Promote standard solutions to accommodate changes; encourage communications to anticipate impacts. |

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| **Los Alamos** | | | | | |
| 1 | Platform plans change or deliveries delayed. | High | High | High | Control: Promote standard solutions to accommodate changes; encourage communications to anticipate impacts. |
| 2 | Delivered hardware or software may be unstable or not perform as expected. | Moderate | High | Medium | Control: Promote source availability for faster diagnosis and fix; encourage early initial hardware deliveries when possible to identify problems early. |
| 3 | Difficulty hiring and attrition may lead to wrong skill mix. | Moderate | Moderate | Medium | Control: Train existing staff when possible; shuffle staff to highest priority efforts. |
| 4 | Commercial platform or ISV partners may have changes in business plan or organization that impact deliverables or discontinue service. | Moderate | Low | Medium | Control: Promote standard solutions; have secondary sources; promote open source products. |
| 5 | Security Rules may change, impacting security software infrastructure. | Low | Low | Low | Control: Promote standard solutions to accommodate changes; encourage communications to anticipate impacts. |
| 6 | User software environments continue to diverge across tri-lab sites and platforms reducing productivity of the user community. | Moderate | High | Medium | Control: Promote standard user software environment and tools across tri-lab computing community as far as possible. |

# SECTION 4: UNIVERSITY PARTNERSHIPS

The University Partnerships program has three key elements: the Academic Strategic Alliance Program (ASAP), ASC Institutes, and Graduate Fellowship Programs in computational science and high-performance computer science. Training and recruiting individuals with skills critical to the SSP are integral components of each of these three program elements.

The ASAP engages the U.S. academic community in making significant advances in science-based modeling and simulation technologies. Research conducted through this partnership contributes to the knowledge base required to demonstrate the capabilities of modeling and simulation across a broad spectrum of science and engineering applications using the most powerful computers in the world. The computing problems tackled by the ASAP are not classified and do not involve nuclear weapons research, nevertheless, they mirror in complexity the simulation problems faced by the SSP. Furthermore, the concepts and tools being developed to solve these problems are broadly useful to the SSP as well as to other U.S. national security efforts.

Each of the three DP laboratories has established a computer science institute to advance basic and applied research initiatives in computational sciences in support of the ASC Program. The Institutes attract university experts to work with laboratory staff in these research initiatives, and further engage U.S. universities by providing central facilities at each laboratory to encourage extended visits by faculty and students and to serve as a focal point for interaction with laboratory scientists. The Institutes also jointly fund and manage the High-Performance Computer Science Graduate Fellowship Program, encouraging the training of computer scientists in areas of critical need to the ASC Program. The Krell Institute administers this four-year program. Fellows participating in the program are required to do at least one practicum (usually for three months) at a defense laboratory.

The Computational Science Graduate Fellowship Program, jointly funded by the DOE Office of Science and NNSA/DP, is administered by the Krell Institute to support highly capable individuals pursuing doctorates in applied science or engineering disciplines with applications in high-performance computing. The fellowship program requires completion of a program of study that provides a solid background in three areas: a scientific or engineering discipline, computer science, and applied mathematics. A practicum working with researchers at a DOE or NNSA/DP laboratory is required of every fellow for at least one three-month period during the term of the fellowship.

## *4A: University Partnerships Activities*

### 4.1 Academic Strategic Alliance Program

The ASAP strategy is to accelerate the emergence of new scientific methods and associated technology for high-performance, computer-based modeling and simulation by supporting strategically chosen research at U.S. universities. High-performance modeling and simulation have become key partners with theoretical and experimental studies. Together they are proving to be invaluable tools for acquiring a fundamental understanding of the scientific and engineering problems critical to the success of ASC and the SSP. The applications being developed and run on ASC computing resources by the ASAP university teams are unclassified and focus on significant scientific needs outside of the Nuclear Weapons Program, but they are similar in difficulty and complexity to the problems encountered in the SSP.

The major goals of the ASAP strategy are as follows:

- Solve science and engineering problems of national importance using large-scale, multidisciplinary modeling and simulation
- Establish and validate large-scale, multidisciplinary modeling and simulation as a viable scientific methodology across stewardship-related applications (such as, those requiring coupled multi-physics and complex simulation sequences)
- Enhance the overall ASC goals by engaging external expertise in computer science, computational mathematics, and simulation science and engineering fields of interest
- Couple ASAP efforts with ongoing ASC and SSP projects in the NNSA/DP laboratories
- Leverage relevant basic science, high-performance computing systems, and problem-solving environment research in the academic community
- Strengthen academic training and research in areas critical to the long-term success of ASC and the SSP
- Strengthen ties among LLNL, LANL, SNL, and U.S. universities

### 4.1.1 Relationship to Other Advanced Simulation and Computing Strategies

The Alliance strategy is well coordinated with all aspects of ASC. A number of ASC personnel are active participants in all phases of the Alliance collaborations from writing initial solicitations to selecting awardees, setting priorities, monitoring ongoing work, and interacting on research of common interest. In this way, the ASAP projects encourage mutually beneficial collaborations among the university partners and ASC researchers at the NNSA/DP laboratories.

### 4.1.2 Implementation

The Alliance strategy has two program levels to engage universities in meeting both near- and long-term goals:

- Level 1, Strategic Alliances: Major centers engaged in long-term, large-scale, unclassified, integrated, multidisciplinary simulation projects along with supporting computer science and computational mathematics representative of ASC-class problems
- Level 3, Individual Task Collaborations: Focused projects initiated by individual ASC laboratory researchers working on near-term, ASC-related problems

The five strategic Alliance Centers are in their second five years of funding. Each center has selected a large-scale application of national importance for analysis that requires coupling and integrating computer-based simulations from multiple disciplines. In addition to major advances in the areas of application, these efforts provide unprecedented opportunities for important discoveries in basic and applied science areas especially relevant to ASC goals and the broader SSP. These applications are unclassified and highly relevant to nationally significant scientific, engineering, and economic priorities. In support of their research activities, the centers are collectively given access to approximately 5 percent of ASC computing resources or their equivalent at the NNSA/DP laboratories. An additional 10 percent of the San Diego Supercomputer Center system, Blue Horizon, is also available to the centers.

The Individual Task Collaborations (Level 3) are funded across ASC by the three NNSA/DP laboratories to work on specific problems where outside expertise is required. They typically are smaller awards ranging from $50K to $100K per year.

### 4.1.3 Alliance Program Management

The ASAP is a joint management responsibility of DOE/NNSA and LLNL, LANL, and SNL. An Alliance Strategy Team (AST) has overall responsibility for the Level 1 programs and coordinates the following:

- Computer Resource Team (CRT), which manages the computing resources for the Alliance
- Tri-Lab Sponsor Teams (TSTs), which facilitate interactions among each of the Level 1 centers and the three NNSA/DP laboratories

#### *4.1.3.1 The Alliance Strategy Team*

The AST manages and coordinates ASAP activities. The AST ensures that the ASAP strategic goals are met, provides a unified strategy for the NNSA/DP laboratories and other Alliance projects, and organizes annual reviews of each center and other projects as needed. Specific management tasks include: working with NNSA to enable success of the ASAP and with the CRT to ensure that computer resources and access are in place for Level 1 centers, establishing annual external reviews of the centers, identifying—with the TST—issues needing resolution in each research program and coordinating interaction responsibilities with the TSTs.

Specific AST management milestone activities planned for FY05 are listed below.

- **External Review of Level 1 Centers**: To provide an effective review of each year's progress, the AST organizes two-day site reviews at each of the five centers, usually in October following the just-concluded project year. External review teams (one per center) conduct the reviews. Team members are knowledgeable technical experts from across the disciplines relevant to the center's work. Also in attendance are representatives from DOE/NNSA HQ, the defense laboratories, and the center's TST. The review's objective is to examine the center's progress. Each review concludes with a written report to NNSA, the DP laboratory ASC program leaders, and the center director.
- **Center Project Lead Meetings and Workshops**: While five ASAP centers of excellence are working on distinct simulation problems, each has technical challenges in common with the other centers that include computer science, computational math, physics, and engineering issues. To facilitate cross-center awareness, potential collaborations among centers, and laboratory interaction, at least one center meeting/workshop normally is held for participants from the centers and laboratories each year. The AST facilitates the organization of this meeting in collaboration with the TSTs and centers.
- **Center Reporting**: Each Level 1 center is contractually obligated to update annually its simulation development roadmaps and timelines, implementation plans, and budget and staffing plans, and to provide cross-center interaction plans, ASC computer utilization plans, and annual reports. All except the annual report are due in September; the annual report is due by November. The AST reviews these reports.

### 4.1.3.2 The Computer Resource Team

ASC has committed up to approximately 5 percent of its computational resources to the Alliance Program for Level 1 center access. Because of technical difficulties in switching ASC platforms from running in classified mode to unclassified modes, the laboratories make systems available to the Centers that are running in only unclassified modes. Access needed for Level 3 researchers may be arranged at the discretion of individual laboratories. DOE has also made available 10 percent of the computational resources of the Blue Horizon system at the San Diego Supercomputer Center, specifically targeted for use by foreign nationals from sensitive countries, but available to all Alliance Center users. The CRT provides uniform computer access policies and procedures toward achieving efficient use of the machines for ASC Alliance universities, the principal university users of these assets.

The highest milestone is ensuring that the Level 1 centers get access to up to approximately five percent of ASC platform capabilities to meet their goals. To support this, access mechanisms and procedures for the Alliance participants are currently in place and will be updated as required. These include procedures for obtaining accounts and any required approvals for the use of the platforms. Usage by Level 1 centers is monitored monthly, and mechanisms ensuring balanced access across the centers are in place. Training and technical assistance in the use of ASC platforms is offered as needed. A monthly teleconference among the CRT members is held to ensure communication between the laboratories and the Level 1 centers is maintained.

Each center works with a TST of two technical representatives from each laboratory; one represents the application topic for the university and the other represents computational mathematics and computer science. Each center has a different TST.

The TSTs facilitate interactions between the laboratories and the centers. They also monitor the progress of the center against contractual requirements and strategic direction. The TSTs meet with their respective centers individually and collectively as needed during the year. The TST lead, in particular, interacts extensively with the center director during the year on a range of technical, contractual, and other matters. In addition, the TSTs participate in informal mid-year project reviews. The AST also meets with selected TST members as issues of importance to various aspects of the project arise. For FY05, the following TST milestones are scheduled at each center:

- **Annual External Review of Level 1 Centers**: TSTs will make recommendations to the AST for the review team members. They also will assist the AST and the centers in arranging the agenda for the site visits. Finally, they will be present at the reviews to answer any questions from the review team related to the TST's role.
- **Project Reviews**: TSTs will meet with the centers at least twice a year (this could be more often depending upon the need). At these informal reviews, the TSTs will provide technical comments and suggested opportunities for laboratory collaborations.
- **Center/Laboratory Facilitation**: TSTs will work with the NNSA/DP laboratories and the centers to encourage collaboration and information exchange. In addition, TST members will take responsibility for forwarding access exceptions for approval if required by the Foreign National Access Policy.
- **TST Briefing of Laboratory Upper Management**: TST members will join with ASC project managers and AST members in briefing their laboratories' upper level management on the progress of Level 1 centers and benefits accruing to the DP laboratories from laboratory/center interactions.

- **Yearly One Program–Three Laboratories (OPTL) Milestone**: All funding budgeted for the ASAP must go to the universities via contracts. Miscellaneous expenses incurred by the laboratories in support and management of the ASAP are funded on an individual case basis by ASC OPTL program. OPTL provides resources and management as appropriate to meet specific management needs. For FY05, activities sponsored by OPTL will include working with AST, CRT, and TST to ensure effective interactions through Center visits by laboratory personnel and others, laboratory/center meetings, cross-Center meetings and workshops, and NNSA and TST reviews. OPTL funding also pays travel expenses of external reviewers and meeting expenses. In addition, OPTL contract managers will work with the AST to ensure the satisfaction of contractual obligations and efficient placement of university contracts.

### 4.1.4 Level 1 Strategic Alliance Centers

#### *4.1.4.1 California Institute of Technology, Center for Simulating Dynamic Response of Materials*

**Project Description.** The primary goal of the Center is the development of an integrated simulation capability that comprises the Virtual Test Facility (VTF), a suite of computational engines that are capable of conducting high-performance computations relevant to the simulation of high velocity impact experiments. The simulation capability is validated using carefully coordinated experiments. The chief components are a 3D parallel unigrid Eulerian solver with level set capability, a three-dimensional parallel AMR computational fluid dynamics solver utilizing the Grid Adaptive Computational Engine adaptive grid environment, a three-dimensional parallel Lagrangian solid mechanics solver with adaptive meshing, facilities for checkpointing and visualization, and a Python scripting environment (Pyre) to integrate the computational engines and provide a uniform environment for running the simulations. In addition, the VTF implements a fluid-solid coupling algorithm that employs level set technology to enable coupled simulations in which the fluid mechanics is performed using the Eulerian facility, and the solid mechanics is performed using the Lagrangian facility.

**FY05 Goals:**

- Integration Capability Simulation. Detonation-fracture simulations: We will carry out detailed simulations of detonation fracture simulations with full and reduced reaction chemistry. Converging shock simulations: We will carry out large scale converging shock large eddy simulations (LESs) utilizing AMR for both phase 0 and phase 1 validation experiments.
- Compressible turbulence. Converging shock experiment: The completion of Phase 0 and Phase 1 simulations of the converging- shock validation experiment, and comparison with data from the validation experiment. Turbulence modeling: Extension of the LES of Richtmyer-Meshkov instability, driven by incident self-similar shocks, to both cylindrical and spherical geometries. The AMR in Object oriented C++ (AMROC) framework will be essential for this work. Completion of LES of the plane turbulent combusting jet and extension of this to the axisymmetric combusting jet. Development of a sub-grid-scale model for subgrid flame holes.
- Solid Dynamics. First principles calculations: We plan to calculate diffusion barriers for aluminum vacancies near dislocation, diffusion barriers for Al vacancies near grain boundaries, transition paths for iron phase transformations, and twin-boundary energies for Fe, and to implement the Car-Parrinello tight-binding model for Fe. Mesoscopic calculations: We plan to implement the level set model of void coalescence and integrate models of twinning and dislocation structures into our

direct numerical simulation polycrystal model. Macroscopic calculations: We plan to integrate variational r-adaption as well as variational integrators into the Virtual Test Facility. We plan to verify our graph-implementation of fragmentation and contact into the VTF. Validation: We plan to continue validation runs for the tube-detonation experiment, validation runs for shear-compression experiment and validation runs for our dynamic fracture experiment.

- Computational and Computer Science. Development of component based solid and fluid solvers: The existing solid and fluid solvers are currently undergoing a major redesign with an emphasis on generic programming. First public release of pyre: We expect to be able to release pyre 1.0 by the third quarter of FY05. Pyre on the grid: The advent of pyGlobus from Lawrence Berkeley National Laboratory will allow the framework to discover available remote hosts, storage facilities and other computational resources.
- Materials Property Methodology. Software: FY05 will see the integration of the comprehensive molecular dynamics framework with Pyre. The framework computational engines will be exposed to Pyre methods, allowing full-scale simulations to utilize domains of atomistic calculations. Quantum Monte Carlo methods will be finalized and delivered to allow arbitrarily accurate predictions of structures and energies along reactive pathways and will be compared to DFT methods for basis set development.
- Validation. Detailed experiments of shear compression of Tantalum and Iron – comparison with direct numeric simulation. Comparison of detonation fracture data with simulation. Phase 0 and Phase 1 converging shock experiments with comparison to simulation. Detailed validation of cohesive law and fracture phenomena for homalite.

#### *4.1.4.2 Stanford, Center for Integrated Turbulence Simulation*

**Project Description:** The goal of the ASC Alliance Program at Stanford University's Center for Integrated Turbulence Simulations is to build a detailed computational simulation of a jet engine. This requires modeling the key engine components, including the compressor, combustor, and turbine. The major challenges involve not only developing models for the individual components but integrating them into a unified model in order to study their interactions. The resulting integrated models examine many characteristics, including turbine blade vibrations, rotating stall in the compressor, instabilities as the jet fuel burns in the combustor, and heat transfer from the hot combustion products to the first rows of blades of the turbine. In addition, the streaming supercomputer project aims to develop a scientific computer that offers an order of magnitude or more improvement in performance per unit cost compared to cluster-based scientific computers built from the same underlying semiconductor and packaging technology.

**FY05 Goals:**

- Combuster Group goals include: Complete analysis of single sector Pratt & Whitney combustor simulation, and perform multi-sector combustor simulations to investigate periodicity and patterning/hot streak formation. Complete work on a mesh refinement algorithm and define adaptivity criteria suitable for LES. Complete and validate unstructured particle level set solver. In supporting combustion science, we will validate the extended Flamelet/Progress Variable model with experimental data, and develop, implement, and validate soot models for turbulent combustion based on unsteady flamelet models. We will perform direct numeric simulation of the primary atomization using the LSVS method to further validate it and to develop appropriate large surface structure subgrid models. We will implement and validate models to account for finite-size effects in dense spray. We will continue to work closely with Pratt & Whitney to integrate Charles David Pierce into their design cycle and to develop a suite of validation cases.

- Turbomachinery Group goals include: complete the implementation and demonstrate/validate the capability of conservative mismatched block interfacing, the Lower/Upper Symmetric Gauss Seidel scheme, the non-linear frequency domain (real approach) method, adaptive wall functions, and enhancements to the v2-f model (for rotational behavior). Begin implementation of the preconditioned, semi-coarsening multigrid approach for the solution of the governing equations. Demonstrate 5x–10x speedup on both steady-state (external aerodynamics) and unsteady (NASA stage35 and isolated rotor) test cases derived from the use of the algorithms described above. Make improvements to the v2-f model for flows in turbines and compressors and develop transition prediction methodologies and corrections for turbulence models in flows with strong rotation. Conduct large-scale simulations: three-dimensional rotating stall calculations, flutter/aeroelastic analysis of industrial cases with a full non-linear approach, and Immersed Boundary Reynolds-Averaged Navier Stokes simulations of the cooling flow inside turbine blades.
- Integration Group goals include: The main goal for FY05 is to perform an integrated LES/Reynolds-averaged Navier Stokes computation for the reactive flow in the combustor and the first part of the turbine using the PW6000 geometry. The purpose of this simulation is to analyze the migration of hot streaks from the combustor into the turbine. In preparation for integrated compressor/combustor/turbine simulations with the goal of studying combustion instabilities, interface boundary conditions for fully compressible reactive flows have to be formulated. The emphasis will be on the accurate description of the dynamics of the pressure field.
- Merrimac Group goals include: The high-radix network technology will be transferred to Cray. The optimized Brook to Merrimac compiler will be completed. Performance results for complex, multi-node applications on the Merrimac simulator and a controlled comparison of stream processor to conventional processor will be carried out. Architecture studies on conditionals, aspect ratio, variable-rate streams, and scatter-add will be performed. Finally, an analysis of how stream processing can be integrated into conventional and vector processors will be completed.
- Merrimac Applications Group goals include: Present a complete study of the multi-node Merrimac for various applications. The goal is to evaluate the performance of the applications, and design of the language and compiler and to assess memory consistency, cache coherency and segmentation. The implementation of streaming-based flow solver with multigrid will be completed. Getting good performance for multigrid is challenging since there is little computational work to perform on coarse grids. Implementation of parts of Charles David Pierce will be completed in particular the weighted essentially non-oscillatory discretization scheme. Testing performance for this particular algorithm will give us representative results for the entire code. Finally we will start working on other applications, in particular hydrocodes of interest to NNSA.

#### *4.1.4.3 University of Chicago, Center for Astrophysical Flash Phenomena*

**Project Description.** The goal of the Center is to solve the long-standing problem of thermonuclear flashes on the surfaces of compact stars, such as neutron stars (x-ray bursts) and white dwarfs (novae), and in the interior of white dwarfs (Type Ia supernovae). This remarkable problem includes physical phenomena such as the accretion flow onto the surfaces of these compact stars; shear flow and Rayleigh-Taylor instabilities on the stellar surfaces and interiors; ignition of nuclear burning under conditions leading to convection; and either deflagration or detonation, stellar envelope expansion, and the possible creation of a common envelope binary star system. The Center's scientific goal is realized by means of the construction of a multi-dimensional, multi-physics, simulation code, which is able to carry out numerical simulations of the various aspects of the "FLASH problem."

**FY05 Goals:**

- Astrophysics. The primary scientific objective of the center during the next two years will be to carry out large-scale, integrated, multi-physics simulations of Type Ia supernovae. Specific milestones for Type Ia supernova simulations for FY05 include: extensive 3D simulations of the deflagration phase, enabling us to explore the sensitivity of the outcome to the location and the number of ignition points; and extensive 2D simulations of the detonation phase, enabling us to determine the energy and the nucleosynthetic yield of the explosion.
- Computational Physics and Validation. Specific milestones for FY05 include: applications—development of a data interface for the radiation transfer code that will be used to calculate light curves and spectra from our Type Ia supernovae models; and code validation—initiation of a collaboration with Harry Robey and Bruce Remington (LLNL) and Paul Drake (University of Michigan) on laser-driven experiments.
- Code. Specific milestones for FY05 include: migrating the remaining physics modules to FLASH 3, refining it, and making it robust enough to replace FLASH 2.
- Visualization, Computer Science, and Basic Physics. The important efforts of these groups in support of the FLASH code and the FLASH problem will continue in FY05.

#### *4.1.4.4. University of Illinois, Center for Simulation of Advanced Rockets*

**Project Description.** The goal of the Center is the detailed, whole-system simulation of solid propellant rockets from first principles under both normal and abnormal operating conditions. The design of solid propellant rockets is a sophisticated technological problem requiring expertise in diverse subdisciplines, including the ignition and combustion of composite energetic materials; the solid mechanics of the propellant, case, insulation, and nozzle; the fluid dynamics of the interior flow and exhaust plume; the aging and damage of components; and the analysis of various potential failure modes. These problems are characterized by very high energy densities; extremely diverse length and time scales; complex interfaces; and reactive, turbulent, and multiphase flows.

**FY05 Goals:**

- Re-usable solid rocket motor (RSRM) simulations — Semi-annual simulations of RSRM are planned to exercise the then-most recent features of Rostar. RSRM simulations will increase in complexity and machine demand through the end of DOE/NNSA support, concluding with a 10,000 +/- processor simulation run in 2007. — March 2005, September 2005, semi-annually thereafter
- Titan IV case rupture accident — In this simulation, the pressure builds up until the case fails. In test firing an early design, a rocket motor exploded violently destroying the test stand, but there was no propellant detonation. (By the time we implement the required remeshing capability, we expect to have an advanced material model for the propellant that includes the effects of voids and dewetting.) — 2005

- RSRM complete normal burn — The ignition transients for the Space Shuttle booster are well characterized in the open literature, and we have access to extensive test data. An especially difficult aspect of simulating the entire history of a large motor is reducing the run time. For a fluids mesh that is fine enough to allow accurate turbulence modeling, for example, time zooming techniques under consideration will be required to reach 120 seconds of physical problem time. — 2006
- Algorithm for propellant regression along case implemented
- Automatic insertion of cohesive elements in Rocfrac verified
- Implementation of remeshing for tetrahedral meshes completed

#### *4.1.4.5 University of Utah, Center for Simulation of Accidental Fires and Explosions*

**Project Description.** The focus of the Center is to provide state-of-the-art, science-based tools for the simulation of accidental fires and explosions, especially in the context of handling, transporting, and storing highly flammable materials. The ultimate goal of C-SAFE is to simulate fires spanning a wide range of accident scenarios. Such problems require knowledge of the fundamental chemistries of gases and solids that drive fires and explosions, the turbulent flows that feed the fires, the convective and radiative heat transfers, and the underlying response of the structures that causes them to explode.

FY05 Goals:

- Our Uintah simulation software is designed to support team integration by separating parallelism from the application component scientific codes. The major ongoing projects within the Computer Science team to support this integration strategy are: use the BlueGene/L architecture to push the limits of parallel scaling properties; investigate porting our code to the Red Storm architecture; scheduler redesign to improve MPI efficiency, perhaps using threads; particle AMR research and implementation; computational fluid dynamics AMR improvements; miscellaneous machine and framework fixes, performance analysis and improvements; ongoing work in dynamic load balancing; visualization methods for AMR; methods for volume rendering AMR grids; better integration of other visualization methods; better particle visualization; combustion visualization; and time-varying remote visualization (data management).
- The focus of the Fire Spread team during the next year will be the verification, validation, and qualification of the fire components and algorithms. Our goal is to critically assess the confidence we have in fire simulation results via a well-defined methodology. This methodology includes verification and validation at five levels: unit problems, coupled problems, benchmark cases, subsystem cases, and the complete system. The unit problem level represents the decomposition of the complete system into the components of the multiphysics problem.
- The Container Dynamics team will have three main areas of focus in FY05: implementation of the Fire Spread models for mixing, reaction and radiation into the integrated ICE/MPM code for performing the integrated end-to-end simulation; incorporation of functional AMR technology in both the ICE and MPM components; and creation of a formal verification and validation effort for the individual components (MPM and ICE) and our combined solution strategy. Several large-scale parallel simulations will be run in conjunction with the efforts described above. Note: ICE (Implicit-Continuous-Fluid-Eulerian) is a computational fluid dynamics code originally developed at LANL, and MPM (Material Point Method) is a

computational algorithm for treating the motion of solid materials on a structured Eulerian computational grid.

- The Molecular Fundamentals team is tasked with providing the scientific underpinnings for subgrid-scale models that allow the macroscale simulation to properly reflect the underlying chemical and physical properties of the materials in the computational domain. Some of the specific ongoing tasks are: kinetics of soot formation; optical properties of soot; reaction rate constant calculations from quantum molecular dynamics; reaction mechanisms for condensed-phase high-melting explosive decomposition; combustion simulations with advanced kinetics; coarse-grained simulations of model estane/ high-melting explosive/plasticizer systems; and mesoscale simulations of granular materials.
- Validation has been a major theme since the inception of the center. Major tasks for FY05 include: continuing a formal verification and validation program for soot formation in fuel fires, including both laboratory experiments and predictive computational modeling; continuing our efforts to model initiation and growth of soot particles at a molecular scale, and connecting those models to grid scale computational models; and planning three large-scale explosion tests at the Alliances Technologies, Inc., Thiokol facility with a focus on predicting explosion violence and measuring effects of nonuniform heating of the container.

## 4.2 Institutes

The ASC Institutes at each laboratory serve both as vehicles to foster basic and applied scientific research at the laboratories and as focal points for laboratory-university interactions in support of the ASC Program. The Institutes enable cutting-edge research activities in computer science, scientific computing, and computational mathematics at the laboratories relevant to the ASC Program. In addition, the Institutes facilitate laboratory scientists and academic collaborators to work together to explore challenging computer/computational problems that cut across ASC Program elements or are likely to have long-term impact on our modeling and simulation capabilities.

Each institute provides an open facility to support extended visits by faculty and students. Since these facilities are located outside secure areas, they provide a simplified way to enhance interactions between visiting faculty/students and laboratory scientists.

Recognizing the scarcity of U.S. citizens enrolling for advanced degrees in fields crucial to the success of ASC, we have enhanced these institutes by establishing High Performance Computer Science Graduate Fellowships. This fellowship program is open to highly qualified U.S. citizens who are senior undergraduates or in their first or second year of graduate study at a university within the United States. Applicants must be pursuing or planning to pursue a Ph.D. in computer science with an emphasis on high-performance computing. In addition to receiving a year-round stipend, equipment, and travel funds, students spend at least one practicum (research assignment) for an extended period working with researchers at the sponsoring DP laboratory. The time spent in the practicum provides students with an opportunity to discover both the level of technical excellence at the laboratories and the exciting challenge of applying supercomputers to complex physics and engineering problems.

### 4.2.1 Sandia Computer Science Research Institute

The CSRI has established a research center in areas of computer and computational science critical to the laboratories' and the DOE's mission. It works to identify external research collaboration that will impact ASC objectives and funds, primarily work by university researchers (faculty and students) working onsite at SNL. The CSRI projects respond to the need for computer science and applied mathematics research with a portfolio of exploratory research and development activities that will provide computational-enabling technologies for SNL code development and application to weapon design and manufacturing organizations.

The CSRI provides a mechanism by which university researchers will learn about problems in computer and computational science at DOE laboratories, conduct leading-edge research, interact with scientists and engineers at the laboratories, and help transfer the results of their research to programs at the laboratories. The CSRI also enables the laboratories to maintain and expand the computer science and mathematics expertise required for the SSP projects and initiatives to be successful. The CSRI is a focal point, both physically and in terms of research collaborations, for university researchers, students, and laboratory staff engaged in computer and computational science, modeling, and simulation.

**Research Efforts:**

The CSRI sponsors research in computer science, computational science, and mathematics that impact large-scale modeling and simulation. One of the key technical issues is that of scaling; the CSRI is interested in developing algorithms and software that scale both as the size and complexity of the problems increase and as the number of processors increase to the thousands or tens of thousands. The CSRI is also interested in computer platforms, including hardware and system software that scale to thousands of processors. Technical focus areas of the CSRI include the following:

**Algorithms and Computational Mathematics Focus Area:** This area includes efforts in design and optimization, solvers, finite-element methods, adaptivity, uncertainty quantification, graph-theoretic methods and multiscale methods. The solver efforts include research in linear solvers, nonlinear solvers, and time integrators. This work focuses on scalable algorithms, particularly multilevel preconditioners and multi-time scale problems. Other work in this area impacts our ability to use massively parallel processing machines. In particular, the graph-theoretic methods form the basis of the dynamic load balancing work, as well as much of the work in resource management, for example, processor allocation and routing. There is also a strong link between this area and ASC validation efforts. In particular, the design and optimization research together with the adaptivity and uncertainty quantification research impact our ability to understand and characterize physical systems and to validate codes. Finally, we are engaging the research community to develop multiscale methods for use in ASC modeling efforts.

**Enabling Technologies Focus Area:** This area includes efforts in meshing, visualization, and dynamic load balancing. The meshing research focuses on the generation of high-quality hex meshes, mesh connectivity, mesh optimization, and mesh refinement. Of particular interest in this area is the flow of information from the design phase through the analysis phase. Dynamic load balancing is a key aspect of massively parallel processing implementations and will be come even more important as machines like Red Storm come on line. Current research questions in this area include hypergraph partitioning, which is particularly important in applications such as electrical modeling and simulation. This area also includes research in visualization. Emphasis in this area will be on scalable visualization tools and algorithms for very large data sets and in feature identification and knowledge extraction.

**Computer Science Focus Area:** The last focus area of the CSRI includes efforts in operating systems, I/O, advanced architectures, networking, and environments. Current research includes the development of light-weight kernels, RAS systems, hardware and protocols for interprocessor communications and I/O subsystems, including libraries and interfaces. As with other areas of research, the focus is on scalability and performance. The goal of the advanced architectures effort is to develop a roadmap that will enable ASC to move beyond the current architectures used in machines like Red Storm to enable computing at petaops and beyond.

The CSRI provides several mechanisms for focused collaborative research on DOE computer and computational science problems. CSRI activities are conducted almost entirely onsite at SNL. In addition to projects in the areas described above, activities include the following.

- An active visitor program for faculty and students, including short-term and long-term visits such as sabbaticals, post-doctoral appointments, summer faculty, and summer student positions.
- A regular series of workshops focusing on specific research areas is offered. These workshops range in length from one week to one month.

Support of fellowships offered through the National Physical Science Consortium and the Krell Institute (High-Performance Computing System Fellowship).

### 4.2.2 Lawrence Livermore ASC Institute for Terascale Simulation

The LLNL ASC ITS collaborates with academia on research topics in computer science, computational mathematics, and scientific computing that are relevant to the SSP. The ITS is an intellectual and geographic nexus for LLNL's research activities and academic collaborations in these areas. Specifically, the ITS brings the world's leading computer scientists and their students to LLNL to work with laboratory researchers on challenging problems facing ASC.

**Products and Capabilities**

Presently, the ITS concentrates on scalable numerical algorithms, advanced meshing and discretization techniques, scientific computing methods, and software technologies—all with an emphasis on scalability to tens of thousands of processors. More specifically, the ITS has expertise in parallel multigrid methods, linear and nonlinear solvers, structured AMR, compiler technology, parallel radiation transport, and laser plasma simulation. A critical goal of the ITS is to ensure the transfer of its research results in these areas into the ASC simulation codes.

**Planned Efforts**

This LLNL ITS Implementation Plan consists of four technical projects, each corresponding to a major technical area. Each of these technical areas is led by a Center for Applied Scientific Computing (CASC) permanent staff member and some are co-led by a university collaborator. A fifth project coordinates an academic outreach program. In addition, the ITS will take steps to build new research projects in a few key areas.

- Numerical Algorithms

  The goal of this project is the development of state-of-the-art algorithms and software to enable the large-scale scientific simulations of interest to ASC. The work involves primarily research in the areas of nonlinear and linear solvers. In FY05, the focus will be on the development of algorithms that scale up to one-hundred-thousand processors, needed for BlueGene/L. In FY05/06, coarsening algorithms will be developed for algebraic multigrid based on new ideas of compatible relaxation, aggressive coarsening, and a theoretical framework for algebraic multigrid recently developed in CASC.

- Simulation Software Technology

  The goal of this project is to enable large-scale scientific simulations through research and development of software frameworks and related technologies. The primary effort in this project is the structured AMR applications infrastructure (SAMRAI). In FY05, the focus will be on the development of algorithms to extend parallel scaling for adaptive problems on very large-scale parallel machines like BlueGene/L, and on integrating support for parallel adaptivity into the Defense and Nuclear Technology Directorate's CALE code (B Division). In FY06, we will continue to enhance support for large-scale parallel adaptive applications based on our current and new collaborations with LLNL programs, with an emphasis on Defense and Nuclear Technology Directorate needs.

- Advanced Meshing and Discretization

  The goal of this project is the research and development of novel meshing and discretization techniques applicable to the modeling of physical phenomena relevant to ASC. The techniques currently being investigated are ALE-AMR methods for modeling shock hydrodynamics. In FY05, the focus will be on the extension of single-fluid gas dynamics ALE methods with AMR to include a full stress tensor formulation and elastic-plastic constitutive relations. Of particular importance will be the development of inter-level transfer operators and inter-level AMR methods for stress tensors and plasticity history variables. In FY06, work will begin to extend the strength model to include damage and failure.

- Scientific Applications

  The goal of this project is to develop prototype applications in critical problem areas of interest to ASC in the exploration of new solver technologies. The main application areas currently under investigation in the project are transport algorithms and laser plasma simulation. In FY05/06, we will perform scaling studies on BG/L of a new electron transport package for laser plasma simulations. We will complete the analytical derivation of diffusion synthetic acceleration for AMR grids, and implement a diffusion synthetic acceleration accelerator based on the Fast Adaptive Composite Grid method in a B-Division AMR Boltzmann transport code. We also will investigate scaling of current methods for transport sweeps when running on BlueGene/L, as well as consider novel new multilevel algorithms in this context.

- Academic Collaborations

  The goal of this project is to complement the long-term academic collaborations of the technical projects above with a variety of shorter-term research and dissemination thrusts, such as one-time technical workshops, sabbatical visitors, and the ITS lecture series.

There are a number of other technical areas that the ITS is interested in pursuing. Uncertainty quantification is a field that is extremely important to ASC's verification and validation efforts, and CASC already has experts in the related area of sensitivity analysis. We will work with the V&V program to explore potential new research projects in this area. The ITS is also interested in performance analysis and modeling questions, especially as they relate to massively parallel architectures such as BlueGene/L. In particular, algorithm performance on recent hardware has become much less predictable than on earlier architectures. Understanding the causes of this behavior from an application-based model point-of-view would be beneficial to the purchase of future platforms.

**Expected Deliverables**

The ITS expects to develop new algorithms and technologies in the technical areas mentioned above. The results of this research will appear in refereed journals, coauthored wherever possible with our academic collaborators. Most importantly, suitable steps will be taken to insure the delivery of this technology to the major ASC simulation codes. The ITS also expects to interact extensively with the world's top researchers in the fields of interest. This will be done through a variety of mechanisms as described in Section 4B. Finally, the ITS expects to aid in the training and recruiting of young researchers through its student programs.

### 4.2.3 Los Alamos Computer Science Institute

The LACSI has the overarching purpose of fostering computer science research efforts that are both internationally recognized for their quality and relevant to the goals of the ASC Program and LANL.

LACSI engages researchers at LANL and at partner academic computer science departments at Rice, Houston, North Carolina, New Mexico, and Tennessee. They focus on five strategic, long-term thrusts of critical importance to LANL, which are discussed below. The goal of all these thrusts is to increase the productivity of LANL computing for the ASC program: better algorithms, increased use of software development methodologies, systems with better usability at lower cost, improved performance of applications, and enhanced collaborations.

LACSI research produces software technologies and tools of value to code teams (performance measurement and analysis tools, component technologies, numerical methods, systems software stacks) that contribute to LANL's Computer Science level 2 milestones.

The LACSI community annually revises its priorities and strategies document to publish plans which guide joint efforts in pursuit of the research thrusts. See *LACSI Priorities and Strategies* for additional detail on LACSI work plans.

#### *4.2.3.1. Software Component Technology*

The long-term goal is to make application development easier via modular codes that integrate components at a high level of abstraction. Components allow developers to focus on their own areas of expertise and provide an increased economy of scale, so resources can be shifted to areas such as performance, testing, and platform dependencies, thus improving software quality, portability, and application performance. Since developers cannot afford to sacrifice performance for this clearly useful functionality, it is important to explore integration strategies that perform context-dependent optimizations automatically as a part of the integration process.

**FY05–06 Goals**

**Marmot as the LACSI Component Integration Challenge Problem:** The problem of integrating data structure (for example, sparse matrices) with functional (for example, linear algebra) components is a difficult challenge because the frequency of invocation of data access methods places a premium on high performance of the component interfaces. We will work closely with the Marmot code team to define a challenge problem by specifying the interfaces and functionality of components within Marmot that implement abstract meshes on which computations are carried out.

**Supporting Technologies for Component Integration:** The goal is compiler and library technologies for automatic construction of domain-specific development environments for applications built from components. Programmers would use high-level (Matlab, Python) or conventional (Fortran, C++) languages to coordinate invocation of library components. A simple source-to-source translation results in long compilation times and precludes exploitation of domain knowledge from library developers. A new approach, telescoping languages, does extensive and expensive, but one-time, analysis of library components in advance to generate a domain-specific compiler. This processes applications that invoke components to produce a highly optimized program in a base language in reasonable compile time.

**Retargetable High-Performance Components and Libraries:** Retargeting applications for new architectures is an ongoing problem as the machines change rapidly. We propose to harness high-performance computing to assist in this effort by exploiting recent work in automatic tuning libraries for new machines. We will explore new approaches to building adaptive numerical software that selects a suitable algorithm based on application data, selects a parallel implementation based on resource availability, and optimizes code based on architectural details.

#### *4.2.3.2. Systems Software*

Systems software transforms bare hardware boxes into usable, reliable, and predictable systems that strive to deliver high performance to applications and high productivity to programmers. The ASC program at LANL needs new systems software, and this work concentrates on areas of collective expertise where significant impact can be had. The following table identifies three desirable characteristics of systems software and two technical areas of concentration.

**Organization of the System Software Thrust**

| | Performance | Reliability | Utility |
|---|---|---|---|
| Networking/ Messaging | Endpoint hardware/software design; layering/modularization | Network and process fault tolerance | Standards: MPI, MPI-2, MPI-IO, ARMCI |
| Clustering software | Clustermatic work; integrated monitoring | Compiler-driven checkpoint; fault prediction; failover | Cluster admin; improve SSI; V9FS |

**FY05-06 Goals**

**Networking and messaging:** Near-term, distributed systems are cost-effective, so performance, reliability and utility of network hardware and messaging software continue to be important. Network hardware will soon overwhelm the I/O bandwidth of nodes, so node hardware and software co-design is required to exploit these networks. Reliability issues continue in distributed systems and at future scales, more fault tolerance must be handled in processes with an extended monitoring infrastructure. To successfully incorporate the latest networks and low-level libraries, adherence to applicable standards is mandatory.

**Clustering software:** LACSI-funded research has provided the Clustermatic software stack for Linux clusters with a myriad of advantages over conventional approaches; deployment on near-term ASC platforms at LANL forms an important resource for application execution. More automated support for checkpoint/restart and redundant administration is required. The software stack must be polished to provide friendlier development and execution environments.

### *4.2.3.3. Foundations of Computational Science*

This thrust focuses on the development, analysis, and verification and validation of numerical solution techniques for physical models embodied within large-scale multi-physics simulation tools. The effort can be divided into three principal research areas: algorithms and models for specific physical phenomena of interest, numerical methods for the algorithmic coupling of these physical phenomena, and metrics for correctness and robustness of these models and algorithms.

**FY05-06 Goals**

This thrust complements the LANL ASC Computational Sciences program element, whose principle mission is to deploy verified and validated software components embodying shock hydrodynamics, radiative and neutron transport, and linear/nonlinear solvers. In particular, this thrust will deliver software to the three ASC weapons performance code projects at LANL

### *4.2.3.4. Application and System Performance*

Building applications that can effectively exploit extreme-scale parallel systems has proven very difficult: massive parallelism poses major challenges in achieving scalable performance; architectural complexity (complex processors, deep memory hierarchies, heterogeneous interconnects) is difficult for applications to exploit effectively; at this scale component failure is inevitable, so long-running applications must be resilient in order to run to completion.

**FY05-06 Goals**

**Modeling Application and System Performance:** Research in this area will span a wide range of topics: continue modeling applications to cover all types of computations important to ASC; enhance current models to include effects of operating system, architecture, and other system activity; explore using models for application steering; simplify the complicated process of model creation; and use developed models for scalability analysis, procurement and software development

**Better Tools for Measurement and Analysis of Application Performance:** On large systems performance problems are complex, so a wide range of performance evaluation methods must be supported. Research will address determining the appropriate level for implementing different instrumentation and measurement strategies, how to support a modular and extensible framework for performance evaluation as well as the appropriate compromise between instrumentation cost, the level of detail of measurements, and the volume of data to be gathered.

**Automatic Application Tuning:** We want to apply automatic techniques for tuning libraries to whole applications. This requires algorithms for identifying critical loop nests that could potentially benefit from tuning. A promising direction is to use data from hardware performance counters to guide empirically driven tuning approaches by identifying performance bottlenecks.

**Compiler Technology for Exploiting Modern Processors:** A compiler must generate code to simultaneously address a number of challenging performance problems. Solutions often conflict in optimizing different behaviors, so combining optimizations poses a difficult challenge.

**Application Mapping, Dynamic Adaptation and Steering:** Mapping and performance steering can adjust a running program for more efficient execution or to adapt to changing resources (for example, failures or sharing). Challenges include developing strategies that enable applications to monitor and adjust their behavior to optimize performance; and measuring environmental conditions on nodes to balance checkpoint frequency and partition allocation based on likelihood of failures.

**Compiler Technology for Extreme-Scale Systems:** Global address space programming models (in contrast to messaging models supported by MPI) are simpler to program and more efficient because compilers can yield perform complex optimizations that programmers would not do. For widespread success, these languages require sophisticated compiler technology to perform well both on today's loosely-coupled clusters and tightly-coupled petascale platforms of the future.

#### *4.2.3.5. Computer Science Community Interactions*

LACSI supports several mechanisms to support collaborations in the LACSI community:

- Individual researchers visit each other to share ideas and to actively collaborate on projects
- LACSI organizes technical workshops at LANL on topics related to the technical vision
- An annual symposium showcases LACSI results and provides a forum for discussing research results from the national community

## *4B: University Partnerships Integration*

**Lawrence Livermore University Partnerships Integration**

The ITS engages academia in the full range of its research activities through a variety of mechanisms. The emphasis is on bringing visitors to LLNL for extended periods, supplemented with subcontracts to maintain focused effort at the visitor's home institution. Specifically, the ITS:

- Supports an extensive visitor program for faculty and students, including single-day seminars, summer stays, and year-long sabbatical leaves;
- Runs a postdoctoral program for recent graduates in the computational sciences;
- Hosts a series of workshops focused on specific topics.

The ITS coordinates its activities with those of the two other ASC Institutes. For example, ITS expects to leverage LANL's expertise in run-time systems and SNL's expertise in optimization. Close ties have been established with ASAP centers, and these collaborations will ensure that relevant research results of the ITS benefit these centers.

The ITS works with the ASC PSE, DVS, and Applications efforts to ensure the relevance and utility of its research program. In general, the ITS engages in longer term research in collaboration with academia, whereas the PSE, DVS, and Applications efforts are more focused on development, nearer-term research, and deployment activities. Existing ties to LC are exploited to establish insertion paths for the results of our computer science research and development efforts. Our strong ties to the ASC code groups serve as the insertion paths for our algorithmic research and development results. To facilitate the timely integration of ITS algorithmic advances, CASC personnel are co-located with code groups in the Defense & Nuclear Technologies Directorate.

**Los Alamos University Partnerships Integration**

LACSI engages in collaboration with academic research groups through an ongoing contract with Rice and subcontracts with North Carolina, Tennessee, Houston, and New Mexico. In addition to ad-hoc interactions, LACSI organizes special-purpose workshops and meetings at LANL to maximize the availability of the expertise of our academic partners and to maximize their understanding of our research issues. LACSI also supports the DOE High Performance Computer Science Fellowship Program to influence the research that these students perform and to improve our chances of hiring them upon graduation. The annual LACSI symposium affords our academic partners and other academic researchers the opportunity to publish results and meet to form new collaborations. Beginning in October 2004, the LACSI symposium will have one or more regular sessions devoted to research progress reports from ASC Alliance projects.

Internally, the PSE program at LANL is a partner. Several successful projects that LACSI has funded are being transferred to PSE funding for advanced development and deployment. Performance tools have also been deployed on ASC platforms directly for code teams in Applied Physics Division, in partnership with support people in the Computing, Communications and Networking Division at LANL.

**Sandia University Partnerships Integration**

The CSRI at Sandia integrates with other program elements by selecting projects, visitors, and workshops that impact these program elements directly.

## *4C: University Partnerships Risk Assessment*

The following table summarizes top risks and mitigation approaches for University Partnerships:

**Table 4C-1. Top Risks for University Partnerships**

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| **Alliances** | | | | | |
| 1 | Experimental data will not be available to validate material models and codes developed by Alliance Centers. | High | Very High | High | Control: Increase program emphasis on V&V; survey open literature and leverage other programs at the universities that can generate relevant data. |
| 2 | Available computer resources will not be sufficient to meet Alliance needs. | High | Moderate | Medium | Control: Focus program planning to integrate Alliance requirements into ASC platform plans; acquire resources from NSF supercomputing centers for Alliance applications. |

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| **Sandia Computer Science Research Institute** | | | | | |
| 1 | Failure to engage external community in research | Moderate | Moderate | Medium | Control: Aggressively recruit CSRI participants, participate in external activities (for example, conferences and reviews) |
| 2 | Failure to maintain a core competency in Computer Science | Moderate | Moderate | Medium | Control: Control through reviews and project selection |
| 3 | Pressure to focus on near-term deliverables | Moderate | Moderate | Low | Control: Control through project selection and management |
| **Lawrence Livermore ASC Institute for Terascale Simulation** | | | | | |
| 1 | Reduce interactions with leaders in the world scientific research community | Moderate | Moderate | Medium | Control: Encourage outside interactions via workshops, sabbaticals, conferences |
| 2 | Poor alignment with future ASC goals | High | Low | Medium | Control: Coordinate strategic planning with other ASC elements; communicate goals to ITS participants |
| 3 | Pressure to focus on near-term deliverables | High | Low | Medium | Control: Continue to successfully move research into ASC simulation activities. |
| **Los Alamos Computer Science Institute** | | | | | |
| 1 | Failure to maintain computer science competency | High | Moderate | Medium | Control: Select projects to retain expertise |
| 2 | Pressure to focus on short term | High | Moderate | Medium | Control: Design projects with long-term goals, short term deliverables |

# SECTION 5: ASC INTEGRATION

Continual collaboration between ASC, Campaigns, and DSW is a major strength of the SSP. Joint efforts in software development, code verification and validation, and tool-suite application are good examples of this collaboration.

- Software Development. ASC 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 stockpile life extension programs.
- Code Verification and Validation. The verification and validation of ASC codes is conducted by ASC and DSW, as part of the formal stockpile stewardship verification and validation process. Experiments designed to address specific weapons issues are used to validate codes. Codes are also verified against idealized scenarios, with known solutions.
- Tool-Suite Application. Weapons designers use the ASC simulation and modeling tool suite to assess unresolved surveillance SFIs, by using 3D simulations and new numerical techniques in the ASC simulation codes. These capabilities are vital to stockpile life extension program 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:
    - LANL and LLNL are using the ASC tools and technologies to address physics and engineering issues associated with the W88, W76, W78, B61, and W80.
    - SNL was able to reduce the number of development tests in a stockpile-engineering product, because of the high confidence in validated ASC simulations. This reduction in development tests allowed acceleration of the development schedule and an improved allocation of existing resources.
    - ASC simulations and tools are being used to refine and optimize casting and manufacturing processes. As a result of collaborative efforts with manufacturing experts and a strong verification and validation process, increased confidence in casting simulations has resulted in improved mold designs and manufacturing processes.

**Integration with Directed Stockpile Work**

Coordination between ASC and DSW is a significant aspect 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 safety, security, and reliability in the future.

**Integration with Defense Programs Science Campaigns**

The development of predictive capabilities relies on a strong experimental program to support the assessment of stockpile issues and to provide physics and materials data needed to validate new scientific models and theories incorporated into the simulation codes. DP's Science Campaigns provide the science development, testing, and experiments needed to manage the nuclear weapons stockpile. In the previous era of test-based confidence, DP provided direct answers about the safety, security, and reliability of the stockpile. In the current era, the focus has shifted to a simulation-based confidence, which requires a close connection between ASC and the Science Campaigns. Using facilities such as NIF at LLNL, the Dual Axis Radiographic Hydrodynamic Testing Facility at LANL, and the MESA facility at SNL, the Science Campaigns produce significant quantities of high-quality physics data. Working together with the Science Campaigns, ASC simulation tools are employed in the design of experiments. Data from these experimental programs provide ASC with the raw material necessary to evaluate and improve physics models to better characterize weapons' performance and aging.

**Integration with the Department of Energy Office of Science and Other Government Agencies**

Certain technical problems that arise in terascale computing are generic to scientific simulation and apply equally well to applications within the NNSA, DOE's Office of Science, and other government agencies such as NSA, DoD, and the Defense Advanced Research Projects Agency. This includes I/O and archival 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 scientific 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 ASC. Both programs are collaborating to identify areas of common interest and to establish appropriate coordination of efforts.

# *5A: ASC Integration Activities*

## 5.1 One Program/Three Labs

The One Program/Three Laboratories program element funds several critical coordination and integration activities essential to the success of ASC. These crosscut and outreach activities seek to facilitate cooperation and collaboration among the weapons laboratories, improve program visibility within the high-performance computing community, and enhance the overall operations of the ASC program. Principal efforts within One Program/Three Laboratories include:

- The ASC Executive Committee, a tri-lab management structure including DOE-HQ program managers and an executive and deputy from each of the labs
- Quarterly meetings of the ASC Executive Committee
- Annual principal investigator meetings that expose attendees to technical and programmatic efforts at the three laboratories
- SAIC contract to provide various administration support

## 5.2 SuperComputing 2004

The international high-performance supercomputing conference advances the science and application of high-performance computing and communication technology in a way unmatched by any other industry event. The ASC research exhibit at SuperComputing 2004 (SC04) will promote ASC's HPC computer science applications and accomplishments to the wider supercomputing community. Attendees and other exhibitors are provided with information about all of the ASC program elements contributed from collaborative activities within the tri-labs, alliances, the nuclear weapons complex plants (Y-12 and Pantex), and our industry partners.

This year, ASC's exhibit theme is "ASC…The Next Decade" with a subtitle of "Enhancing Predictive Capability for Stockpile Stewardship and National Security." The downsized booth (to reduce cost to the program) will showcase ASC technical presentations and 3D simulations, demonstrations of innovative ASC technologies, a 10-minute video highlighting ASC's three strategy elements, and a compact disc for visitors to take away, which will contain the *ASC Strategic Plan* and the *ASC Program Plan,* along with ASC-funded and -developed open source software.

# VI. ASC Level 1 and 2 Milestones

**Table VI-1. Level 1 Milestone Dependencies**

| Milestone ID | DOE Programs / Subprograms | Milestone Title | FY | Completion Date | Level | Sites | Depends on another milestone | Milestone ID | Has another milestone depending on it | Milestone ID |
|---|---|---|---|---|---|---|---|---|---|---|
| 342 | ASC Advanced Applications Development | Document the requirements to move beyond a 100TF ASC computing platform to a petaflop platform | 2005 | Dec-04 | 1 | HQ<br>LANL<br>LLNL<br>SNL | | | | |
| 349 | ASC Advanced Applications Development | Develop, implement, and validate an initial physics/engineering capability in advanced ASCI simulations and benchmark for the W76 and W80 against legacy codes and experiments. | 2006 | Jun-06 | 1 | HQ<br>LANL<br>LLNL<br>SNL | | | | |
| 350 | ASC S&CS | Provide a 100TF Platform environment supporting to the tri-laboratory DSW & Campaign simulation requirements. | 2007 | Dec-06 | 1 | HQ<br>LLNL | Yes | 461, 464, 1348 | Yes | 359 (and many more) |
| 359 | ASC Advanced Applications Development | Complete modern baseline of all enduring stockpile systems with ASC codes. | 2009 | Sep-09 | 1 | HQ<br>LANL<br>LLNL<br>SNL | | | | |

## Table VI-2. Level 2 Milestone Dependencies for FY05

| Milestone ID | DOE Programs / Subprograms | Milestone Title | FY | Completion Date | Level | Sites | Depends on another Milestone | Milestone ID | Has another Milestone depending on it | Milestone ID |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | ASC Verification and Validation | Validate the application of ALEGRA-HEDP for Z-Pinch Experimental Design and Analysis. | 2005 | Sep-05 | 2 | SNL | No | | Yes | FY07 L2 (B) |
| 9 | ASC Verification and Validation | Apply the validation process at the sub-system level to support W76-1 qualification in hostile blast and impulse environments. | 2005 | Sep-05 | 2 | SNL | Yes | 27 | Yes | FY06 L1 (#349)<br>FY06, L2 (A) |
| 12 | ASC Materials and Physics Modeling | Develop, implement and test advancements in geological material models for use in a realistic simulation of an earth penetrating weapon. | 2005 | Sep-05 | 2 | SNL | No | | Yes | FY06 L2 (C) |
| 14 | ASC Advanced Applications Development | Deploy computer codes for modeling trajectory and response of earth penetrating weapons. | 2005 | Sep-05 | 2 | SNL | No | | Yes | FY06 L2 (C) |
| 15 | ASC Materials and Physics Modeling | Develop MEMS subgrid models for thermal simulations of MEMS features. | 2005 | Sep-05 | 2 | SNL | Yes | 28 | Yes | FY07 L2 (F) |
| 17 | ASC S&CS | Transition Red Storm platform to Limited Availability. | 2005 | Sep-05 | 2 | SNL | Yes | 30 | Yes | FY06 L2 (F) |
| 18 | ASC S&CS | Deploy a limited availability Red Storm user environment. | 2005 | Sep-05 | 2 | SNL | Yes | 30, 31 | Yes | FY06 L2 (G) |
| 19 | ASC S&CS | Initial Productionization of Design Through Analysis Environment. | 2005 | Sep-05 | 2 | SNL | Yes | 32 | Yes | FY06 L2 (H) |
| 23 | ASC Advanced Applications Development | Deliver scalable multilevel solvers for use in ASC simulation codes. | 2005 | Sep-05 | 2 | SNL | No | | Yes | FY06 L2 (B-D)<br>FY07 L2 (A-E) |
| 369 | ASC Advanced Applications Development | Analysis of Supercomputing Systems Architectures for ASC Applications. | 2005 | Sep-05 | 2 | SNL | Yes | FY05 L1 (#342) | Yes | FY07 (I) |
| 1312 | ASC Advanced Applications Development | Demonstrate the loose coupling of planned ASC early-time neutron damage modeling codes. | 2005 | Sep-05 | 2 | SNL | No | | Yes | FY07 L2 (E) |

| Milestone ID | DOE Programs / Subprograms | Milestone Title | FY | Completion Date | Level | Sites | Depends on another Milestone | Milestone ID | Has another Milestone depending on it | Milestone ID |
|---|---|---|---|---|---|---|---|---|---|---|
| 1313 | ASC S&CS | Provide visualization for capability calculations on Red Storm. | 2005 | Sep-05 | 2 | SNL | Yes | 30, 31 | Yes | FY06 L2 (G) |
| 455 | ASC Advanced Applications Development | Perform and profile a high quality W80 3D secondary burn calculation with advanced physics. | 2005 | Jun-05 | 2 | LLNL | Yes | 459 | Yes | 349, 1358 |
| 457 | ASC Advanced Applications Development | Investigate advanced primary performance and safety simulation capabilities for future stockpile activities to move towards a more predictive capability | 2005 | Sep-05 | 2 | LLNL | | | | |
| 458 | ASC Advanced Applications Development | Implement enhancements of nuclear weapon simulation codes to support new designer needs | 2005 | Jun-05 | 2 | LLNL | | | | |
| 459 | ASC Verification and Validation | Secondary burn code initial validation of focused physics capability | 2005 | Mar-05 | 2 | LLNL | | | Yes | 1391, 334, 342, 359, 455, 1353 |
| 461 | ASC S&CS | Deploy First Phase of I/O Infrastructure for Purple | 2005 | Sep-05 | 2 | LLNL | No | | Yes | 350 |
| 464 | ASC S&CS | Complete Phase 1 Integration of Site-Wide Global Parallel File System (SWGPFS) | 2005 | Sep-05 | 2 | LLNL | No | | Yes | 350 |
| 465 | ASC S&CS | Deploy Remote Computing Environment for Red Storm | 2005 | Sep-05 | 2 | LLNL | Yes | 17 | Yes | 349 |
| 1348 | ASC ICS | TSF Activation | 2005 | Jun-05 | 2 | LLNL | No | | Yes | 350 |
| 1349 | ASC Materials and Physics Modeling | Develop and apply the computational capability to give detailed term (line) treatment of radiation opacities for programmatic applications in DSW, NNSA Science campaigns and High Energy Density Experiments | 2005 | Sep-05 | 2 | LLNL | No | | No, none on the current FY05 Campaigns list, but it does support upcoming DSW and Campaign activities. | |
| 1350 | ASC Verification and Validation | V&V 4th Stockpile Summary / Annual: V&V status and results of simulation capability relevant to LLNL stockpile weapon systems. Theme: The PMP Model Set | 2005 | Jun-05 | 2 | LLNL | Yes | 459 | Yes | 1391, 334, 342, 343, 1416, 349, 359 |

| Milestone ID | DOE Programs / Subprograms | Milestone Title | FY | Completion Date | Level | Sites | Depends on another Milestone | Milestone ID | Has another Milestone depending on it | Milestone ID |
|---|---|---|---|---|---|---|---|---|---|---|
| 1353 | ASC Advanced Applications Development | Implement an advanced physics capability in 3D secondary performance code and prototype its use through a 3D secondary burn calculation | 2005 | Dec-04 | 2 | LLNL | Yes | 455 | | |
| 1358 | ASC Verification and Validation | Code and Solution Verification of Selected Primary and Secondary Capabilities | 2005 | Sep-05 | 2 | LLNL | Yes | 1350, 459 | Yes | 1391, 334, 342, 343, 1416, 349, 359 |
| 470 | ASC Advanced Applications Development | Simulate casting of the Qual Type 126 pit and compare the results of the simulation to the available experimental data for the same process. | 2005 | Sep-05 | 2 | LANL | | | | |
| 476 | ASC Advanced Applications Development | The Capsaicin Project will demonstrate a robust and accurate 2D-RZ discrete ordinates radiation transport capability. | 2005 | Mar-05 | 2 | LANL | | | | |
| 477 | ASC Materials and Physics Modeling | Model for Damage with Accompanying Data implemented into Project B Code & validated. | 2005 | Mar-05 | 2 | LANL | | | | |
| 500 | ASC S&CS | Fully functioning 64-bit software environment deployed on the LANL Lightning capacity computing system functioning at full scalability | 2005 | Sep-05 | 2 | LANL | | | | |
| 501 | ASC Advanced Applications Development | Deliver and demonstrate an interface steepening component to Code Project A | 2005 | Mar-05 | 2 | LANL | | | | |
| 502 | ASC Verification and Validation | Organizational SQA Standards in Place and Assessments conducted of IWA Performance Code Projects. | 2005 | Sep-05 | 2 | LANL | | | | |
| 1351 | ASC ICS | SCC Infrastructure Upgrade (Phases 2 & 3) | 2005 | Jun-05 | 2 | LANL | | | | |
| 1352 | ASC S&CS | Immersive Visualization Environment Deployed for ASC Users | 2005 | Mar-05 | 2 | LANL | | | | |
| 1354 | ASC S&CS | Performance study against LANL workload of potential systems considered for the next LANL capability platform procurement | 2005 | Sep-05 | 2 | LANL | | | | |

| Milestone ID | DOE Programs / Subprograms | Milestone Title | FY | Completion Date | Level | Sites | Depends on another Milestone | Milestone ID | Has another Milestone depending on it | Milestone ID |
|---|---|---|---|---|---|---|---|---|---|---|
| 1355 | ASC Materials and Physics Modeling | HE EOS model for PBX9502 products, validated against fundamental data, delivered to Code B | 2005 | Sep-05 | 2 | LANL | | | | |
| 1356 | ASC Materials and Physics Modeling | High Fidelity Nuclear Library | 2005 | Sep-05 | 2 | LANL | | | | |
| 1357 | ASC Verification and Validation | Code Verification, Calculation Verification and Solution Error Analysis for LANL Physics and Engineering Codes | 2005 | Sep-05 | 2 | LANL | | | | |
| 1360 | ASC Advanced Applications Development | Final Project B code release supporting major primary design requirements for W76-1 LEP | 2005 | Mar-05 | 2 | LANL | | | | |
| 1361 | ASC Advanced Applications Development | A specific transport capability in-line in Project A & B codes | 2005 | Mar-05 | 2 | LANL | | | | |
| 1362 | ASC Advanced Applications Development | Intermediate Project A code release supporting major secondary design requirements for W76-1 LEP | 2005 | Mar-05 | 2 | LANL | | | | |

## Table VI-3. Preliminary Level 2 Milestone Dependencies for FY06

| Milestone ID | DOE Programs / Subprograms | Milestone Title | FY | Completion Date | Level | Sites | Depends on another Milestone | Milestone ID | Has another Milestone depending on it | Milestone ID |
|---|---|---|---|---|---|---|---|---|---|---|
| New SNL 06-A | ASC Verification and Validation | Apply the validation process to the coupled electromagnetics and radiation transport model of the W76-1 Cavity System Generated Electromagnetic Pulse (SGEMP) response in a hostile environment. | FY06 | Sep-06 | 2 | SNL | | | | |
| New SNL 06-B | ASC Advanced Applications Development | Demonstrate algorithms for simulating electrical systems with multi-time behavior in STS environments. | FY06 | Dec-05 | 2 | SNL | | | | |
| New SNL 06-C | ASC Advanced Applications Development | Demonstrate capability to model computationally the structural response of a MEMs device. | FY06 | Sep-06 | 2 | SNL | | | | |
| New SNL 06-D | ASC Materials and Physics Modeling | Demonstrate ability to compute material response coupled across two or more length scales. | FY06 | Sep-06 | 2 | SNL | | | | |
| New SNL 06-E | ASC Advanced Applications Development | Develop coupled error estimation/uncertainty quantification capabilities. (APPS/Algorithms) | FY06 | Sep-06 | 2 | SNL | | | | |
| New SNL 06-F | ASC Simulation and Computer Science | Transition Red Storm to General Availability. | FY06 | Jun-06 | 2 | SNL | | | | |
| New SNL 06-G | ASC Simulation and Computer Science | Deploy a general availability Red Storm user environment. | FY06 | Jun-06 | 2 | SNL | | | | |
| New SNL 06-H | ASC Simulation and Computer Science | Deploy a fully operational Design Through Analysis (DTA) environment. | FY06 | Sep-06 | 2 | SNL | | | | |
| New SNL 06-I | ASC Simulation and Computer Science | Down select technologies for research and implementation from the roadmap developed in FY05. Begin research and implementation of the necessary technologies to develop the supporting computing environment for Sandia's next generation platform. | FY06 | Sep-06 | 2 | SNL | | | | |

| Milestone ID | DOE Programs / Subprograms | Milestone Title | FY | Completion Date | Level | Sites | Depends on another Milestone | Milestone ID | Has another Milestone depending on it | Milestone ID |
|---|---|---|---|---|---|---|---|---|---|---|
| New SNL 06-J | ASC Simulation and Computer Science | Deliver prototype data analysis models and demonstrate their use in support of Verification and Validation program goals. (DVS / V&V) | FY06 | Sep-06 | 2 | SNL | | | | |
| New SNL 06-K | ASC Simulation and Computer Science | Deploy Security Infrastructure for ASC Tri-Lab. | FY06 | Jun-06 | 2 | SNL | | | | |
| New LLNL 06-01 | ASC Advanced Applications Development | Demonstrate high quality full system capability in a 2D secondary performance code with the addition of one or more physics model improvements needed for DSW simulations. | FY06 | Mar-06 | 2 | LLNL | | | | |
| New LLNL 06-02 | ASC Advanced Applications Development | Apply enhanced 3D secondary simulation capability to calculations required for DSW activities. | FY06 | Sep-06 | 2 | LLNL | | | | |
| New LLNL 06-03 | ASC Advanced Applications Development | Enhance capabilities of nuclear weapon simulation codes to support current and planned design efforts. | FY06 | Jun-06 | 2 | LLNL | | | | |
| New LLNL 06-04 | ASC Advanced Applications Development | Explore and assess new opportunities to enhance the predictive capability of primary performance and safety codes for future stockpile activities. | FY06 | Sep-06 | 2 | LLNL | | | | |
| New LLNL 06-05 | ASC Advanced Applications Development | Demonstrate a mixed implicit-explicit nonlinear thermo-mechanical simulation capability in a 3D engineering simulation code for STS modeling. | FY06 | Jun-06 | 2 | LLNL | | | | |
| New LLNL 06-14 | ASC Verification and Validation | Complete and document initial focused validation of primary simulation capability. | FY06 | Mar-06 | 2 | LLNL | | | | |
| New LLNL 06-06 | ASC Verification and Validation | V&V 5th Stockpile Summary / Annual: V&V status and results of simulation capability relevant to LLNL stockpile weapon systems. Theme: When Confidence Bounds Overlap. | FY06 | Jun-06 | 2 | LLNL | | | | |
| New LLNL 06-13 | ASC Materials and Physics Models | Produce and provide initial assessment for a first generation complex material model for strength and plasticity of | FY06 | Dec-05 | 2 | LLNL | Yes | 393 | No | |

| Milestone ID | DOE Programs / Subprograms | Milestone Title | FY | Completion Date | Level | Sites | Depends on another Milestone | Milestone ID | Has another Milestone depending on it | Milestone ID |
|---|---|---|---|---|---|---|---|---|---|---|
| 06-13 | Models | weapons materials based on theory, microscale calculations, and experimental data. | | | | | | | | |
| New LLNL 06-07 | ASC Materials and Physics Models | Next-generation Pu multiphase EOS delivered for QMU and stockpile certification. | FY06 | Mar-06 | 2 | LLNL | | | | |
| New LLNL 06-08 | ASC Materials and Physics Models | Produce and provide advanced assessment of a complex physics model using the full compliment of verification and validation tools and techniques available. | FY06 | Sep-06 | 2 | LLNL | | | | |
| New LLNL 06-09 | ASC S&CS | Deploy Security Infrastructure for ASC Tri-Lab. | FY06 | Jun-06 | 2 | LLNL | | | | |
| New LLNL 06-10 | ASC S&CS | Deploy Next-Generation Delivery Infrastructure for Visualization Imagery | FY06 | Jun-06 | 2 | LLNL | | | | |
| New LLNL 06-11 | ASC ICS | BlueGene/L System Ready for Limited Availability | FY06 | Jun-06 | 2 | LLNL | | | | |
| New LLNL 06-12 | ASC ICS | Purple System Ready for Limited Production | FY06 | Jun-06 | 2 | LLNL | | | | |
| New LANL 06-01 | Simulation and Computer Science | Deploy production commodity cluster visualization to theaters and designer desktops | FY06 | FY06/Q2 | 2 | LANL | | | | |
| New LANL 06-02 | | Intermediate Project B code release supporting W88 primary certification (may change to B61 support) | FY06 | | 2 | LANL | | | | |
| New LANL 06-03 | | Model for Damage with Accompanying Data implemented into Project A Code & validated | FY06 | | 2 | LANL | | | | |
| New LANL 06-04 | | Final Project A code release supporting major secondary design requirements for W76-1 LEP | FY06 | | 2 | LANL | | | | |

| Milestone ID | DOE Programs / Subprograms | Milestone Title | FY | Completion Date | Level | Sites | Depends on another Milestone | Milestone ID | Has another Milestone depending on it | Milestone ID |
|---|---|---|---|---|---|---|---|---|---|---|
| New LANL 06-05 | | Placeholder for an additional IWA milestone | FY06 | | 2 | LANL | | | | |
| New LANL 06-06 | | Placeholder for an additional CompSci milestone | FY06 | | 2 | LANL | | | | |
| New LANL 06-07 | | Secondary V&V Assessment Supporting W76-1 LEP Certification (Intermediate) | FY06 | | 2 | LANL | | | | |
| New LANL 06-08 | | Engineering V&V Assessment of W76 Aft Mount Surrogate Assembly Shock Response Supporting W76-1 LEP Certification (Final) | | | | | | | | |
| New LANL 06-09 | | Primary V&V Assessment Supporting W76-1 LEP Certification (Final) | | | | | | | | |
| New LANL 06-10: | | Secondary V&V Assessment Supporting W76-1 LEP Certification (Final) | | | | | | | | |

# VII. ASC Integration

Continual collaboration between ASC, Campaigns, and DSW is a major strength of the SSP. Joint efforts in software development, code verification and validation, and tool-suite application are good examples of this collaboration.

- Software Development. ASC 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 stockpile LEPs.
- Code Verification and Validation. The verification and validation of ASC codes is conducted by ASC and DSW, as part of the formal stockpile stewardship verification and validation process. Experiments designed to address specific weapons issues are used to validate codes. Codes are also verified against idealized scenarios, with known solutions.
- Tool-Suite Application. Weapons designers use the ASC simulation and modeling tool suite to assess unresolved surveillance SFIs, by using 3D simulations and new numerical techniques in the ASC simulation codes. These capabilities are vital to stockpile LEP 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:
  - LANL and LLNL are using the ASC tools and technologies to address physics and engineering issues associated with the W88, W76, W78, B61, and W80.
  - SNL was able to reduce the number of development tests in a stockpile-engineering product, because of the high confidence in validated ASC simulations. This reduction in development tests allowed acceleration of the development schedule and an improved allocation of existing resources.
  - ASC simulations and tools are being used to refine and optimize casting and manufacturing processes. As a result of collaborative efforts with manufacturing experts and a strong verification and validation process, increased confidence in casting simulations has resulted in improved mold designs and manufacturing processes.

## Integration with Directed Stockpile Work

Coordination between ASC and DSW is a significant aspect 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 safety, security, and reliability in the future.

## Integration with Defense Programs Science Campaigns

The development of predictive capabilities relies on a strong experimental program to support the assessment of stockpile issues and to provide physics and materials data needed to validate new scientific models and theories incorporated into the simulation codes. DP's 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 safety, security, and reliability of the stockpile. In the current era, the focus has shifted to a simulation-based confidence, which requires a close connection between ASC and the Science Campaigns. Using facilities such as NIF at LLNL, the Dual Axis Radiographic Hydrodynamic Testing Facility at LANL, and the MESA facility at SNL, the Science Campaigns produce significant quantities of high-quality physics data. Working together with the Science Campaigns, ASC simulation tools are employed in the design of experiments. Data from these experimental programs provide ASC with the raw material necessary to evaluate and improve physics models to better characterize weapons' performance and aging.

### Integration with the Department of Energy Office of Science and other Government Agencies

Certain technical problems that arise in terascale computing are generic to scientific simulation and apply equally well to applications within the NNSA, DOE's Office of Science and other government agencies such as the National Security Agency, DoD, and Defense Advanced Research Projects Agency. This includes I/O and archival 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 scientific 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 ASC. Both programs are collaborating to identify areas of common interest and to establish appropriate coordination of efforts.

# VIII. ASC Risk Management

Risk management is a process for identifying and analyzing risks, executing mitigation and contingency planning to minimize potential consequences of identified risks, and monitoring and communicating up-to-date information about risk issues. Risk management is about identifying opportunities and avoiding losses. A "risk" is defined as (1) a future event, action, or condition that might prevent the successful execution of strategies or achievement of technical or business objectives, and (2) the risk exposure level, defined by the likelihood or probability that an event, action, or condition will occur, and the consequences, if that event, action, or condition does occur. Table VIII-1 summarizes ASC's top ten risks, which are managed and tracked.

**Table VIII-1. ASC's Top 10 Risks**

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| 1 | Compute resources are insufficient to meet capacity and capability needs of designers, analysts, DSW, or other Campaigns. | High | High | High | Integrate program planning with DSW and other Campaigns, to ensure requirements for computing are understood and appropriately set; maintain emphasis on platform strategy as a central element of the program; pursue plans for additional and cost-effective capacity platforms. |
| i2 | Designers, analysts, DSW, or other Campaign programs lack confidence in ASC codes or models for application to certification /qualification. | Very High | Low | Medium | Maintain program emphasis on V&V; Integrate program planning with DSW and other Campaign programs to assure requirements needed for certification/qualification are properly set and met. |
| 3 | Inability to respond effectively with Modeling & Simulation (M&S) capability and expertise in support of stockpile requirements – near or long term, planned or unplanned (Sockpile LEP, SFIs, etc.). | Very High | Low | Medium | Integrate program planning, particularly technical investment priority, with DSW and other Campaign programs to ensure capability and expertise is developed in most appropriate areas; retain ability to apply legacy tools, codes, models. |

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| 4 | Base of personnel with requisite skills, knowledge, and abilities erodes. | High | Low | Medium | Maintain emphasis on "best and brightest" personnel base, with Institutes, Research Foundations, and University programs, as central feeder elements of the program. |
| 5 | Advanced material model development more difficult, takes longer than expected. | Moderate | High | Medium | Increase support to physics research; pursue plans for additional computing capability for physics model development |
| 6 | Data not available for input to new physics models or for model validation. | High | Moderate | Medium | Work with Science Campaigns to obtain needed data; propose relevant experiments. |
| 7 | Infrastructure resources are insufficient to meet designer, analyst, DSW, or other Campaign program needs. | High | Low | Medium | Integrate program planning with DSW and other Campaigns, to ensure requirements for computing are understood and appropriately set; maintain emphasis on system view of infrastructure and PSE strategy, as central elements of the program. |
| 8 | External regulatory requirements delay program deliverables by diverting resources to extensive compliance-related activities | Moderate | Low | Medium | Work with external regulatory bodies to assure that they understand NNSA's mission, ASC's mission, and the processes to set and align requirements and deliverables, consistent with applicable regulations. |
| 9 | Inadequate PSE impedes development and use of advanced applications on ASC platforms. | Moderate | Very Low | Low | Integrated planning between program elements to anticipate application requirements and prioritize PSE development and implementation. |

| No. | Risk Description | Risk Assessment | | | Mitigation Approach |
|---|---|---|---|---|---|
| | | Consequence | Likelihood | Risk Exposure | |
| 10 | Fundamental flaws discovered in numerical algorithms used in advanced applications require major changes to application development. | Moderate | Very Low | Low | Anticipate or resolve algorithm issues through technical interactions on algorithm research through the Institutes, ASC Centers, and academia, and focus on test problem comparisons as part of software development process. |

# Appendix A. Performance Measures

**Table A-1. ASC Performance Measures**

| ADVANCED SIMULATION AND COMPUTING (ASC) CAMPAIGN | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Goal**: Provides leading edge, high-end simulation capabilities to meet weapons assessment and certification requirements, including weapon codes, weapon science, platforms, and computer facilities. | | | | | | | | |
| **INDICATOR** | **ANNUAL TARGETS** | | | | | | | **ENDPOINT TARGET DATE** |
| | **FY04** | **FY05** | **FY06** | **FY07** | **FY08** | **FY09** | **FY10** | |
| Peer-reviewed progress in completing milestones, according to a schedule in the Advanced Simulation and Computing Campaign Program Plan, in the development and implementation of improved models and methods into integrated weapon codes and deployment to their users (long-term output).<br>Panel Criteria: (1) Delivery and implementation of validated models into code projects, and (2) Documented verification of approximations. | High Fidelity Primary Code | Initial baseline Primary Code | Initial validated simulation code for W76 and W80 | W80 code baseline | Conduct modern baseline of all enduring stockpile systems | Complete modern baseline of all enduring stockpile systems | Quantify margins and uncertaintie s of modern baseline simulations | By 2015, accomplish full transition from legacy design codes to modern ASC codes with documented quantification of margins and uncertainties of simulation solutions. |

| ADVANCED SIMULATION AND COMPUTING (ASC) CAMPAIGN | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **Goal**: Provides leading edge, high-end simulation capabilities to meet weapons assessment and certification requirements, including weapon codes, weapon science, platforms, and computer facilities. | | | | | | | | |
| **INDICATOR** | **ANNUAL TARGETS** | | | | | | | **ENDPOINT TARGET DATE** |
| | **FY04** | **FY05** | **FY06** | **FY07** | **FY08** | **FY09** | **FY10** | |
| Cumulative percentage of the 31 weapon system components, primary/secondary/engineering system, analyzed using ASC codes, as part of annual assessments and certifications (long-term output). | 32% | 38% | 51% | 67% | 87% | 96% | 100% | By 2010, analyze 100 percent of 31 weapon system components using ASC codes, as part of annual assessments and certifications (interim target). |
| The maximum individual platform computing capability delivered, measured in trillions of operations per second (teraflops) (long-term output). | 40 | 100 | 200 | 200 | 200 | 350 | 350 | BY 2009, deliver a maximum individual platform computing capability of 350 teraops. |
| Total capacity of ASC production platforms attained, measured in teraflops, taking into consideration procurements & retirements of systems (long-term output). | 75 | 172 | 160 | 360 | 470 | 980 | 980 | By 2009, attain a total production platform capacity of 980 teraops. |
| Average cost per teraflops of delivering, operating, and managing all SSP production systems in a given fiscal year (efficiency measure). | $8.15M | $5.7M | $3.99M | $2.79M | $1.96M | $1.37M | $0.96M | By 2010, attain an average cost of $0.96 M per teraflops of delivering, operating, and managing all SSP production systems. |

# Appendix B. Glossary

| | |
|---|---|
| **ALC** | Advanced Simulation and Computing Linux Cluster |
| **ALE** | Arbitrary Lagrangian-Eulerian |
| **AMR** | Adaptive Mesh Refinement |
| **ASAP** | Academic Strategic Alliance Program |
| **ASC** | Advanced Simulation and Computing (formerly ASCI) |
| **ASCI** | Accelerated Strategic Computing Initiative |
| **ASIC** | Application Specific Integrated Circuit |
| **AST** | Alliance Strategy Team |
| **CASC** | Center for Applied Scientific Computing |
| **CCF** | Central Computing Facility at Los Alamos |
| **CCS** | Computer and Computational Sciences Division at Los Alamos |
| **CEI** | Computational Engineering International |
| **CRT** | Computer Resource Team |
| **CSRI** | Computer Science Research Institute at Sandia |
| **DARPA** | Defense Advanced Research Projects Agency |
| **DCE** | Distributed Computing Environment |
| **DisCom** | Distance Computing |
| **DoD** | Department of Defense |
| **DOE** | Department of Energy |
| **DP** | Defense Programs |
| **DSW** | Directed Stockpile Work |
| **DVS** | Data and Visualization Sciences |
| **EDTV** | Early Development Technology Vehicle |
| **GPFS** | Global Parallel File System |
| **HPC** | High-Performance Computing |
| **HPSD** | High Performance Systems Division at Lawrence Livermore |
| **HPSS** | High-Performance Storage System |

| | |
|---|---|
| **I/O** | Input/Output |
| **ICCD** | Integrated Computing and Communications Department at Lawrence Livermore |
| **ICN** | Integrated Computing Network |
| **ICS** | Integrated Computing Systems |
| **ITS** | Institute for Terascale Simulation at Lawrence Livermore |
| | |
| **LACSI** | Los Alamos Computer Science Institute |
| **LANL** | Los Alamos National Laboratory |
| **LC** | Livermore Computing |
| **LDCC** | Laboratory Data Communication Center at Los Alamos |
| **LEP** | Life Extension Program |
| **LES** | Large Eddy Simulation |
| **LLNL** | Lawrence Livermore National Laboratory |
| | |
| **M&PM** | Materials and Physics Models |
| **MCR** | Multiprogrammatic Capability Cluster |
| **MESA** | Microsystems and Engineering Sciences Applications |
| **MPI** | Message Passing Interface |
| **MPICH** | Message Passing Interface-Chameleon |
| **MPP** | Massively Parallel Processing |
| | |
| **NIF** | National Ignition Facility |
| **NNSA** | National Nuclear Security Administration |
| **NPR** | Nuclear Posture Review |
| **NSD** | Networks and Services Division at Lawrence Livermore |
| | |
| **OCF** | Open Computing Facility |
| **OPTL** | One Program – Three Laboratories |
| | |
| **pEDTV** | IBM Power 4+ processor early development technology vehicle |
| **petaops** | 1,000 teraops |
| **PI&P** | Physical Infrastructure and Platforms |
| **PSE** | Problem Solving Environment |
| **PYRE** | Python Scripting Environment |

| | |
|---|---|
| **RAS** | Reliable, available, and secure |
| **RSRM** | Re-Usable Solid Rocket Motor |
| | |
| **S&CS** | Simulation and Computer Science |
| **SAMRAI** | Structured Adaptive Mesh Refinement Applications Infrastructure |
| **SARAPE** | Synchronized Account Request Automated Process |
| **SCC** | Strategic Computing Complex at Los Alamos |
| **SCF** | Secure Computing Facility |
| **SDD** | Services and Development Division at Lawrence Livermore |
| **SDM** | Scientific Data Management |
| **SFI** | Significant Finding Investigation |
| **SGI** | Silicon Graphics International |
| **SMP** | Symmetric Multiprocessor |
| **SNL** | Sandia National Laboratories |
| **SP** | Scalable POWERparallel |
| **SPMD** | Single-Program-Multiple-Data |
| **SSP** | Stockpile Stewardship Program |
| **STS** | Stockpile to Target Sequence |
| | |
| **teraops** | Trillions of floating point operations per second |
| **TSF** | Terascale Simulation Facility at LLNL |
| **TST** | Tri-Lab Sponsor Team |
| | |
| **V&V** | Verification and Validation Program |
| **VTF** | Virtual Test Facility |
| | |
| **WAN** | Wide Area Network |
| | |
| **xEDTV** | Intel Pentium 4 Xeon processor early development technology vehicle |

# Appendix C. Points of Contact

| IP Section | Title | Contact |
|---|---|---|
| 2.1.0 | Tri-Lab Problem Solving Environment Activities | Jeff Brown (tri-lab contact), LANL, 505-665-4655, jeffb@lanl.gov<br>Mary Zosel, LLNL, 925-422-4002, zosel1@llnl.gov<br>Pete Dean, SNL, 925-294-2656, pwdean@sandia.gov |
| 2.2.0 | Tri-Lab Distance Computing Activities | Mike Sjulin (tri-lab contact), SNL, 505-845-8550, mrsjuli@sandia.gov<br>Dave Wiltzius, LLNL, 925-422-1551, wiltzius@llnl.gov<br>Bob Tomlinson, LANL, 505-665-6599, bob@lanl.gov<br>Jim Handrock, SNL, 925-294-3444, jlhandr@sandia.gov |
| 2.3.0 | Tri-Lab PathForward Activities | Dick Watson (tri-lab contact), LLNL, 925-522-9216, dwatson@llnl.gov<br>Jeff Brown, LANL, 505-665-4655, jeffb@lanl.gov<br>Jim Tomkins, SNL, 505-845-7249, jltomki@sandia.gov |
| 2.4.0 | Tri-Lab Data and Visualization Activities | Steve Louis (tri-lab contact), LLNL, 925-422-1550, stlouis@llnl.gov<br>Bob Tomlinson, LANL, 505-665-6599, bob@lanl.gov<br>Rob Leland, SNL, 505-845-8439, leland@sandia.gov |
| 3.1.1 | LLNL Platforms | Lynn Kissel, LLNL, 925-422-5864, kissel1@llnl.gov |
| 3.1.2 | LANL Platforms | Charlie Slocomb, LANL, 505-664-0569, cas@lanl.gov |
| 3.1.3 | SNL Platforms | Jim Tomkins, SNL, 505-845-7249, jltomki@sandia.gov |
| 3.2.1 | LLNL Computational Systems | Doug East, LLNL, 925-424-4148, east1@llnl.gov |
| 3.2.2 | LANL Computational Systems | Cheryl Wampler, LANL, 505-667-5243, clw@lanl.gov |
| 3.2.3 | SNL Computational Systems | John Noe, SNL, 505-844-5592, jpnoe@sandia.gov |
| 3.3.1 | LLNL Simulation Support | Brian Carnes, LLNL, 925-423-9181, carnes1@llnl.gov |
| 3.3.2 | LANL Simulation Support | Cheryl Wampler, LANL, 505-667-5243, clw@lanl.gov |
| 3.3.3 | SNL Simulation Support | John Noe, SNL, 505-844-5592, jpnoe@sandia.gov |
| 4.1 | Academic Strategic Alliance Program | Dick Watson, LLNL, 925-522-9216, dwatson@llnl.gov<br>Paul Dotson, LANL, 505-667-6107, dotson@lanl.gov<br>Tony Chen, SNL, 505-284-3959, aachen@sandia.gov |
| 4.1.4.1 | Caltech, Center for Simulating Dynamic Response of Materials | Dan Meiron, 626-395-3424, dim@its.caltech.edu<br>Michael Aivazis, 626-395-3424, aivazis@caltech.edu<br>Paul Dimotakis, 626-395-6811<br>Bill Goddard, 626-395-2731, wag@wag.caltech.edu<br>Michael Ortiz, 626-395-4530, ortiz@aeor.caltech.edu<br>Dale Pullin, 626-395-6081, dale@galcit.caltech.edu |

| IP Section | Title | Contact |
|---|---|---|
| 4.1.4.2 | Stanford, Center for Integrated Turbulence Simulation | Parviz Moin, 650-723-9713, moin@stanford.edu<br>Juan Alonso, 650-723-9954, jjalonso@stanford.edu<br>Heinz Pitsch, 650-736-1995, h.pitsch@stanford.edu<br>William Dally, 650-725-8945, billd@csl.stanford.edu<br>Pat Hanrahan, 650-723-8530, hanrahan@cs.stanford.edu |
| 4.1.4.3 | University of Chicago, Center for Astrophysical Flash Phenomena | Donald Q. Lamb, 773-702-7194, d-lamb@uchicago.edu<br>Robert Rosner, 773-702-0560, r-rosner@uchicago.edu<br>Todd Dupont, 773-702-3485, Dupont@cs.uchicago.edu<br>Rusty Lusk, 630-252-7852, lusk@mcs.anl.gov<br>Tomasz Plewa, 773-834-3227, tomek@flash.uchicago.edu<br>Andrew Siegel, 773-834-8501, siegela@flash.uchicago.edu<br>Jim Truran, 773-702-9584, truran@nova.uchicago.edu |
| 4.1.4.4 | University of Illinois, Center for Simulation of Advanced Rockets | Michael T. Heath, 217-333-6268, m-heath@uiuc.edu<br>William A. Dick, 217, 244-7235, wdick@uiuc.edu<br>Robert A. Fiedler, 217-333-3247, rfiedler@uiuc.edu |
| 4.1.4.5 | University of Utah, Center for Simulation of Accidental Fires and Explosions | David W. Pershing, 801-581-5057, David.Pershing@utah.edu<br>Chuck Wight, 801-581-8796, Chuck.Wight@utah.edu<br>Tom Henderson, 801-581-3601, tch@cs.utah.edu<br>Philip Smith, 801-585-3129, smith@crsim.utah.edu<br>Greg Voth, 801-581-7272, voth@chem.utah.edu<br>Patrick McMurtry, 801-581-3889, mcmurtry@eng.utah.edu<br>Eric Eddings, 801-585-3931, eddings@che.utah.edu<br>Steve Parker, 801-585-1504, sparker@cs.utah.edu |
| 4.2.1 | Lawrence Livermore ASC Institute for Terascale Simulation | Rob Falgout, LLNL, 925-422-4377, rfalgout@llnl.gov |
| 4.2.2 | Los Alamos Computer Science Institute | Rod Oldehoeft, LANL, 505-665-3663, rro@lanl.gov |
| 4.2.3 | Sandia Computer Science Research Institute | David Womble, SNL, 505-845-7471, dewombl@sandia.gov |

# Appendix D. ASC Risk Management Process

Risk Management is a process for identifying and analyzing risks, encouraging mitigation and contingency planning to minimize the potential consequence of identified risks, and monitoring and communicating up-to-date information about risk issues. It is a process to support better decision-making by contributing to a greater insight into project uncertainties and their potential consequences. It is as much about identifying opportunities as it is about avoiding losses.

A "risk" is defined in this context as: (1) a future event, action, or condition that might prevent successfully executing strategies or achieving technical or business objectives; (2) the risk exposure level defined by the likelihood or probability that an event, action, or a condition will occur and the consequences if that event, action, or condition does occur. Associated with a risk may be the mitigation/contingency planning developed for managing that risk.

Risk management in ASC consists of three major components: assessment, handling/mitigation, and tracking.

## Risk Assessment

Risk assessment is the identification, analysis, and mitigation/contingency planning associated with risk management. The objective of risk assessment is to prioritize the risks to help focus management efforts on mitigating top risks.

Identification is the exploration for issues surrounding goals, milestones, deliverables, schedules, costs, technical performance, dependencies and any other factors that may introduce an element of uncertainty into a given project.

Analysis is where expertise and judgment are used to evaluate the consequence a given identified risk may have on a project's cost, schedule, or performance, and the likelihood that a given identified risk may have a programmatic or technical impact. Analysis also includes evaluation of ownership of an issue and evaluation of potential interdependencies that may influence the ability to manage or control an issue.

Mitigation/contingency planning is the action that is proactively undertaken to lessen consequence or likelihood, and/or develop contingency actions, in the event that risk issues develop.

Risks are annually identified during program planning and development of milestones.

Criteria for evaluating risks must be consistently applied to effectively prioritize risks. Table D-1 lists criteria for evaluating consequences against cost, performance, and schedule. Table D-2 lists criteria for evaluating likelihood against programmatic or technical risks. Table D-3 is a matrix for defining the risk exposure level, based on consequence and likelihood.

**Table D-1. Consequence Criteria**

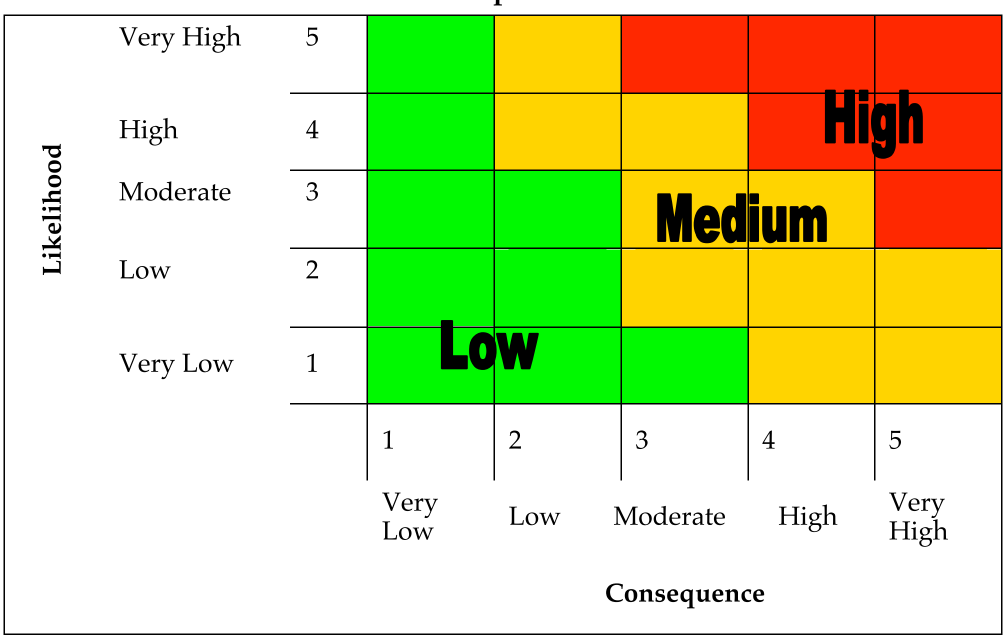
| Consequence | Criteria |
|---|---|
| Very Low | Cost: Negligible impact on cost. Impact is contained within the strategic unit and results in neither under or over costing of spend plan.<br>Performance: Negligible impact on function or performance. Requirements are clearly met.<br>Schedule: Negligible impact on schedule. Impact is managed within the strategic unit. Results in no impact to critical path and no impact to other strategic units. Milestones are clearly met. |
| Low | Cost: Minor impact on cost. Impact is contained within the strategic unit and results in less than 5% under or less than 5% over costing of spend plan.<br>Performance: Minor impact on function or performance. Requirements are clearly met.<br>Schedule: Minor impact on schedule. Impact may be managed within the strategic unit. Results in no impact to critical path and no impact to other strategic units. Milestones are clearly met. |
| Moderate | Cost: Recognizable impact on cost. Impact is not contained within the strategic unit and may result in less than 5% under or greater than 5% over costing of spend plan.<br>Performance: Recognizable impact on function or performance. Requirements may not all be met.<br>Schedule: Recognizable impact on schedule. Impact may not be managed within the strategic unit. May result in impact to critical path or may impact other strategic units. Milestones may not be met. |
| High | Cost: Significant impact on cost. Impact is not contained within the strategic unit and may result in less than 10% under or greater than 10% over costing of spend plan.<br>Performance: Significant impact on function or performance. Requirements will not all be met.<br>Schedule: Significant impact on schedule. Impact will not be managed within the strategic unit. Will result in impact to critical path or will impact other strategic units. Milestones will not be met. |
| Very High | Cost: Major impact on cost. Impact will not be contained within the strategic unit and will result in less than 10% under or greater than 10% over costing of spend plan.<br>Performance: Major impact on function or performance. Requirements cannot be met.<br>Schedule: Major impact on schedule. Impact cannot be managed within the strategic unit. Will result in failure in critical path or will significantly impact other strategic units. Milestones cannot be met. |

**Table D-1. Likelihood Criteria**

| Consequence | Criteria |
|---|---|
| Very Low | Programmatic: No external, environment, safety, and health (ES&H), security or regulatory issues. Qualified personnel, resources, and facilities are available.<br>Technical: Non-challenging requirements. Simple design or existing design. Few and simple components. Existing technology. Well-developed process. |

| Consequence | Criteria |
|---|---|
| Low | Programmatic: Minor potential for external, ES&H, security or regulatory issues. Minor redirection of qualified personnel, resources, or facilities modification is necessary.<br>Technical: Low requirements challenge. Minor design challenge or minor modification to existing design. Moderate number or complex components. Existing technology with minor modification. Existing process with minor modification. |
| Moderate | Programmatic: Moderate potential for external, ES&H, security or regulatory issues. Moderate redirection of qualified personnel, resources, or facilities modification is necessary.<br>Technical: Moderate requirements challenge with some technical issues. Moderate design challenge or significant modification to existing design. Large number or very complex components. Existing technology with significant modification. Existing process with significant modification. |
| High | Programmatic: Significant potential for external, ES&H, security or regulatory issues. Significant redirection of qualified personnel, resources, or facilities modification is necessary.<br>Technical: Significant requirements challenge with major technical issues. Significant design challenge or major modification to existing design. Large number and very complex components. New technology. New process. |
| Very High | Programmatic: Major potential for external, ES&H, security or regulatory issues. Major redirection of qualified personnel, resources, or facilities modification is necessary.<br>Technical: Major requirements challenge with possibly unsolvable technical issues. Major design challenge or no existing design to modify. Extreme number and extremely complex components. Possibly no technology available. Possibly no process available. |

**Table D-3. Risk Exposure Level Matrix**



## Risk Exposure

The risk exposure values and the resulting matrix chart categorize risks as high, eedium, and low. The rating matrix is intentionally skewed toward weighing consequence more than likelihood. Subjectively, a low-consequence risk is of little consequence, while a high or very high consequence risk, even if very unlikely to develop, is still a high or very high consequence, which may require more active management.

| | |
|---|---|
| High | Risk exposure is High if consequences are severe and likelihood is significant. Some mitigating or contingency plan is required. Dependencies and impacts on other strategic units must be explored, and potentially affected units engaged. |
| Medium | Risk exposure is Medium if consequences are significant and likelihood is moderate. Some mitigating or contingency plan is recommended. Dependencies and impacts on other strategic units must be explored, and potentially affected units engaged. |
| Low | Risk exposure is Low if consequences are minimal and likelihood is minor. Some mitigating or contingency plan is optional. Dependencies and impacts on other strategic units should be explored, and potentially affected units may be engaged. |

## Risk Types

There are various methods to identify the type and/or source of risks. ASC has five different risk types: programmatic, technical, cost, schedule, and performance.

| | |
|---|---|
| Programmatic Risks | Those risks that flow from (or impose) an impact on program governance, and those risks that impact program performance. The risks for governance may be external (political, statutory, litigious, or contractual) or internal [business priorities, staff limitations, return-on-investment (ROI) constraints, and learning curves]. |
| Technical Risks | Performance risks associated with end items. From the customer's perspective, there is concern that the system will not perform as required. From the performing organization's perspective, the concern is that the system will not meet its specifications. |
| Cost Risks | Not enough money at the highest level to do the job required in the time allocated, including reserves for reasonable contingencies. The causes of such risks can be estimating errors, low-ball bids, business decisions, lack of understanding of requirements and political expediency. |
| Schedule Risks | Not enough time exists at the highest level of concern to do the required job with the resources allocated. Problems with resources may be of a programmatic nature, but at a managerial level, the concern is more focused. For example, how does one allow for flexibility at the end of the schedule for coping with problems that will inevitably occur as time and resources diminish? |

| | |
|---|---|
| Performance Risks | At the highest level of concern, one or more performance requirements may not be met. Problems meeting performance requirements may be technical, but at a managerial level, the concern is more focused on evaluating flexibility in choosing technology option alternatives and evaluating outcomes associated with not meeting specific performance requirements. Risks that impact program performance generally flow from issues of competence, experience, organizational culture, and management team skills. |

## Risk Handling/Mitigation

Handling/mitigation is the action that is proactively undertaken to lessen consequence or likelihood, and/or develop contingency actions, in the event that risk issues develop. The following is a list of various methods in handling risks:

| | |
|---|---|
| Avoidance | Use an alternative approach, with no risks, if feasible. There are programs that deliberately involve high risks in the expectation of high gains. However, avoidance is the most effective risk management technique. This approach can be applied to high and medium risks. |
| Control | Controlling risks involve the development of a risk mitigation approach/action and tracking the progress of that risk under control. This approach is mostly applied to High and Medium risks. |
| Assumption | Simply accepting the risk and proceeding. This approach is usually applied to low risk items. |
| Risk Transfer | An attempt to pass the risk to another program element. This approach can be applied to external risks outside the control of ASC program. |

## Risk Tracking

Risk tracking is the process of tracking the progress of mitigation actions and the status of risks. Risk status and an updated evaluation of risks are included in quarterly progress reports from the three laboratories, and DP status reporting.

# Appendix E. Detailed Level 2 Milestones

## SANDIA FY05 MILESTONES

**Milestone (8): Validate the application of ALEGRA-HEDP for Z-Pinch Experimental Design and Analysis.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Verification and Validation

Description: Assess processes and methodologies of the Sandia ASC V&V program when applied to the application of the ALEGRA-HEDP code to the design and analysis of Z-pinch experiments. This milestone supports the development of predictive z-pinch modeling applied to Campaign (2,4,7,10) activities on z-pinch facilities. Such modeling impacts use and optimization of the current Z-machine; and contributes to the design and projected use of new facilities, including the refurbished Z-machine (ZR), scheduled to begin operations in FY06.

Integration/Interfaces: This is a V&V milestone. Milestone execution and success relies upon close collaboration between the Sandia Z-machine experimental program, the Sandia ASC ALEGRA-HEDP code development project, and the Sandia ASC V&V program.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: Assess processes and methodologies of the Sandia ASC V&V program when applied to the application of the ALEGRA-HEDP code to the design and analysis of Z-pinch experiments. This milestone supports the development of predictive z-pinch modeling applied to Campaign (2,4,7,10) activities on z-pinch facilities. Such modeling impacts use and optimization of the current Z-machine; and contributes to the design and projected use of new facilities, including the refurbished Z-machine (ZR), scheduled to begin operations in FY06.

SNL Integration/Interfaces: This is a V&V milestone. Milestone execution and success relies upon close collaboration between the Sandia Z-machine experimental program, the Sandia ASC ALEGRA-HEDP code development project, and the Sandia ASC V&V program.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (9): Apply the validation process at the sub-system level to support W76-1 qualification in hostile blast and impulse environments.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Weapons System: Multiple Systems

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Verification and Validation

Description: State-of-the-art structural dynamics validation processes will be demonstrated on a series of test articles supporting the mechanical response prediction of the W76-1 AF&F for the blast test environment. The validation process will accommodate parametric uncertainties, test variabilities, and unit-to-unit assembly variation. Specific elements of the milepost will include development of foam models, AF&F bolted joint representations, and combined effects in a low fidelity mock-up of the AF&F. The Salinas structural dynamics code will be used to predict structural response to hostile environments.

Integration/Interfaces: This is a V&V milestone collaboratively supported by Applications and C6 and supporting W76-1 LEP. Physics based understannding of joint and faom behavior with uncertainty will aid SLEPs for the W80 and B61.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: State-of-the-art structural dynamics validation processes will be demonstrated on a series of test articles supporting the mechanical response prediction of the W76-1 AF&F for the blast test environment. The validation process will accommodate parametric uncertainties, test variabilities, and unit-to-unit assembly variation. Specific elements of the milepost will include development of foam models, AF&F bolted joint representations, and combined effects in a low fidelity mock-up of the AF&F. The Salinas structural dynamics code will be used to predict structural response to hostile environments.

SNL Integration/Interfaces: This is a V&V milestone collaboratively supported by Applications and C6 and supporting W76-1 LEP. Physics based understannding of joint and faom behavior with uncertainty will aid SLEPs for the W80 and B61.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (12): Develop, implement and test advancements in geological material models for use in a realistic simulation of an earth penetrating weapon.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11 Weapons System: Multiple Systems

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Materials and Physics Modeling

Description: This milestone is responsible for the development of an advanced geological material model that will be used by the advanced ASC codes for modeling earth penetrators. The high-rate model will be enhanced to include (1) a tensile cracking capability and (2) a ubiquitous joint capability for field scale analyses. The high-rate model will be fitted to available hard rock shock data. The material model will be documented either in a Sand report or submitted to a peer reviewed journal. The model will be implemented into Alegra and Presto and tested in a demonstration calculation.

Integration/Interfaces: This milestone is strongly integrated with the ASC Advanced Applications FY05 Level 2 milestone for HDBT. The Advanced Applications milestone will involve a realistic demonstration of a earth penetrator simluation both Alegra and Presto. In order to perform a demonstration calculation the advanced geological model will require implementation into Alegra and Presto. The ASC M&PM Solid Mechanics Project will be responsible for implementation of the advanced material models into the material model library, LAME. Implementation of this model will allow analyst to investigate if this model can be used effectively when advecting target material through a mesh although detailed understanding of this issue will not be part of the milestone deliverable.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: This milestone is responsible for the development of an advanced geological material model that will be used by the advanced ASC codes for modeling earth penetrators. The high-rate model will be enhanced to include (1) a tensile cracking capability and (2) a ubiquitous joint capability for field scale analyses. The high-rate model will be fitted to available hard rock shock data. The material model will be documented either in a Sand report or submitted to a peer reviewed journal. The model will be implemented into Alegra and Presto and tested in a demonstration calculation.

SNL Integration/Interfaces: This milestone is strongly integrated with the ASC Advanced Applications FY05 Level 2 milestone for HDBT. The Advanced Applications milestone will involve a realistic demonstration of a earth penetrator simluation both Alegra and Presto. In order to perform a demonstration calculation the advanced geological model will require implementation into Alegra and Presto. The ASC M&PM Solid Mechanics Project will be responsible for implementation of the advanced material models into the material model library, LAME. Implementation of this model will allow analyst to investigate if this model can be used effectively when advecting target material through a mesh although detailed understanding of this issue will not be part of the milestone deliverable.

SNL Status: ?

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (14): Deploy computer codes for modeling trajectory and response of earth penetrating weapons.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11 Weapons System: Multiple Systems

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: This milestone is the development and deployment of a computational capability to predict penetration depth and mechanical loading experienced by a penetrator body during penetration. This will be accomplished by developing capabilities in Alegra to model earth penetration using an advanced geological material model and developing an Alegra output capability to export penetrator load histories (for subsequent detailed modeling of subsystem and component response). These capabilities will be demonstrated with simulations relevant to DSW.

Integration/Interfaces: The successful completion of this milestone will require contributions from DSW (representative target geology, representative EP design information), and Campaign 6 (representative geologic material properties, validation data for earth penetrator performance). This milestone is strongly integrated with the ASC M&PM Level 2 milestone to develop advanced geological material models for HDBT.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: This milestone is the development and deployment of a computational capability to predict penetration depth and mechanical loading experienced by a penetrator body during penetration. This will be accomplished by developing capabilities in Alegra to model earth penetration using an advanced geological material model and developing an Alegra output capability to export penetrator load histories (for subsequent detailed modeling of subsystem and component response). These capabilities will be demonstrated with simulations relevant to DSW.

SNL Integration/Interfaces: The successful completion of this milestone will require contributions from DSW (representative target geology, representative EP design information), and Campaign 6 (representative geologic material properties, validation data for earth penetrator performance). This milestone is strongly integrated with the ASC M&PM Level 2 milestone to develop advanced geological material models for HDBT.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (15): Develop MEMS subgrid models for thermal simulations of MEMS features.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11 Weapons System: Multiple Systems

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Materials and Physics Modeling

Description: This milestone is responsible for the development and documentation of subgrid models required to accurately predict thermal transport in microsystems where the accuracy of continuum assumptions is questionable. Two subgrid models will be required for MEMS thermal analysis: novel conductivity models for micro structural polysilicon and advanced models for energy transfer in rarified gases between micro features. These subgrid models will be developed through the use of Direct Simulation Monte Carlo simulations that accurately captures non-continuum effects. These subgrid models will be documented and integrated into the necessary continuum codes.

Integration/Interfaces: This milestone will be heavily leveraged with ASC Advanced Applications microsystems projects. The Advanced Applications program has a level 3 milestone in FY05 that will be responsible for delivering the demonstration calcuation that takes advantage of these advanced subgrid models.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: This milestone is responsible for the development and documentation of subgrid models required to accurately predict thermal transport in microsystems where the accuracy of continuum assumptions is questionable. Two subgrid models will be required for MEMS thermal analysis: novel conductivity models for micro structural polysilicon and advanced models for energy transfer in rarified gases between micro features. These subgrid models will be developed through the use of Direct Simulation Monte Carlo simulations that accurately captures non-continuum effects. These subgrid models will be documented and integrated into the necessary continuum codes.

SNL Integration/Interfaces: This milestone will be heavily leveraged with ASC Advanced Applications microsystems projects. The Advanced Applications program has a level 3 milestone in FY05 that will be responsible for delivering the demonstration calcuation that takes advantage of these advanced subgrid models.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (17): Transition Red Storm platform to Limited Availability.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 03/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: In Q2 FY05 the Red Storm computer system will be placed into Limited Availability status following successful installation, verification, testing and acceptance by Sandia. Stockpile Stewardship capability sized simulations (i.e. requires more than 3000 processors) from Los Alamos, Lawrence Livermore and Sandia will be eligible to run on a stablized system in both classified and unclassified modes. Red Storm will be fully integrated into the Sandia computing environment(s), accessible from the DisCom WAN, running multiple applications from each laboratory and will be supporting file transfers to pre- and post-processing support systems at Sandia, at Los Alamos and at Lawrence Livermore.

Integration/Interfaces: This is a Computational Systems milestone collaboratively supported by VIEWS, PSE, DisCom, and, most importantly, Platforms and by the Construction & Infrastructure program.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: In Q2 FY05 the Red Storm computer system will be placed into Limited Availability status following successful installation, verification, testing and acceptance by Sandia. Stockpile Stewardship capability sized simulations (i.e. requires more than 3000 processors) from Los Alamos, Lawrence Livermore and Sandia will be eligible to run on a stablized system in both classified and unclassified modes. Red Storm will be fully integrated into the Sandia computing environment(s), accessible from the DisCom WAN, running multiple applications from each laboratory and will be supporting file transfers to pre- and post-processing support systems at Sandia, at Los Alamos and at Lawrence Livermore.

SNL Integration/Interfaces: This is a Computational Systems milestone collaboratively supported by VIEWS, PSE, DisCom, and, most importantly, Platforms and by the Construction & Infrastructure program.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (18): Deploy Red Storm user environment.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: Demonstrate a user environment that provides application development and execution, data analysis and visualization, and distance computing in accordance with ASC Red Storm and application requirements as defined in the Red Storm Usage Model. PSE, together with VIEWS and DisCom, will build on the limited environment developed in FY04 to deliver both a local and distance-computing environment for a limited user base.

Integration/Interfaces: PSE works closely with the ASC platform deployment teams, ASC code developers, and analysts in planning and standing up of new platforms and software systems. PSE and VIEWS will both collaborate with DisCom to ensure that the remote ASC supercomputer resources are accessible and that the WAN supports the distance environments enabled through the problem-solving environment and visualization programs. In addition, PSE will work closely with Ongoing Computing for production support.

Participating Sites: HQ, LANL, LLNL, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: Demonstrate a user environment that provides application development and execution, data analysis and visualization, and distance computing in accordance with ASC Red Storm and application requirements as defined in the Red Storm Usage Model. PSE, together with VIEWS and DisCom, will build on the limited environment developed in FY04 to deliver both a local and distance-computing environment for a limited user base.

SNL Integration/Interfaces: PSE works closely with the ASC platform deployment teams, ASC code developers, and analysts in planning and standing up of new platforms and software systems. PSE and VIEWS will both collaborate with DisCom to ensure that the remote ASC supercomputer resources are accessible and that the WAN supports the distance environments enabled through the problem-solving environment and visualization programs. In addition, PSE will work closely with Ongoing Computing for production support.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (19): Initial Productionization of Design Through Analysis Environment.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: An initial problem setup environment defined by the Design Through Analysis (DART) roadmap published in FY04 will be in a production state for supporting mechanics finite-element analyses performed with the SIERRA and Nevada code suites, as well as some commercial analysis codes. The metadata functionality will provide data continuity for the DART processes from design initiation through post processing and archiving. The engineering sciences analysis process will be supported with automated analysis QA procedures and data pedigree tracking. In the post-processing arena, emphasis will be on capabilities that enable office visualization for a spectrum of data sizes associated with mechanics problems at Sandia.

Integration/Interfaces: This is a PSE milestone collaboratively supported by VIEWS and supporting all DSW and S&T high- performance finite-element analysis. This milestone requires buy-in and close cooperation form the Sandia NWIE and DSW communities.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: An initial problem setup environment defined by the Design Through Analysis (DART) roadmap published in FY04 will be in a production state for supporting mechanics finite-element analyses performed with the SIERRA and Nevada code suites, as well as some commercial analysis codes. The metadata functionality will provide data continuity for the DART processes from design initiation through post processing and archiving. The engineering sciences analysis process will be supported with automated analysis QA procedures and data pedigree tracking. In the post-processing arena, emphasis will be on capabilities that enable office visualization for a spectrum of data sizes associated with mechanics problems at Sandia.

SNL Integration/Interfaces: This is a PSE milestone collaboratively supported by VIEWS and supporting all DSW and S&T high- performance finite-element analysis. This milestone requires buy-in and close cooperation form the Sandia NWIE and DSW communities.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (23): Deliver scalable multilevel solvers for use in ASC simulation codes.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: The solution of linear and nonlinear systems of equations is a key computational kernel within many ASC simulation codes. In this milestone, we will design and implement new algebraic multilevel capabilities that build on our existing multilevel solvers. This new functionality is necessary to successfully apply multilevel techniques to truly complex simulations. The new capabilities will include arbitrary matrix coarsenings, adaptive multilevel kernels (built on run-time analysis of solver performance), and extensions of current multilevel transfers to higher order techniques. The new components will be delivered in ML as a part of the Trilinos framework. A key aspect of this milestone will be the application of the new multilevel technology to several ASC simulations. This includes the utilization of ML within Premo as well as improvements to solvers in ALEGRA. Other potential applications include Ceptre, Xyce, Salinas, and Calore.

Integration/Interfaces: Applications: Code Development. The successful completion of this milestone will depend on a related investment by the code development teams, particularly the PREMO team, to integrate and test multilevel solvers within the codes.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: The solution of linear and nonlinear systems of equations is a key computational kernel within many ASC simulation codes. In this milestone, we will design and implement new algebraic multilevel capabilities that build on our existing multilevel solvers. This new functionality is necessary to successfully apply multilevel techniques to truly complex simulations. The new capabilities will include arbitrary matrix coarsenings, adaptive multilevel kernels (built on run-time analysis of solver performance), and extensions of current multilevel transfers to higher order techniques. The new components will be delivered in ML as a part of the Trilinos framework. A key aspect of this milestone will be the application of the new multilevel technology to several ASC simulations. This includes the utilization of ML within Premo as well as improvements to solvers in ALEGRA. Other potential applications include Ceptre, Xyce, Salinas, and Calore.

SNL Integration/Interfaces: Applications: Code Development. The successful completion of this milestone will depend on a related investment by the code development teams, particularly the PREMO team, to integrate and test multilevel solvers within the codes.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (1312): Demonstrate the loose coupling of planned ASC early-time neutron damage modeling codes.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Weapons System: Multiple Systems

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: Address a degenerate case starting with a threat weapon neutron spectrum, proceeding through the generation of neutron-induced recoil particles, the evolution of the displacement cascade, the early-time annealing of the defects, and ending with a hand-off of the defect definition to a device-level simulation code. This milestone demonstrates that the project has a clear definition of the interfaces between the modules being developed to simulate the early-time neutron damage. This is a crucial point in establishing that we have properly posed the problem and considered the steps in the simulation. We start with the neutron radiation environment and end with the time evolved defect definition.

Integration/Interfaces: This milestone addresses the critical issue of alternatives to SPR-III. It builds on ASC M&PM supported work in modeling the early-time annealing of neutron damage, is guided by C7 RES experimental measurements of the transient response of radiation damaged devices, interfaces with ASC Apps NuGET code for the time and energy-dependent neutron/gamma damage environment, interfaces with ASC Apps HPEM/Xyce code for the response of radiation-damaged circuits, and complements the MESA work on the development of a radiation hardened toolkit. This milestone helps lay a foundation for addressing how to certify future modifications of the fuze in the W78 or W88 systems to neutron radiation hardness requirements.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: Address a degenerate case starting with a threat weapon neutron spectrum, proceeding through the generation of neutron-induced recoil particles, the evolution of the displacement cascade, the early-time annealing of the defects, and ending with a hand-off of the defect definition to a device-level simulation code. This milestone demonstrates that the project has a clear definition of the interfaces between the modules being developed to simulate the early-time neutron damage. This is a crucial point in establishing that we have properly posed the problem and considered the steps in the simulation. We start with the neutron radiation environment and end with the time evolved defect definition.

SNL Integration/Interfaces: This milestone addresses the critical issue of alternatives to SPR-III. It builds on ASC M&PM supported work in modeling the early-time annealing of neutron damage, is guided by C7 RES experimental measurements of the transient response of radiation damaged devices, interfaces with ASC Apps NuGET code for the time and energy-dependent neutron/gamma damage environment, interfaces with ASC Apps HPEM/Xyce code for the response of radiation-damaged circuits, and complements the MESA work on the development of a radiation hardened toolkit. This milestone helps lay a foundation for addressing how to certify future modifications of the fuze in the W78 or W88 systems to neutron radiation hardness requirements.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

**Milestone (1313): Provide visualization for capability calculations on Red Storm.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: The VIEWS program will provide the systems necessary to interprete the data arising from a leading-edge capability calculation employing a majority of the available compute nodes on Red Storm. We will support interactive volume visualization with time evolution and will demonstrate remote image delivery from a central visualization server to both theater and desktop environments. The theater environment will provide display resolution at least an order of magnitude greater than that available on a typical desktop scientific workstation.

Integration/Interfaces: This is a VIEWS milestone collaboratively supported by PSE and supporting all DSW and S&T high-performance finite element analysis. This requires buy-in and close cooperation from the Sandia NWIE and DSW communities.

Participating Sites: HQ, SNL

NNSA POC: KUSNEZOV,DIMITRI F

SNL Information

SNL Implementation: The VIEWS program will provide the systems necessary to interprete the data arising from a leading-edge capability calculation employing a majority of the available compute nodes on Red Storm. We will support interactive volume visualization with time evolution and will demonstrate remote image delivery from a central visualization server to both theater and desktop environments. The theater environment will provide display resolution at least an order of magnitude greater than that available on a typical desktop scientific workstation.

SNL Integration/Interfaces: This is a VIEWS milestone collaboratively supported by PSE and supporting all DSW and S&T high-performance finite element analysis. This requires buy-in and close cooperation from the Sandia NWIE and DSW communities.

SNL M&O Contractor POC: VAHLE,MICHAEL O.

## SANDIA FY06 PRELIMINARY MILESTONES

**New SNL 06-A: Apply the validation process to the coupled electromagnetics and radiation transport model of the W76-1 Cavity System Generated Electromagnetic Pulse (SGEMP) response in a hostile environment.**

**New SNL 06-B: Demonstrate algorithms for simulating electrical systems with multi-time behavior in STS environments.**

**New SNL 06-C: Demonstrate capability to model computationally the structural response of a MEMs device.**

**New SNL 06-D: Demonstrate ability to compute material response coupled across two or more length scales.**

**New SNL 06-E: Develop coupled error estimation/uncertainty quantification capabilities. (APPS/Algorithms)**

**New SNL 06-F: Transition Red Storm to General Availability.**

**New SNL 06-G: Deploy a general availability Red Storm user environment.**

**New SNL 06-H: Deploy a fully operational Design Through Analysis (DTA) environment.**

**New SNL 06-I: Down select technologies for research and implementation from the roadmap developed in FY05. Begin research and implementation of the necessary technologies to develop the supporting computing environment for Sandia's next generation platform.**

**New SNL 06-J: Deliver prototype data analysis models and demonstrate their use in support of Verification and Validation program goals. (DVS / V&V)**

**New SNL 06-K: Deploy Security Infrastructure for ASC Tri-Lab.**

# LAWRENCE LIVERMORE FY05 MILESTONES

**Milestone (455): Perform and profile a high quality W80 3D secondary burn calculation with advanced physics.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 06/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: To be added

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: Perform a high quality secondary burn simulation, employing advanced physics capabilities in a 3D secondary performance code, for the W80. This is the next logical step beyond the corresponding FY05/Q1 Milestone (#1353). In contrast to the FY05/Q1 milestone, which is a prototype calculation, the advanced physics capabilities will be more mature, having been initially demonstrated in FY05/Q1. In addition, results of this calculation will be compared to an underground nuclear test. If possible more advanced physics capabilities will be brought to bear on this milestone. This simulation will make use of 3D parallel setup and meshing tools that will be employed in a production mode by secondary code developers and/or designers to prepare calculations to address 3D issues related to stockpile systems. Computer performance of the secondary code will be measured.

LLNL Integration/Interfaces: Advanced physical materials models generated by M&PM are required to successfully complete the milestone. Significant computer resources will be required. The selection of the system to simulate is intimately coordinated with DSW program element. The successful completion of this milestone demonstrates to the DSW and Science Campaign 4 program elements the continuing increase in capability of this secondary burn code.

LLNL M&O Contractor POC:

**Milestone (457): Investigate advanced primary performance and safety simulation capabilities for future stockpile activities to move towards a more predictive capability**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: To be added

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: Identify and research appropriate 2D and 3D primary performance and safety codes issues that are seen as necessary to make advances toward the vision of a predictive capability for future stockpile simulation work needed for DSW deliverables. The principal focus of this milestone will be on neutron transport methods. The investigations may include new physics options, new numerical techniques, new methods of utilizing the codes, new computer or code architectures, and/or comparison of methods and demonstrations to quantify uncertainties (e.g., numerical convergence, or algorithm and model sensitivity), as needed to contribute to the use of QMU methodology. The product of this milestone will be the identification of the investigation area, or areas, an evaluation of the studies performed, with a view towards enhancing predictive capability, and recommendations for the future path forward.

LLNL Integration/Interfaces: This milestone directly supports the future needs of DSW and the Science Campaigns (especially Campaign 1), and will address V&V objectives, so requires close coordination with these activities. Code project personnel will need ready access to adequate computing resources for code development, debugging, execution of a range of calculations, and analysis of code results.

LLNL M&O Contractor POC:

**Milestone (458): Implement enhancements of nuclear weapon simulation codes to support new designer needs**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 06/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: to be added

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: Implement and evaluate significant improvements to weapons codes and their models or algorithms to meet needs by designers for current or anticipated DSW deliverables. The enhancements will focus on implementation and evaluation by the code projects of advanced material models developed in M&PM projects. Some of the designer needs may arise as a result of work on the FY04 Level 2 milestones. While the principal focus for this milestone will be on primary performance and safety codes, the enhanced capabilities may be applicable to secondary, full system, or nonnuclear experiment simulations. Progress on this milestone will be evident first through the identification and documentation of specific needs for code enhancements. The product of this milestone will be the code enhancements, either the completion or status report on development for major enhancements, user documentation, and examples of their application to test problems, prototype applications, or other demonstrations of their use to meet the identified needs.

LLNL Integration/Interfaces: This milestone directly supports the accomplishment of DSW, Science Campaign (especially Campaigns 1, 2, and 3), and V&V objectives, so requires close coordination with these activities. Designers and code project personnel will need ready access to adequate computing resources for code development, debugging, execution of a range of calculations, and analysis of code results.

LLNL M&O Contractor POC:

**Milestone (459): Secondary burn code initial validation of focused physics capability**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 03/2005

DOE Programs/Subprograms: ASC Verification and Validation

Description: 2B added

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: An initial, focused validation evaluation by the V&V program will be performed and documented for this stockpile system simulation capability. A detailed, quantitative comparison of simulations with key output metrics derived from relevant experimental data will be made, as well as a determination of the uncertainty of these metrics due to uncertainties in the focused physics models. The extent of the focused validation will depend, in part, on the availability of computing resources.

LLNL Integration/Interfaces: Significant computer resources will be needed to perform the initial validation of focused physics. The selection of the system to simulate is intimately coordinated with DSW program element. The successful completion of this milestone demonstrates to the DSW and Science Campaign 4 program elements the continuing increase in capability of this secondary burn code.

**Milestone (461): Deploy First Phase of I/O Infrastructure for Purple**

Level: 2
Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: To be added

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: External networking infrastructure installation and performance analysis will be completed for the initial delivery of Purple. The external networking infrastructure includes incorporation of a new 10 Gigabit Ethernet fabric linking the platform to the LLNL High Performance Storage System (HPSS) and other center equipment. The LLNL archive will be upgraded to HPSS Release 5.1 to support the requirements of the machine and performance analysis will be completed using the newly deployed I/O infrastructure. Demonstrated throughput to the archive for this infrastructure will be a minimum of 1.5GB/s with a target of 3GB/s. Since Purple delivery is not scheduled until late Q3, demonstration of these performance goals will use parts of Purple and/or an aggregate of other existing resources.

LLNL Integration/Interfaces: Deployment of this phase of the I/O infrastructure for Purple requires integration and interface between Ongoing Computing, Physical Infrastructure & Platforms, and S&CS program elements at LLNL. Success will depend on the combined effort of these ASC program elements along with collaboration with IBM platform and archive personnel as well as 10 Gigabit Ethernet vendors.

LLNL M&O Contractor POC:

**Milestone (464): Complete Phase 1 Integration of Site-Wide Global Parallel File System (SWGPFS)**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: to be added

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: At LLNL, the Lustre file system will be deployed to create a new Site-Wide Global Parallel File System (SWGPFS) for both the open and classified networks. On the open network, SWGPFS will be the primary data resource for capacity systems, BlueGene/L, and visualization resources and will have high-speed access to the HPSS archive. Deployment on the classified network will follow at a later date when appropriate multi-cluster security plans are in place. For this milestone, Phase 1 of the SWGPFS will be deployed and scalable file system functionality will be demonstrated between a minimum of two LLNL ASC platforms and archival storage on the open network. File system performance will be demonstrated using the IOR test suite to show transfers between the Lustre-enabled clusters with a minimum of 60% of the effective measured aggregate network and I/O bandwidth available and a target of 80%. Archive performance of at least one GigaByte per second will also be demonstrated using HPSS interfaces to the archive.

LLNL Integration/Interfaces: Integration of an initial SWGPFS requires continued cooperation between ICC, PSE, and VIEWS program elements at LLNL. The Lustre file system PathForward effort also requires continued tri-lab cooperation with LANL and SNL. The SWGPFS team will work closely with the HPSS project and file system and platform vendors to ensure successful early deployment of this new file system model.

**Milestone (465): Deploy Remote Computing Environment for Red Storm**

Level: 2
Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: To be added

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: Deploy initial Red Storm production environment needed by LLNL application codes targeted to run on Red Storm. This milestone will be done in conjunction with the Sandia Red Storm deployment milestone, extending appropriate access and software to meet the needs of remote users from LLNL. This will include general availability to ASC resource (storage, visualization, computational) access, basic code development tools, and data archive capabilities. The deployment will include all the necessary elements for authorization, remote access and utilization from LLNL. This milestone is complete when the required LLNL application code services are generally available and the targeted LLNL application codes have successfully run in production mode on Red Storm.

LLNL Integration/Interfaces: This requires integration and interface between VIEWS, DisCom, PSE, SS, and CS program element efforts at Sandia and LLNL. It also requires interface with potential users from the LLNL DNT program for requirements, and the Sandia Red Storm team for details of the system and environment for ensuring we meet LLNL program requirements and that capabilities work as efficiently and seamlessly as practicable.

**Milestone (1348): TSF Activation**

Level: 2
Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 06/2005

DOE Programs/Subprograms: ASC Integrated Computing Systems (ICS)

Description: 2B added

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: Activate the Terascale Simulation Facility for classified and unclassified computing and complete all staff relocation into the TSF. Classified and unclassified networking must be in operation. Critical classified and unclassified servers must be in operation. The computer operations center and the hotline call center must be in operation. The first set of compute and visualization platforms have been moved into the TSF's computer rooms. All this must be accomplished with minimal downtime of LC services and minimal disruption of services to our customers. Decisions for planning moves that affect customers will be made in cosultation with our customers.

LLNL Integration/Interfaces: Cooperation among VIEWS, SS, CS, and Platforms will be required since these program elements have responsibility for equipment or services that will be affected by this effort.

LLNL M&O Contractor POC:

**Milestone (1349): Develop and apply the computational capability to give detailed term (line) treatment of radiation opacities for programmatic applications in DSW, NNSA Science campaigns and High Energy Density Experiments**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Materials and Physics Modeling

Description: 2B added

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: Our new code, the world's first relativistic detailed term opacity code, will be completed and applied both to benchmark three initial programmatic opacities and also to drive and analyze the results from upcoming laser based radiative transfer and opacity experiments. Accurate analysis of the transport and spectral emission characteristics of programmatic plasmas is complicated by the presence of numerous closely spaced transitions. It is known from computations and experiments for mid-Z elements at low density and temperature that a detailed line approach is often required because of significant "porosity" between the transitions. At higher Z, the number of relevant quantum mechanical states and transitions explodes, necessitating novel, scalable parallel atomic physics algorithms. These are being implemented in the new code.

LLNL Integration/Interfaces: This milestone directly supports the accomplishments and goals of DSW and the Science Campaigns, as well as the high energy density physics experimental effort (NIF), therefore requiring close coordination with these activities. Successful completion of this milestone will require access to adequate computing and programming resources.

LLNL M&O Contractor POC:

**Milestone (1350): V&V 4th Stockpile Summary / Annual: V&V status and results of simulation capability relevant to LLNL stockpile weapon systems. Theme: The PMP Model Set**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 06/2005

DOE Programs/Subprograms: ASC Verification and Validation

Description: 2B

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: Results of verification and validation evaluations will be rolled-up in a user-friendly summary for physics models and stockpile system simulations. Focus will be on the V&V of high priority capabilities relevant to the weapons program. Results will include model and system simulation V&V status, references supporting the completed V&V evaluations, appropriate mesh resolution and physical parameter ranges for model use, identification of appropriate verification test problems and validation data, sensitivities of some performance metrics to variations in model input parameters, and example input decks. Formal V&V standards for high priority computational capability evaluations will be developed for capabilities in each focus area to enable systematic, quantified interpretation of summary results. Each guidance document will include code and solution verification and model validation guidance as well as software process improvement guidance for V&V evaluations. This milestone represents a roll-up of all current V&V evaluations performed to date; the model and stockpile system simulation summary will be updated annually to reflect additional V&V quantification progress.

LLNL Integration/Interfaces: This milestone directly supports the NNSA-wide Annual Assessment process, the SFI process handled formally within DSW, and the SLEP Planning process within DSW, so requires close coordination with these activities. Designers and code project personnel will need ready access to adequate computing resources for code development, debugging, execution of a range of calculations, and V&V analysis of model results.

LLNL M&O Contractor POC:

**Milestone (1353): Implement an advanced physics capability in 3D secondary performance code and prototype its use through a 3D secondary burn calculation**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 12/2004

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: 2B

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: Implement an advanced physics capability in the 3D secondary performance code and perform a prototype 3D secondary burn simulation of a stockpile system. This will demonstrate the availability of these physics capabilities for future secondary performance simulations to meet stockpile objectives. One or more of several physics capabilities under development will be selected for this milestone. This milestone directly supports development of a secondary burn capability for stockpile performance assessments, for resolution of stockpile issues (e.g., SFIs), and determination of uncertainty in secondary margin estimates. First and second generation EOS, opacity, and nuclear material models generated through advanced computational models will be used as available.

LLNL Integration/Interfaces: As explicitly stated in the milestone description advanced physical materials models generated by M&PM are required to successfully complete the milestone. Significant computer resources will be needed. The selection of the system to simulate is intimately coordinated with DSW program element. The successful completion of this milestone demonstrates to the DSW and Science Campaign 4 program elements the continuing increase in capability of this secondary burn code.

LLNL M&O Contractor POC:

**Milestone (1358): Code and Solution Verification of Selected Primary and Secondary Capabilities**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Verification and Validation

Description: 2B

Integration/Interfaces:

Participating Sites: HQ, LLNL

NNSA POC: KUSNEZOV,DIMITRI F

LLNL Information

LLNL Implementation: In FY05, the third Level 2 Milestone will be focused on Verification of particular code simulation capabilities for specific applications against analytic and semi-analytic solutions. Code Verification demonstrates the ability, in a spatially, temporally, and iteratively converged model, to duplicate exact analytical solutions to the theory as coded. Solution Verification is an assessment of the rate of spatial, temporal, and iterative convergence. Verification problems relevant to primary, secondary, and materials modeling issues will be developed and applied to relevant to primary, secondary, and materials modeling issues will be developed and applied to the major primary and secondary performance codes. These analyses will include both code and solution verification evaluations, with comparisons of simulation results to known solutions, and demonstrations of mesh convergence. Solution verification activities and computational requirements will contribute to the justification of a substantial part of future platform capability needs.

LLNL Integration/Interfaces: Completing this milestone requires significant collaboration and involvement from several ASC Program Elements including the Advanced Applications, and Materials and Physics Modeling, the Physical Data Research Program, and interfacing with Assessment and Certification, and the Theoretical/Experimental Campaign elements (C1, C3, C4) of the weapons program. This milestone will require support from the members of the design, experimental, and code development groups and is strongly coupled to the weapon certification mission of A and B Divisions and their DSW, Campaigns 1, 2, 3, and 4 milestones.

LLNL M&O Contractor POC:

# LAWRENCE LIVERMORE FY06 PRELIMINARY MILESTONES

**New LLNL 06-01: Demonstrate high quality full system capability in a 2D secondary performance code with the addition of one or more physics model improvements needed for DSW simulations.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q2

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: Perform a "button to boom" calculation of a stockpile system including relevant primary and secondary physics models with the addition of one or more physics model improvements beyond the models used in the corresponding FY04 milestone. This code will continue to be used to address stockpile issues and contribute to determination of uncertainty in full system performance margin estimates.

LLNL Integration/Interfaces: Successful completion of this milestone requires integration of materials models developed by the M&PM technical element as well as access to adequate computing resources. The milestone supports the execution of the DSW and Science Campaign 4 program elements. The specifics of the milestone will be selected in close coordination with these elements.

LLNL M&O Contractor POC: Jim Rathkopf, (925)422-4602, rathkopf@llnl.gov

**New LLNL 06-02: Apply enhanced 3D secondary simulation capability to calculations required for DSW activities.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q4

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: Complete a high-quality 3D secondary implosion and explosion simulation for a UGT or stockpile system in support of DSW activities. This simulation will make use of advanced physics models and/or increased resolution beyond that used in the FY05 milestone. Physics capabilities used in this simulation will be made generally available in a corresponding release of the production code. This simulation will make use of 3D parallel setup and meshing tools that will be employed in a production mode by secondary code developers and/or designers. The results of the simulation will be compared to available nuclear and above ground experimental data. Computer performance of the secondary code will be measured.

LLNL Integration/Interfaces: Depending on the physics model improvement selected advanced physical materials models generated by M&PM may be needed to successfully complete the milestone. Significant computer resources will be required. The selection of the system to simulate is intimately coordinated with DSW program element. The successful completion of this milestone demonstrates to the DSW and Science Campaign 4 program elements the continuing increase in capability of this secondary burn code.

LLNL M&O Contractor POC: Jim Rathkopf, (925)422-4602, rathkopf@llnl.gov

**New LLNL 06-03: Enhance capabilities of nuclear weapon simulation codes to support current and planned design efforts.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q3

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: Implement and evaluate improvements to weapons codes and their models or algorithms to provide designers with more capable tools to meet current or anticipated DSW deliverables, baselines, advanced concepts, or efforts to quantify uncertainty. The principal focus of this milestone is expected to be on capabilities to simulate laser-driven and other high energy-density experiments. Additional needs for increased capability may arise from user experience with previous code improvements, availability of advanced models developed in M&PM projects, deficiencies identified in V&V studies, or high-leverage areas identified in QMU analyses. While the principal focus for this milestone will be on primary performance and safety codes, the enhanced capabilities may be applicable to secondary, full system, or nonnuclear experiment simulations. Progress on this milestone will be evident first through the identification and documentation of specific needs for code enhancements. The product of this milestone will be the code enhancements, either the completion or status report on development for major enhancements, user documentation, and examples of their application to test problems, prototype applications, or other demonstrations of their use to meet the identified needs.

LLNL Integration/Interfaces: This milestone directly supports the accomplishment of DSW, Science Campaign (especially Campaigns 1, 2, and 3), and V&V objectives, so requires close coordination with these activities. Code project personnel will need ready access to adequate computing resources for code development, debugging, execution of a range of calculations, and analysis of code results.

LLNL M&O Contractor POC: Tom Adams, (925)422-1248, adams35@llnl.gov

**New LLNL 06-04: Explore and assess new opportunities to enhance the predictive capability of primary performance and safety codes for future stockpile activities.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q4

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: Identify and research innovative approaches that have the potential to increase the predictive capability of 2D and 3D primary performance and safety codes for DSW deliverables. The principal focus of this milestone is expected to explore and assess approaches to quantifying and improving the ability to predict effects of 3D geometric features and perturbations in systems of interest. The approaches will be based on exploratory work carried out in FY05 or follow from experimental observations or uncertainties recognized in Science Campaign or DSW activities. The investigations may include new physics options, numerical techniques, methods of utilizing the codes, computer or code architectures, and/or contributions toward applying QMU methodology by addressing numerical convergence, or algorithm and model sensitivity. The product of this milestone will be the identification of the investigation area, or areas, an evaluation of the studies performed, with a view towards enhancing predictive capability, and recommendations for the future path forward.

LLNL Integration/Interfaces: This milestone directly supports the future needs of DSW and the Science Campaigns (especially Campaign 1), and will address V&V objectives, so requires close coordination with these activities. Code project personnel will need ready access to adequate computing resources for code development, debugging, execution of a range of calculations, and analysis of code results.

LLNL M&O Contractor POC: Tom Adams, (925)422-1248, adams35@llnl.gov

**New LLNL 06-05: Demonstrate a mixed implicit-explicit nonlinear thermo-mechanical simulation capability in a 3D engineering simulation code for STS modeling.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q3

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: Perform a nonlinear simulation of an NEP subsystem subject to STS environments representing mixed time scales, e.g., thermal stress and mechanical shock. While the Diablo project has focused to date on only implicit capabilities, this milestone motivates examination of software architecture and performance issues that may arise during eventual unification of our mechanical engineering modeling capabilities.

LLNL Integration/Interfaces: The Engineering STS simulation project supports W Program's DSW, C8 and C6 activities. The ParaDyn code is an explicit structural dynamics production capability supporting both LLNL's W80 LEP and LANL's W76 LEP. Simultaneously, the Diablo code is building new implicit thermo-mechanical capabilities, including a surface chemistry capability already contributing to DSW/C8 activities.

LLNL M&O Contractor POC: Bob Ferencz, (925)422-0571, ferencz@llnl.gov

**New LLNL 06-14: Complete and document initial focused validation of primary simulation capability.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q2

DOE Programs/Subprograms: ASC Verification and Validation

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: Initial V&V evaluation of the primary simulation capabilities of ASCI codes will be performed. By FY05, the first round of detailed V&V evaluations of LLNL code projects' primary simulation capability will be completed, compiled and reported. The report will describe the V&V evaluations performed, the degree to which the code simulation capabilities have been verified and validated, in a particular physical regime, for particular specified stockpile system applications.

LLNL Integration/Interfaces: This milestone directly supports the accomplishment of DSW and Science Campaign 1, so requires close coordination with these activities. Designers and code project personnel will need ready access to adequate computing resources for code development, debugging, execution of a range of calculations, and analysis of code results.

LLNL M&O Contractor POC: Cynthia Nitta, (925)423-3792, nitta@llnl.gov

**New LLNL 06-06: V&V 5th Stockpile Summary/Annual: V&V status and results of simulation capability relevant to LLNL stockpile weapon systems. Theme: When Confidence Bounds Overlap.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q3

DOE Programs/Subprograms: ASC Verification and Validation

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: Results of verification and validation evaluations will be rolled-up in a user-friendly summary for physics models and stockpile system simulations. Focus will be on the V&V of high priority capabilities relevant to the weapons program. Results will include model and system simulation V&V status, references supporting the completed V&V evaluations, appropriate mesh resolution and physical parameter ranges for model use, identification of appropriate verification test problems and validation data, sensitivities of some performance metrics to variations in model input parameters, and example input decks. Formal V&V standards for high priority computational capability evaluations will be developed for capabilities in each focus area to enable systematic, quantified interpretation of summary results. This document will include code and solution verification and model validation guidance as well as software process improvement guidance for V&V evaluations. This milestone represents a roll-up of all current V&V evaluations performed to date; the model and stockpile system simulation summary will be updated annually to reflect additional V&V quantification progress. For this year, there will be primary, secondary, and weaponization engineering V&V status of 1D, 2D and some 3D models, with confidence bounds characterized for performance characteristics of interest. This year's theme will include consideration of the circumstances where requirement and system capability confidence bounds overlap each other.

LLNL Integration/Interfaces: This milestone directly supports the NNSA-wide Annual Assessment process, the SFI process handled formally within DSW, and the SLEP Planning process within DSW, so requires close coordination with these activities. Designers and code project personnel will need ready access to adequate computing resources for code development, debugging, execution of a range of calculations, and V&V analysis of model results.

LLNL M&O Contractor POC: Cynthia Nitta, (925)423-3792, nitta@llnl.gov

**New LLNL 06-13: Produce and provide initial assessment for a first generation complex material model for strength and plasticity of weapons materials based on theory, microscale calculations, and experimental data.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q1

DOE Programs/Subprograms: ASC Materials and Physics Models

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: The efforts of multi scale modeling of constitutive properties will be collected into a complex continuum code model, which will be placed in a primary performance code for assessment. This work builds on earlier efforts to generate an effective, physically reasonable way to handle material models in continuum codes. While some material properties will be based on predictions by multiscale simulation, it is unlikely that the model at this point will include multiscale predictions of all important phenomena.

LLNL Integration/Interfaces: This milestone directly supports the accomplishments of DSW and Science Campaign 2, so requires close coordination with these activities. Successful completion of this milestone will require access to adequate computing resources.

LLNL M&O Contractor POC: Elaine Chandler, (925)422-2482, chandler2@llnl.gov

**New LLNL 06-07: Next-generation Pu multiphase EOS delivered for QMU and stockpile certification.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q2

DOE Programs/Subprograms: ASC Materials and Physics Models

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: A next-generation Pu multiphase EOS will be developed and delivered as a systematic improvement to our existing baseline equation of state by combining advanced quantum-based theory, DAC static experiments on the high-pressure phase diagram and JASPER dynamic EOS experiments. A suitable tabular representation of the multiphase EOS will be developed and delivered for hydrocode application, including QMU and stockpile certification studies.

LLNL Integration/Interfaces: This milestone directly supports DSW and Science Campaign 2 and requires close coordination with these activities. Successful completion of this milestone will require adequate manpower, including the retention of current untenured EOS staff, as well as access to adequate computing resources.

LLNL M&O Contractor POC: Elaine Chandler, (925)422-2482, chandler2@llnl.gov

**New LLNL 06-08: Produce and provide advanced assessment of a complex physics model using the full compliment of verification and validation tools and techniques available.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q4

DOE Programs/Subprograms: ASC Materials and Physics Models

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: A complex physics model will be implemented and assessed using the full range of modern verification and validation tools available. Analytic test problems, experimental data, and DSW design problems will all be considered to accomplish the task. Modifications and enhancements of the model will be implemented as required. The deliverable will be a rigorously-developed and tested model that will serve DSW design needs.

LLNL Integration/Interfaces: This milestone directly supports the Advanced Applications code development activities. Successful completion of this milestone will require access to adequate computing resources.

LLNL M&O Contractor POC: Elaine Chandler, (925)422-2482, chandler2@llnl.gov

**New LLNL 06-09: Deploy Security Infrastructure for ASC Tri-Lab.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q3

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: A new ASC tri-Lab security infrastructure is deployed to replace the existing DCE security infrastructure. This milestone is complete when the inter-site authentication and directory service are generally available and support authentication and authorization to production ASC compute resources by tri-Lab users. Additionally, the new security infrastructure will support an inter-site application to demonstrate the capabilities are functional for transitioning and deploying applications and infrastructure services.

LLNL Integration/Interfaces: The deployment of the tri-Lab security infrastructure will require integration and cooperation between ICC and S&CS program elements at LLNL, LANL, and SNL. Tri-Lab personnel will also work closely with developers of inter-site application and NWC plant sites to ensure successful adoption of the new security infrastructure. Further, as appropriate considering ICSI's (Integrated Cyber Security Initiative) schedule, deliverables, and funding, the tri-Lab security infrastructure will be integrated with the capabilities of the ICSI ESN (Enterprise Secure Network).

LLNL M&O Contractor POC: Dave Wiltzius, (925)422-1551, wiltzius@llnl.gov

**New LLNL 06-10: Deploy Next-Generation Delivery Infrastructure for Visualization Imagery.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q3

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: Existing DVS visual imagery capabilities are now supported by an analog video delivery infrastructure, and ad-hoc session and resource management. New advances in digital networking, graphics hardware, intelligent compression and visualization session orchestration software make it feasible to replace current delivery infrastructures with user-controllable digital image delivery over high-bandwidth networks based on commodity components. As a result, users will have measurably enhanced access to high-resolution, high-frame-rate visualization and rendering resources directly from their office workstations and collaborative workspaces. The milestone will encompass the following four activities: 1) improved video delivery, measured on a cost-benefit basis, will be deployed for user desktops and collaborative displays, 2) in-office access to very-high-bandwidth IP-based networks will be deployed for a large number of users, 3) remote rendering client-server capabilities and rendering abstraction software will be deployed, 4) visualization session orchestration and management software will be deployed.

LLNL Integration/Interfaces: A key focus of this milestone is enhanced access to ASC platform-generated visualization data for SSP users. Scaling and specific design points will be determined based on feedback by the user community to initial FY04-FY05 prototype deployments. Successful next-generation production deployment will require close interaction with end-users, DAM, DisCom, Ongoing Computing, and lab networking infrastructures to ensure proper selection and sizing of both the physical networking layers and the software capabilities required by this milestone.

LLNL M&O Contractor POC: Steve Louis, (925)422-1550, stlouis@llnl.gov

**New LLNL 06-11: BlueGene/L System Ready for Limited Availability.**

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q3

DOE Programs/Subprograms: ASC Integrated Computing Systems

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: The BlueGene/L supercomputer system has completed acceptance testing and early science runs. Tests will include full system runs. This milestone will be complete when the system stability supports access by multiple users to the system for limited availability scientific runs by the designated user community.

LLNL Integration/Interfaces: The operating system and system libraries, code development and performance analysis tools, math and graphics libraries have been installed and are stable enough to open BlueGene/L for access by a limited user community. To achieve this state, close integration of efforts from PSE and IBM is required to assure that the computing environment needed by M&PM codes is available and functional on the system. PSE and SS Lustre team members will provide stable Lustre file system clients. ICC has completed training of system and network administrations, operators, maintenance personnel, and user support personnel. M&PM code teams are working with ICC and PSE to continuing the port, development and tuning of selected applications. A cooperative partnership with Argonne National Laboratory (ANL) will provide coordination and support for access by the broader community from academic and Office of Science sites.

LLNL M&O Contractor POC: Mary Zosel, (925)422-4002, mzosel@llnl.gov

**New LLNL 06-12: Purple System Ready for Limited Production.**

Level: 2
Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06 Q3

DOE Programs/Subprograms: ASC Integrated Computing Systems

Description: To be added

Integration/Interfaces: To be added

Participating Sites: To be added

NNSA POC: To be added

LLNL Information

LLNL Implementation: The ASC Purple system at LLNL will be made available for limited availability classified production usage as soon as the hardware and software systems are deemed suitable stable for applications usage. When this milestone is complete, the system will begin providing useful computing cycles for production needs of NNSA.

LLNL Integration/Interfaces: Deployment of the Purple system requires integration and interface between all parts of the ASC computing organization at LLNL Integrated Computing Systems and Simulation and Computer Science as well as interfaces with ASCI code developers at all three defense laboratories, LLNL, LANL, and SNL. Close integration of efforts from PSE and IBM is required to assure that the computing environment needed by ACS codes is available and functional on the system. ICS has completed training of system and network administrations, operators, maintenance personnel, and user support personnel.

LLNL M&O Contractor POC: Doug East, (925)424-4148, dre@llnl.gov

# LOS ALAMOS FY05 MILESTONES

**Milestone (470): Simulate casting of the Qual Type 126 pit and compare the results of the simulation to the available experimental data for the same process.**

Level: 2
Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: 2B added

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation: The Telluride project seeks to provide simulation software for the manufacturing processes of the nuclear weapons complex. Metal casting is an important aspect of the envisioned pit manufacturing at LANL. This milestone is intended to help the project focus efforts on the physical models, numerical methods, and programming techniques that are required to simulate this specific process. It will also concentrate the activities that are required to perform the simulation. The casting process is complex, and our software contains elements to address each step of the process and each important physical phenomenon that occurs during the casting of Plutonium alloys. The milestone requires the coordination of all the physical models, together with appropriate boundary conditions, material properties, and geometric relationships. Specifically, the milestone simulation will include the preheating of the graphite mold by electromagnetic (Joule) heating imposed physically by a large solenoid. This preheat simulation is necessary to provide accurate initial temperatures, which in turn determine the loss of thermal energy from the liquid Pu alloy during the filling process, and from the solidifying alloy after the pour is complete.

LANL Integration/Interfaces: This milestone supports the Manufacturing Coordination Board milestone for Q2 of FY05 to "Manufacture four Qual and four Prod Type 126 pits". Although our milestone will be complete only a quarter prior to this milestone, intermediate communications will help manufacturing to meet its commitment. The degree of validation possible depends on the availability of experimental data on the pit casting process. NMT-10 intends to perform the necessary experiments late in FY03, but this schedule may well be delayed by more pressing programmatic needs

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (476): The Capsaicin Project will demonstrate a robust and accurate 2D-RZ discrete ordinates radiation transport capability.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 03/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: To be added

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation: The Capsaicin Milestone is the application of a verified deterministic transport capability to a validation problem. The Capsaicin Project will design, deliver, and help integrate verified, massively parallel software that solves the first-order transport equation. The Capsaicin software will be defensible in that verification of its behavior and underlying methods can be demonstrated repeatedly and on-demand. The integration responsibility is shared with the application code team. The execution of the validation problem is the responsibility of the analysts with user support from the application code team and the Capsaicin code team. For transport simulations, deterministic methods are becoming a viable alternative to the predominant Monte Carlo methods. Research and advances in parallel deterministic methods have made them more efficient and accurate than ever before. Not suffering from the statistical noise of Monte Carlo methods, modern deterministic transport methods look to be a useful day-to-day tool for the ASC users, giving them more accuracy faster than they have had before. Having a high-quality, efficient transport capability is one the most important needs of the ASC simulation program.

LANL Integration/Interfaces: The Integrated Weapons Applications Program Element will provide the applications code and the Computational Science Solvers Project will provide a linear solution algorithm.

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (477): Model for Damage with Accompanying Data implemented into Project B Code & validated.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 03/2005

DOE Programs/Subprograms: ASC Materials and Physics Modeling

Description: 2B added

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation: Develop extensions to the TEPLA materials model framework to include damage modeling. Incorporate developments involving void creation and strain-to-failure, validated against experimental data, and implement into Shavano Project codes. This will permit higher fidelity simulations for both the Campaign 1 and Campaign 4 communities, in response to their needs and requests.

LANL Integration/Interfaces: Experimental data on all relevant weapons materials is not assured, as a result of difficulties of working with actinide materials and the extent of the data requested. Not all materials may initially be completely validated. Implementation into codes has already begun, as the TEPLA framework, covering material strength short of damage, already exists in the codes.

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (500): Fully functioning 64-bit software environment deployed on the LANL Lightning capacity computing system functioning at full scalability**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: 2B added

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation: Deploy a production Linux system using initial Linux software environment for systems and users. This environment allows us to leverage the price/performance advantage of Linux systems while improving on manageability of large clusters. Improved manageability will be seen in a shorter mean time to repair for full system outages, as compared to other large clusters.

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (501): Deliver and demonstrate an interface steepening component to Code Project A**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 03/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: To be added

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation: The interface tracking milestone will deliver an alternative method for transporting material interfaces in the Crestone project. Whenever a calculation of the evolution of a material interface is conducted in the Eulerian frame of reference with shock capturing methods that interface can be broadened through numerical diffusion. To combat this tendency a variety of techniques have been employed to mitigate the numerical diffusion while allowing for a stable computation. These approaches include the use of steepened transport algorithms introduced by Harten in 1978 and Woodward & Colella in 1984. These methods modify the basic shock capturing methods reducing the amount of numerical diffusion and limiting the broadening of material interfaces. The material interface remains slightly diffused, but nonetheless compact. This technique is a simple straightforward modification of the methods already in use in the Crestone project. The performance and basic structure of this method merges seemlessly with the existing hydrodynamic integrator. The remaining challenge is when these methods are applied in two or more dimensions where the results are typically less impressive. …

LANL Integration/Interfaces: This milestone supports Laboratory certification L1 milestones (PIB-7, PIB-17) as well as the SIM CB high fidelity physics full system L2

Milestone (SIM 1-6). This milestone is primarily dependant upon the Crestone project and its use for the above milestones and code development in support of these objectives.

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (502): Organizational SQA Standards in Place and Assessments conducted of IWA Performance Code Projects.**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Verification and Validation

Description: 2b

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation: The Integrated Weapons Applications (IWA) Performance Code Projects and major physics- and/or numerical-component projects from the other program elemetns used in the IWA Performance Code projects shall substantially achieve their assigned/negotiated Target Software Quality Engineering Levels as defined in the LANL ASCI Software Engineering Requirements [LA-UR 02-888] (LANL SER) and its follow-on modifications. Evidence of completion will be in the form of the results from a series of LANL-internal, independent assessments of each individual code or component project performed by the staff of the LANL-ASCI Software Quality Assurance team (or other assessors to be determined) with cooperation from the staff of the identified code and component projects.

LANL Integration/Interfaces: Completion of this milestone requires coordination and cooperation between the SQA project staff and the performance code projects in IWA. It also requires coordination and cooperation between the SQA project staff and the component projects that are used in the performance codes.

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (1351): SCC Infrastructure Upgrade (Phases 2 & 3)**

Level: 2
Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 06/2005

DOE Programs/Subprograms: ASC Integrated Computing Systems (ICS)

Description: 2B

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation:

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (1352): Immersive Visualization Environment Deployed for ASC Users**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 03/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: 2B

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation:

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (1354): Performance study against LANL workload of potential systems considered for the next LANL capability platform procurement**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Simulation and Computer Science

Description: 2B

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation:

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (1355): HE EOS model for PBX9502 products, validated against fundamental data, delivered to Code B**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Materials and Physics Modeling

Description: 2B

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

HQ Information

LANL Information

LANL Implementation:

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (1356): High Fidelity Nuclear Library**

Level: 2
Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Materials and Physics Modeling

Description: 2B

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation:

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (1357): Code Verification, Calculation Verification and Solution Error Analysis for LANL Physics and Engineering Codes**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 09/2005

DOE Programs/Subprograms: ASC Verification and Validation

Description: 2B

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation:

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (1360): Final Project B code release supporting major primary design requirements for W76-1 LEP**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 03/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: 2b

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation:

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (1361): A specific transport capability in-line in Project A & B codes**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 03/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: 2b

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation:

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

**Milestone (1362): Intermediate Project A code release supporting major secondary design requirements for W76-1 LEP**

Level: 2

Fiscal Year: 2005

DOE Area/Campaign: C11

Completion Date: 03/2005

DOE Programs/Subprograms: ASC Advanced Applications Development

Description: 2b

Integration/Interfaces:

Participating Sites: HQ, LANL

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information

LANL Implementation:

LANL Integration/Interfaces:

LANL M&O Contractor POC: PEERY,JAMES S.

# LOS ALAMOS FY06 MILESTONES

**New LANL 06-01**: Deploy production commodity cluster visualization to theaters and designer desktops

Level: 2

Fiscal Year: 2006

DOE Area/Campaign: C11

Completion Date: FY06/Q2

DOE Programs/Subprograms: Simulation and Computer Science

Description:

Integration/Interfaces:

Participating Sites:

NNSA POC: KUSNEZOV,DIMITRI F

LANL Information: Visualization is an essential analytical tool for understanding data from ASCI simulations so, as simulation data sets become larger and as more users use ASCI simulations to analyze stockpile issues, users require increasingly more capable visualization hardware. This is being accomplished by adapting commodity personal computer graphics hardware for use in highly parallel graphics systems.

LANL Implementation: This provides a more complete implementation of commodity-based visualization for a broader set of devices on the LANL Visualization Corridor. This deployment will target cluster-based rendering for user desktops, PowerWalls, and Immersive spaces. A user environment which includes CEI EnSight-based tools, movie display tools, and research prototype tools will be supported on the system. The system will be targeted to support analysis of FY06 and beyond milestones and DSW calculations.

LANL Integration/Interfaces: Integration/Interfaces: Successful completion will require integration with the Deployment, Production Visualization, Large Data Visualization & Rendering projects. This milestone will benefit Advanced Applications and Directed Stockpile Work (including the LEP) and related milestones.

LANL M&O Contractor POC: Bob Tomlinson, bob@lanl.gov, (505) 665-6599

**New LANL 06-02**: **Intermediate Project B code release supporting W88 primary certification (may change to B61 support)**

**New LANL 06-03**: **Model for Damage with Accompanying Data implemented into Project A Code & validated**

**New LANL 06-04**: **Final Project A code release supporting major secondary design requirements for W76-1 LEP**

**New LANL 06-05**: **Placeholder for an additional IWA milestone**

**New LANL 06-06**: **Placeholder for an additional CompSci milestone**

**New LANL 06-07**: **Secondary V&V Assessment Supporting W76-1 LEP Certification (Intermediate)**

**New LANL 06-08**: **Engineering V&V Assessment of W76 Aft Mount Surrogate Assembly Shock Response Supporting W76-1 LEP Certification (Final)**

**New LANL 06-09**: **Primary V&V Assessment Supporting W76-1 LEP Certification (Final)**

**New LANL 06-10**: **Secondary V&V Assessment Supporting W76-1 LEP Certification (Final)**

Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551-0808