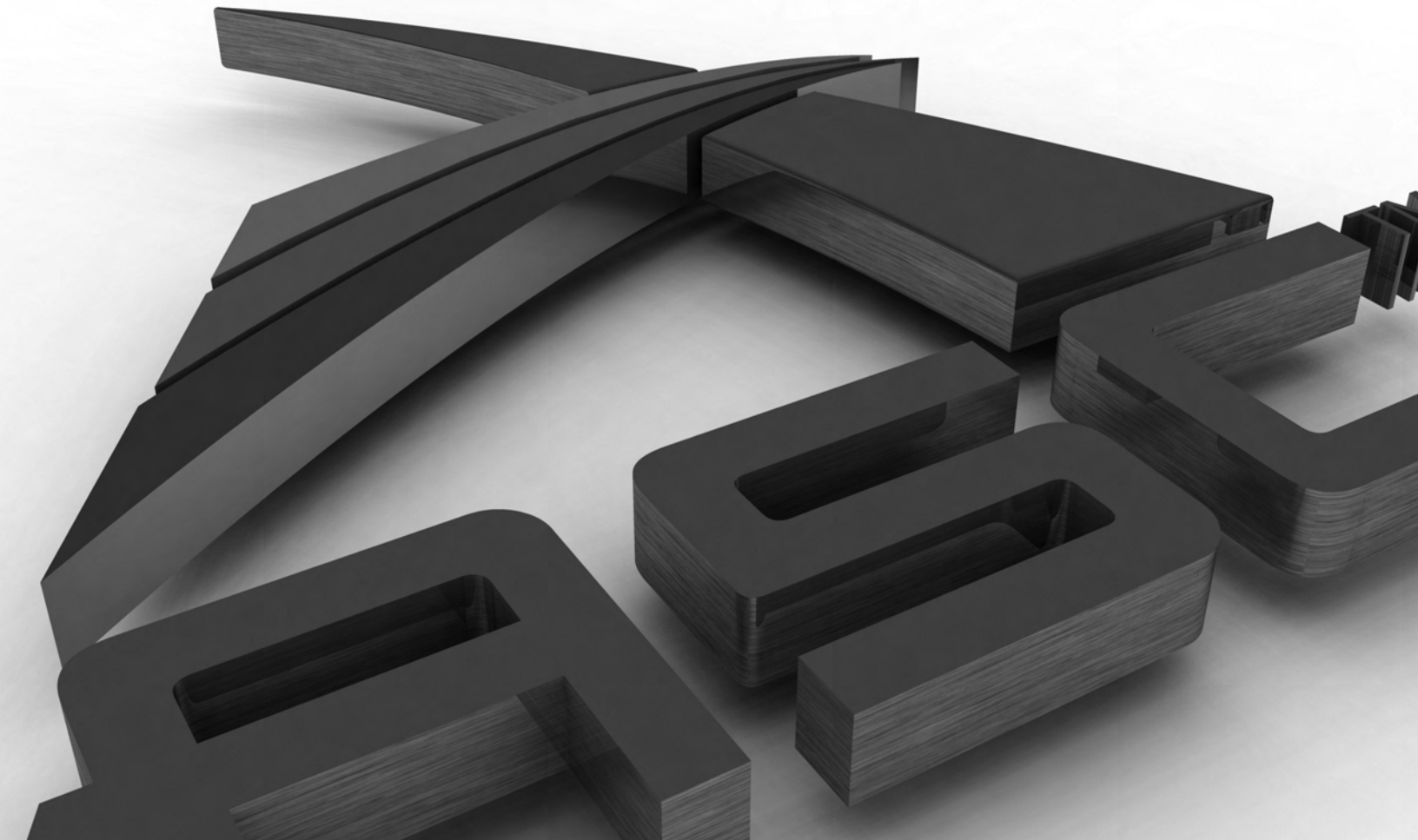
NA-ASC-105R-05-Vol. 2, Rev. 1
UCRL-TR-213013

FY06–07 IMPLEMENTATION PLAN VOLUME 2

August 5, 2005



This work was performed under the auspices of the U.S. Department of Energy by University of California, Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

Advanced Simulation and Computing

FY06–07 IMPLEMENTATION PLAN
Volume 2

August 5, 2005

Approved by:

Dimitri Kusnezov, NNSA ASC Program Director	Signature	*8/5/05* Date
Arthur Hale, SNL ASC Executive	Signature	*8/5/05* Date
Michel McCoy, LLNL ASC Executive	Signature	*8/5/05* Date
James Peery, LANL ASC Executive	Douglas B. Kothe for JSP Signature	*8/5/05* Date

ASC Focal Point
Dimitri Kusnezov
NA 114
Tele.: 202-586-1800
FAX: 202-586-0405
dimitri.kusnezov@nnsa.doe.gov

IP Focal Point
Njema Frazier
NA 114
Tele.: 202-586-5789
FAX: 202-586-7754
njema.frazier@nnsa.doe.gov

Implementation Plan Contents at a Glance

Section No./Title	Vol. 1	Vol. 2	Vol. 3
I. Executive Summary			
II. Introduction			
III. Accomplishments			
IV. Product Descriptions			
V. ASC Level 1 and 2 Milestones			
VI. ASC Integration			
VII. ASC Risk Management			
VIII. Performance Measures			
IX. Budget			
Appendix A. Glossary			
Appendix B. Points of Contact			
Appendix C. 1.5.1.4.12 Alliance Support			

Contents

List of Tables

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 current and 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-weapons design and manufacturing processes, to analyze accident scenarios and weapons aging, and to provide the tools to enable Stockpile Life Extension Programs (SLEPs) and the resolution of Significant Finding Investigations (SFIs). This requires a balanced resource, including technical staff, hardware, simulation software, and computer science solutions.

In its first decade, the ASC strategy focused on demonstrating simulation capabilities of unprecedented scale in three spatial dimensions. In its second decade, ASC is focused on increasing its predictive capabilities in a three-dimensional simulation environment while maintaining the support to the SSP. The program continues to improve its unique tools for solving progressively more difficult stockpile problems (focused on sufficient resolution, dimensionality and scientific details); to quantify critical margins and uncertainties (QMU); and to resolve increasingly difficult analyses needed for the SSP. Moreover, ASC has restructured its business model from one that was very successful in delivering an initial capability to one that is integrated and focused on requirements-driven products that address long-standing technical questions related to enhanced predictive capability in the simulation tools.

ASC must continue to meet three objectives:

- **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. Prediction through Simulation.** 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 performance, 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 simulation capabilities.

[1] In FY02 the Advanced Simulation and Computing (ASC) Program evolved from the Accelerated Strategic Computing Initiative (ASCI).

II. Introduction

The ASC Program supports the National Nuclear Security Administration's (NNSA's) long-term strategic goal of Nuclear Weapons Stewardship: *"ensure that our nuclear weapons continue to serve their essential deterrence role by maintaining and enhancing the safety, security, and reliability of the U.S. nuclear weapons stockpile."*[2]

In 1996, ASCI—the Accelerated Strategic Computing Initiative—was established as an essential element of the SSP to provide nuclear weapons simulation and modeling capabilities.

In 2000, the NNSA was established in 2000 to carry out the national security responsibilities of the Department of Energy, including maintenance of a safe, secure, and reliable stockpile of nuclear weapons and associated materials capabilities and technologies.

Shortly thereafter, in 2002, ASCI matured from an initiative to a recognized program and was renamed the Advanced Simulation and Computing (ASC) Program.

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" (i.e., 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 lifetimes originally envisioned when the weapons were designed.

NNSA will carry out its responsibilities through the 21st century in accordance with the current Administration's vision and the Nuclear Posture Review (NPR) guidance. NNSA Administrator Ambassador Brooks summarized[3] the NNSA objectives for SSP 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 uncovered in our surveillance program; to adapt weapons (achieve a capability to modify or repackage existing warheads within 18 months of a decision to

[2] NNSA Strategic Plan, page 8.

[3] Speech presented to the Heritage Foundation Conference: *U.S. Strategic Command: Beyond the War on Terrorism*, May 12, 2004.

enter engineering development); to be able to design, develop, and initially produce a new warhead within three to four years of a decision to do so;[4] 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 ongoing support efforts are capable of being carried out on a time scale consistent with the Department of Defense'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 begin a modest effort to examine concepts (for example, Advanced Concepts Initiatives, including the Robust Nuclear Earth Penetrator) that could be deployed to further enhance the deterrent capabilities of the stockpile in response to the national security challenges of the 21st 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 development of modern simulation tools that can provide insights into stockpile problems, provide 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 weapons 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 quantify critical margins and uncertainties (QMU), to resolve the increasingly difficult analyses needed for stockpile stewardship. The DSW provides requirements for simulation, including planned SLEPs, stockpile support activities that may be ongoing or require short-term urgent response, and requirements for future capabilities to meet longer-term stockpile needs. Thus, ASC's advancing leading-edge technology in high-performance computing and predictive simulation meets these short- and long-term needs, including the annual assessments and certifications and SFIs. The following section lists past, present, and planned ASC contributions to meet these needs.

ASC Contributions to the Stockpile Stewardship Program

In FY96, ASCI Red was delivered. Red, the world's first teraflops supercomputer, has since been upgraded to more than 3 teraflops.

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 three dimensional (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

[4] While there are no plans to develop new weapons, gaining the capability is an important prerequisite to deep reductions in the nuclear stockpile.

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 an 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 weapons system in a hostile (nuclear) environment; and ASCI delivered an operational 20-teraops platform on the 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. 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 nonnuclear experiments and diagnostics.

In FY05, ASC identified and documented SSP requirements to move beyond a 100-teraops computing platform to a petaflops-class system; ASC delivered a metallurgical structural model for aging to support pit-lifetime estimations, including spiked-plutonium alloy. In addition, ASC provided the necessary simulation codes to support test readiness as part of NNSA's national priorities.

By FY06, ASC will deliver the capability to perform nuclear performance simulations and engineering simulations related to the W76/W80 LEPs to assess performance over relevant operational ranges, with assessments of uncertainty levels for selected sets of simulations. The deliverables of this milestone will be demonstrated through 2D and 3D physics and engineering simulations. The engineering simulations will analyze system behavior in abnormal thermal environments and mechanical response of systems to hostile blasts. Additionally, confidence measures and methods for uncertainty quantification will be developed to support weapons certification and QMU Level 1 milestones.

By FY07, ASC will support the completion of the W76-1 and W88 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 high-capability platform will be sited at Los Alamos National Laboratory (LANL).

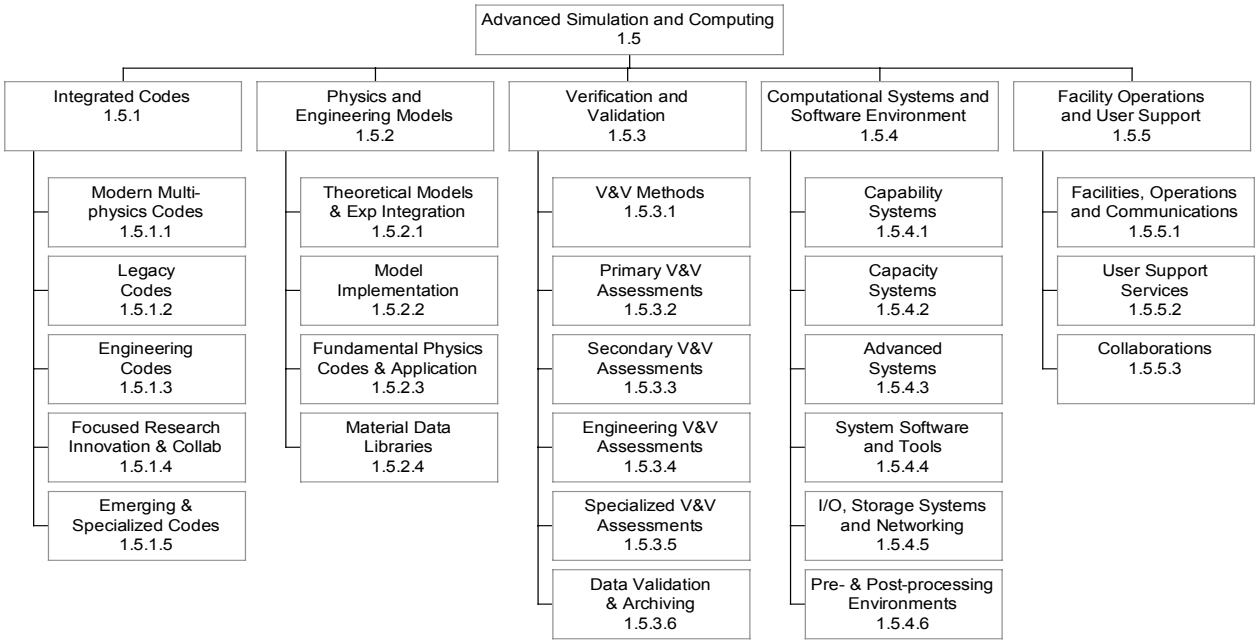
By FY08, ASC will deliver the codes for experiment and diagnostic design to support the CD-4 approval on the National Ignition Facility (NIF).

By FY09, a modern baseline of all enduring stockpile systems, using ASC codes, will be completed.

In FY10 and beyond, ASC will continue to deliver codes for experiment and diagnostic design to support the indirect-drive ignition experiments on the NIF.

The New National Work Breakdown Structure

ASC's program structure is based on the new national work breakdown structure (nWBS), described in the ASC Business Model (NA-ASC-104R-05-Vol.1-Rev.5).



Sub-Programs

As the chart visualizes, ASC is divided into five sub-programs:

- Integrated Codes
- Physics and Engineering Models
- Verification and Validation
- Computational Systems and Software Environment
- Facility Operations and User Support

The first three sub-programs focus on improved models in the modern codes, delivery of validated tools, and response to SSP issues (for example, SFIs, LEPs, annual assessments). Key drivers are to improve the confidence in prediction through simulations; to calculate, measure, and understand the uncertainty in the predictions; and to ensure rapid delivery of simulation capabilities to the SSP.

The fourth sub-program, Computational Systems and Software Environment, ensures the creation of a computing environment needed for all ASC-deployed platforms: capability, capacity, and advanced systems.[5] Not only is this sub-program responsible for related research and technology development, but it is also responsible for planning, procurement, and quality control activities.

The fifth, and last, sub-program, Facility Operations and User Support, provides operational support for production computing and storage; user support services, and collaborative research opportunities with educational institutions, as well as, programmatic support across the ASC program.

[5] The ASC Program is in transition for current platforms. Future platforms will follow the Capital Acquisition Management process identified in the NA-10 *Program Management Manual*.

Product Deliverables

The Product deliverables are described at level 4 and span the full-scope of the program in the context of the nWBS. They describe what the Laboratories expect to provide to a given Product as a result of their activities.

Deliverables can, but do not necessarily, contribute to level 2 milestones chosen in a given fiscal year. Deliverables that do directly contribute to level 2 milestones for the fiscal year will be reviewed in the context of level 2 milestone reviews.

III. Accomplishments for FY04–FY05

ASC accomplishments from Quarter 4, fiscal year 2004 through quarter 3, fiscal year 2005, are reflected below for the newly named Computational Systems and Software Environment and Facility Operations and User Support sub-programs.

HQ is pleased to highlight the outstanding achievements of the Defense Program Contractors.

Computational Systems and Software Environment

LLNL Accomplishments for Computational Systems and Software Environment

At LLNL, the major Computational Systems and Software Environment (CSSE) accomplishments related to L2 milestones are:

- The ASC Purple hardware has arrived in stages, with test systems, followed by the 108-node unclassified uP system initially testing in June, the 1280-node classified section also installed in June, and the final full set of hardware scheduled for September. Associated with the various parts of Purple, there have been system workload tests for acceptance tests, environment testing, file system testing, and a port of the LCRM/SLURM resource management software to AIX for Purple. IBM and LLNL completed an important Purple contract milestone on time at Poughkeepsie, NY this June. This was a critical demonstration of Purple's capabilities.
- The ASC BlueGene/L hardware has arrived in stages, with a quarter-size system deployed and tested, followed by the installation and operation of a half-sized system which is formally recognized as number one on the Top 500 list of systems. At the end of FY05, the full BlueGene/L system should be installed and in test status. The LLNL SLURM and LCRM resource management software packages have also been ported to BlueGene/L. Work on the Lustre file system for BlueGene/L, as well as other scaling, performance, and functionality testing for both system software and applications has been an ongoing FY05 activity. Input/output (I/O) libraries and other tools have been ported and tested.
- The Lustre file system has been the target of development and testing with work to bring it into production status on multiple systems: initially BlueGene/L and the ALC cluster have been deployed as the base of the site-wide file system and other unclassified systems are being added and performance testing will proceed. The performance of the connection to the high-performance storage system (HPSS) has been demonstrated and a multi-cluster Lustre security has been implemented and approved for use on the classified system.

Other accomplishments include the release of HPSS R6.2, which eliminates the need for distributed computing environment (DCE) software and is a major refresh of other components of the infrastructure. Application performance tuning has continued and a database for tracking performance has been deployed. Pre-and Post-Processing Environment accomplishments in FY05 include: completion of unclassified and classified visualization theater and development-lab collaboration areas in Building 453, the Terascale Simulation Facility (TSF), expansion of our production Linux visualization

cluster operation including a new cluster (Sphere), two additional small machines (Klein and Vertex) to drive the TSF classified Powerwall and to explore prototype technologies, procurement of a new, large 256-node visualization cluster to directly support BlueGene/L data analysis needs (expected to be delivered and installed in late September), production release of the Hopper utility featuring powerful search and view capabilities with Windows compatibility, and development of new data management techniques to analyze fluid mix problems, including comparison of simulation to experiments for Richtmyer-Meshkov instabilities and bubble/spike dynamics in Rayleigh-Taylor simulations.

LANL Accomplishments for Computational Systems and Software Environment

The Eclipse Parallel Tools Platform Project is accepted as an official Eclipse foundation project. The project is aimed at providing a high productivity user environment and an integration environment for source code tools.

Prototype Fortran Language support released for the Eclipse IDE. This includes early implementations of prototype Fortran language bindings and a prototype parallel execution environment.

Tutorial on "Performance modeling of large-scale systems and applications" given at the HPCA-11.

Tutorial on "Taking Your MPI [Message Passing Interface] Application To The Next Level" given as Supercomputing 2004.

Organized workshop on "Performance Hardware Design and Functionality" at HPCS-11.

The RADIANT team's Dynamic Right-Sizing technique which enables faster wide-area network transfer and performance is integrated into the Linux kernel (Linux 2.6.x).

A book on ParaView visualization tools is published with chapters co-authored by LANL researchers, Jim Ahrens and Patrick McCormick. These are titled, "Large-Scale Data Visualization and Rendering: A Problem Driven Approach" and "ParaView: An End-User Tool for Large Data Visualization." ParaView is the result of a collaboration, led by Jim Ahrens, that includes LANL, SNL, ANL, and Kitware, Inc.

The state of the art CAVE immersive visualization facility, which provides 3D immersive visualization analysis capabilities, moves into production status. This facility provides never before available ways to interact with the data displayed, aiding greatly in recognizing data set features, and improving analysis capabilities.

The OpenIB Alliance is formed. The consortium is developing an Open Source implementation of the InfiniBand networking stack, which is being supported by the InfiniBand hardware vendors. InfiniBand is a commodity network implementation that appears to be a good candidate to meet a portion of ASC's future high performance networking needs.

The OpenIB software stack is accepted into the official Linux kernel distribution.

For the first time we have shown two sizeable supercomputer clusters which are of different architectures both having scalable simultaneous access to a Scalable Global Parallel File System (GPFS) via a first generation deployment of our Parallel Scalable Back Bone concept (PaScalBB). This is a first for both the Scalable GPFS and PaScalBB projects. A great accomplishment that has taken over five years from inception to reality. This ushers in a new era where multiple heterogeneous supercomputer users will have scalable access to a common GPFS.

The parallel network file system (NFS) project within the NFS version 4 vendor and academic community demonstrated the first working prototype of parallel NFS. The idea for this effort was born at Los Alamos over three years ago. This is the first step in allowing the NFSv4 file system client to have first class (native) access to our scalable GPFSs. The parallel NFS effort entered the IETF standards body about 6 months ago, due to diligent management by the tri-lab.

The NFSv4 project showed the first standards based secure NFS functionality using a third party authentication like Kerberos in the multi site setting. So in the future when this is deployed it will replace the existing tri-lab DFS complex and enable multi-site secure sharing of data with find grained access control.

We have shown the first 32 and 64 bit GPFS clients based on the Secure Object Device model (ANSI T10 1355-D), which allows for highly scalable and secure file system bandwidth.

Coordinator the Lustre file system development project which this year was nominated for an R&D 100 award for innovative file system technology.

HPSS development continues to work towards DCE replacement in the HPSS product. The new HPSS version 6.2 is due out towards the end of this fiscal year. DCE end-of-service is scheduled for Apr 06 and a replacement is necessary for HPSS production capabilities of a 3-petabyte archive to continue.

LANL's first self-integrated capacity Linux platform, Lightning, moves into production status. This includes the LANL developed software, Science Appliance and LA-MPI designed for the special needs of high performance computing (HPC). This also includes the GPFS software from Panasas.

Initial release of Open MPI. This is a collaborative effort to develop a state-of-the-art MPI implementation aimed as addressing both performance and reliability issues of large-scale HPC platform environments. This is a collaborative effort conceived and led by LANL, which also includes participation by Indiana University (LAM/MPI), The University of Tennessee (FT-MPI), the HPC Center (HLRS) at the University of Stuttgart, SNL, and a variety of other contributors.

The development of the distributed memory version of the EnSight client for a rendering cluster was completed by Computational Engineering International working under a subcontract from LANL. This cluster version of EnSight is essential to the FY06 deployment of the ViewMaster rendering cluster which is designed replace three of LANL's older SGI O2K rendering platforms with new commodity-based cluster hardware.

SNL Accomplishments for Computational Systems and Software Environment

In FY05 Sandia met an ASC level 2 milestone by standing up the Red Storm supercomputer and providing for initial operations. Red Storm is an original design massively parallel processor supercomputer consisting of approximately 10 K commodity processors interconnected into a custom engineered modular platform. Cray, Inc. is responsible under contract to Sandia National Laboratories for the development and manufacture of Red Storm. Initial operation of all Red Storm hardware was demonstrated at Sandia by providing functionality needed for early testing of applications codes. We have run the 7X acceptance suite and document the results. This milestone was delayed (from 4QFY04 to 2QFY05) due to design and manufacturing difficulties, but the scope of the milestone was expanded from the original to include running the 7X applications at sufficient scale and duration to minimize risk and accelerate initial user access to Red Storm. This additional risk

mitigation goal added success potential and experience (with the 7X applications) to our effort. LANL users will gain early access to the machine.

In FY05 this product area provided the Sandia's ASC program with critical technical capabilities to staff the Red Storm Risk Mitigation effort. In response to the time criticality of Red Storm, Sandia started the Red Storm Risk Mitigation project with efforts in three key areas: Portals enhancements, PVFS-based parallel I/O capability, and MPI application scaling efforts. These risk mitigation efforts provided Sandia with a much better understanding of the remaining issues and provided the foundation to meet or exceed our projected application scaling by the 2QFY05 due date for this milestone. Continuing Risk Mitigation efforts are directed towards providing LANL with early access to Red Storm for their W76 milestone and meeting the requirements for the remaining three 4QFY05 Red Storm milestones.

Facility Operations and User Support

LLNL Accomplishments for Facility Operations and User Support

The TSF is a new computing facility that was brought into production in FY05. Completion of this milestone was declared on May 23, 2005, a full four months ahead of schedule. This world-class facility has 48,000 square feet of computer floor that is clear span, no air handlers or columns. This allows maximum flexibility for siting large computer systems. The TSF is operating as a fully functioning classified computer center. Over 200 staff was moved into the office tower attached to the building. All system moves into the West and East computer rooms have been accomplished. All accomplished with no safety or security incidents.

Other major accomplishments during the fiscal year have been the siting of the initial deliveries of both Purple and BlueGene/L platforms. By the end of FY05, the hardware for both of these systems should be complete on the floor of the TSF. This effort has involved all parts of the subprogram—with facilities deployment, system administration, security plans, networking, and establishment of user support and documentation for the new systems.

BlueGene/L is the world's fastest supercomputer, according to the latest TOP500 list, released June 22, 2005. BlueGene/L performed 136.8 teraflops, or trillion operations per second.

The next 32,000 nodes of BlueGene/L are being delivered and will be built as a duplicate of the existing BlueGene/L system. After this second system passes its acceptance test, the two sections will be combined into the final system with all 65,000 nodes and a peak of 380 teraflops.

LLNL took delivery of 108 nodes of Purple for an unclassified compute system. This system was put into production a few weeks later. Both LLNL scientists and ASC Alliance partners are running on it now. We took delivery of 252 nodes of Purple, a Federation switch (256 ports), and 300 terabytes of global disk. This is one-sixth of Purple. This 17-teraops compute system was put on the classified network.

The interface cluster for BlueGene/L and the archive HPSS was installed. Four new tape robots were installed in the classified facility. The parallel file system for BlueGene/L is being testing.

LANL Accomplishments for Facility Operations and User Support

The LANL stand-down began shortly into the review period. Throughout the stand-down, Production Computing services continued to operate safely and securely in a

degraded mode as an essential operation, in order to continue to provide computing services as permitted to non-LANL customers and to ensure the health of all systems and data. As the Laboratory developed new policies for the management of accountable classified removable media, Production Computing worked with security personnel to establish acceptable methodologies for the handling of classified media in volume in a production environment. A complete wall-to-wall inventory of all computer center machine rooms, vaults, vault-type rooms, and repositories was successfully conducted. All production operations were converted to the new laboratory accountable classified removable media libraries and management processes. Production Computing operations completed a management self-assessment and was one of the first organizations to resume normal classified computing operations at the Laboratory, in order to provide classified computing services to the rest of the Laboratory as it resumed classified operations.

In the first quarter of FY05, the level 2 milestone for ASC Lightning system general availability was completed. This milestone was delayed one quarter, due to the impact of the stand-down. The completion of the milestone signified the integration of several new technologies into production for the purpose of running large-scale Linux clusters in volume while meeting LANL standards for performance, reliability, and cost efficiency.

A large installation of Panasas GPFS provides the 200 terabytes scratch file system for Lightning. Through the course of the integration, a highly advantageous new technology for the I/O data movement for large Linux clusters was deployed (Parallel, Scalable BackBone, or PaScalBB), which provides high performance in data movement, dramatically increases reliability by eliminating single points of failure, serves as an NFS server for multiple systems, and has potential to scale to very large volumes, first on unclassified systems and later on classified systems.

In addition, Lightning was the first classified cluster to make primary use of the Los Alamos Message Passing Interface, enhancing performance and providing increased reliability in message passing. This product will soon be replaced by OpenMPI.

Lightning was also the first classified cluster to make production use of the Science Appliance systems software stack, including LinuxBIOs and the Bproc modifications to the Linux kernel. This systems software provides dramatic improvements in the manageability of very large clusters in volume, and provides a single process space spanning the entire cluster.

As Lightning production operations spun up, the operations staff took on the role of hardware engineers to provide hardware maintenance in a more cost effective manner to these systems. Operations staff was trained and received A+ certification from Linux Networx (LNXI) in order to assume this responsibility without voiding manufacturer's warranties. This enables LANL to avoid prohibitively high maintenance costs as volume is scaled.

Lightning provides over 13 teraflops peak computing cycles to the weapons community, and has been in production operation since December 2004. At the same time, the highly successful Flash system, a 3-teraops replica of the Lightning technology, was successfully deployed for unclassified weapons computing. The establishment of this new Linux-based production cluster operation is highly significant in the ability of the Weapons Complex to provide the volumes of capacity computing cycles required in a cost effective manner, while still meeting the Program demands for performance, reliability, and maintainability. As of the third quarter of FY05, procurement is well under way for the delivery of approximately 25 teraflops of peak Lightning-like capacity

systems, to be installed in summer, 2005, and a significant ramp-up is expected in 2006 to meet the program's computing requirements.

The ASC Q machine continued to function as the main capacity system providing capacity and capability computing to the tri-lab complex through FY05. By the third quarter, all Alphaserver SC clusters at LANL will be upgraded to the Alphaserver SC v.2.6 "Eagle" release of the operating system, providing performance improvements and additional functionality. In addition to carrying a significant capacity load in FY05, the ASC Q system was also used to run a capability 3D full-system weapons simulation for much of the year. This simulation, still underway, is providing increased resolution and additional physics capabilities for the evaluation of anomalies in weapons systems. In March, ASC Q was used to complete the Verification and Validation program level 2 milestone for the W76 primary. The system is currently being prepared to carry the load of the primary certification effort scheduled to ramp up this summer.

During the third quarter of FY05, the capital equipment project for expanding capacity for distributing conditioned power to the machine room in the Nicolas C. Metropolis Center for Modeling and Simulation (SCC) is nearing completion. This project, which is the next step in a series of infrastructure upgrade projects, makes an additional 3.6 MW of conditioned power available to computing systems in the primary classified computing center at Los Alamos, bringing the total power available for systems in that facility to 7.2 MW. The completion of this project prepares the center to support the growth in computing capacity that is anticipated in FY06. By the end of FY05, a design will also be completed for the next project to be undertaken in FY06, pending availability of funding, to expand this power capacity in preparation for systems anticipated in FY07. Preparations are also being made for upgrading the networking infrastructure in FY06 in preparation for this growth; a request for proposal has been issued for 10 GigE routers.

During FY05, significant achievements were made in the LANL computing centers in the management of machine and facility life cycles. The ASC Bluemountain 3-teraops system was completely decommissioned by November 2005. SGI Origin2000 visualization servers from Bluemountain are still in operation, but have all been consolidated in the computing facility. The classified storage silos were also consolidated into the facility, and all classified storage operations except the Disaster Recovery backup silos were moved into that facility. This work represents a significant accomplishment in reducing the number of classified computing machine rooms that are being managed at Los Alamos.

In the storage arena, an important upgrade was made on the HPSS archival storage systems to HPSS v5.1. This new version has important system restructuring that eliminates the previous reliance upon Transarc's Encina transactional software, replacing that with a standard DB2. This upgrade was essential to ensure continued viability of supporting HPSS in production, and for improving the robustness and reliability of the archive. A Remote Disaster Protection capability using HPSS has also been implemented between LLNL and LANL. By the end of the FY05, this capability will be available for use in managing remote disaster protection needs for the two laboratories.

Finally, FY05 saw the official formulation of the tri-lab Workload Characterization Project. This project team is chartered to implement a tri-lab system in FY06 to deliver quarterly data reports to the Federal ASC managers that will provide details on how ASC machines are being used complex-wide to accomplish programmatic goals. These reports will provide historical data that will assist the program in improving the fidelity of computing resource requirements estimations for future projects, and help to increase credibility of these predictions.

SNL Accomplishments for Facility Operations and User Support

LANL and SNL installed a new OC-48 (2.5 gigabytes per second) link for high speed ASC Wide Area Network connectivity in March 2005 when the new Qwest GeoMax service contract went into effect. This new service replaces the previous OC-48 service at two-thirds the yearly cost. In addition to a cost reduction, the new service provides potential redundancy through alternate paths and offers the opportunity to add additional services such as 10 gigabytes per second Ethernet at very low cost. The 10 gigabytes per second service was ordered with delivery scheduled for August 2005 and will provide the first step in the migration of the ASC wide area network (WAN) from ATM encryption technology to IP encryption technology. To support this new capability and any future services, a new 144-fiber cable has been installed between the SNL telephone building (829) and 880.

Two significant activities related to installation and integration of major platforms were completed in FY05. The delivery of Red Storm began in the last week of FY04 and was completed in the last week of January 2005. Hardware level checkout and software integration was accomplished in phases during this time as the system took final shape on the computing floor in Building 725 in Tech Area I at Sandia's Albuquerque location. The Initial Operation level 2 milestone completed in March reflected contributions from many elements of the ASC program and significant effort by the infrastructure and facilities support organizations at Sandia.

The computing facility itself was designated a Vault Type Room in June 2005 in preparation for classified operations. The system received a 90-day accreditation for classified operation in June as well.

The success of the Institutional Computing Cluster (ICC) and Nuclear Weapons Compute Cluster (NWCC) systems in providing capacity cycles for the ASC program provided us the opportunity to retire the aging CPlant™ home-grown clusters. Retirement and removal of this equipment paved the way for an additional large cluster resource to be procured and integrated into Sandia's infrastructure. The Thunderbird cluster composed of 4096 compute nodes interconnected with Infiniband was delivered and installed in the summer of 2005, following a significant renovation of the south end of the main computing annex in Building 880. Additional power and cooling capacity was added to Room 230 to accommodate the new cluster and to improve the basic infrastructure support systems for that facility.

Also accomplished in FY04 and FY05 was the installation of two new HPSS systems running Release 5.1. These systems are dedicated to the Data Service Cluster systems, which support post processing and visualization needs of the Red Storm Capability platform. The existing HPSS systems, which primarily support ASCI Red, will be upgraded from Release 4.5 to Release 5.1 in preparation for FY06 upgrades to Release 6.2 for all HPSS systems.

There continues to be a significant presence of what we term "commercial platforms" including two large memory SGI platforms and an HP AlphaServer system. The SGI systems supply a large central memory (128GB and 256GB respectively) for use by commercial codes which have not been converted to Massively Parallel Programming models. The large central memory and fast file systems provided by the SGI systems enable extremely large simulation meshes to be generated and visualized prior to being spread across many hundreds or thousands of processors for simulation runs. The HP system provides a code porting vehicle for applications codes destined for production runs on LANL Q, as well as additional capacity for large memory per node problems.

User Support activities for Red Storm included the release of the Collaborative Learning, Information and Knowledge web based tool which will provide the methodology for

tracking issues, maintaining a knowledge base and providing an information search capability for Red Storm and other tri-lab ASC platforms. In addition, the SARAPE web based account request process was put into production, enabling tri-labs and NWC wide requests for accounts to be processed on the web. This electronic system was patterned after the original SecureNet paper based account request system.

IV. Product Descriptions by the National Work Breakdown Structure

WBS 1.5.4: Computational Systems and Software Environment

This sub-program provides to the ASC users a stable, seamless computing environment for all ASC deployed platforms, ranging from capability, capacity and advanced systems. It is responsible for delivering and deploying the ASC computational systems and user environment via technology development and integration at the Defense Programs National Laboratories, in addition to industrial and academic partnerships. The scope of the sub-program includes strategic planning, research, development, procurement, maintenance, testing, integration and deployment, and quality and reliability activities for all ASC computational systems and software environment.

WBS 1.5.4.1: Capability Systems

This level 4 product provides capability production platforms and integrated planning for the overall system architecture commensurate with projected user workloads. The scope of this product includes strategic planning, research, development, procurement, hardware maintenance, testing, integration and deployment, and quality and reliability activities, as well as industrial and academic collaborations. Projects and technologies include strategic planning, performance modeling, benchmarking, and procurement and integration coordination. This product also provides market research for future systems.

Capability Systems Deliverables for FY06

- Purple will be accepted and put into limited availability status for classified NNSA computing.
- LANL product deliverables include planning, preparation, and startup of the project to supply a capability system in the FY08 timeframe. A component of the planning is to understand and document LANL user requirements, which together with requirements from all laboratories, are drivers for the performance and sizing specifications on the system.
- The specific SNL deliverable is to provide capability computing for the Nuclear Weapons Program through the transition to production of the Red Storm computing system in FY06. Red Storm will be a shared capability computing resource for the NNSA tri-lab.

Strategy to Deliver Capability Systems for FY06–FY07

- Develop and acquire capability computing platforms designed to meet the needs of the NNSA scientists and engineers.
- Partner closely with the vendor throughout the contract period from design and build to acceptance and throughout the life of the system.

- Actively partner with off-site labs to develop tri-lab platform strategies and aid in the efforts at the other labs.
- Have tri-lab ASC Platform Strategy team continue to work together with Federal ASC managers to determine system siting and other major considerations.
- Move the Red Storm system to Limited Availability operation at the end of FY05.

1.5.4.1.1 Purple (LLNL)

The Purple contract, a collaboration of the tri-lab community and IBM led by LLNL, will deliver a 93-teraops capability to the SSP in 2005. Purple will be the premier NNSA classified capability computer serving weapons scientists and engineers at all three NNSA labs. This system is a near five-fold increase in scale for a single compute system for NNSA. 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 symmetric multiprocessor is IBM's latest offering in the scalable POWER parallel 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 scalable POWER parallel Switch and scalable POWER parallel Switch2. The cluster-wide storage subsystem is based on IBM's 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.

Purple is currently scheduled for delivery to LLNL in two portions. The first 256-node piece was delivered and was accepted in the third quarter of FY05. The remaining approximately 1280-node portion of Purple will 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—in the third quarter FY06.

In the second quarter of FY07, 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.

1.5.4.1.2 Systems Requirements and Planning (LANL)

This project covers all aspects of planning for capability systems and strategic planning for supporting infrastructure.

The main focus is to define the requirements and the potential system architecture of a capability platform that meets programmatic requirements and drivers. The project will draw upon the skill and experience of the Platforms Project Director's office for planning and project management.

Depending on the outcome of the ASC Platform Strategy, the FY06 focus will be on defining the requirements for systems, performing market surveys of applicable technologies, and planning procurement strategies that meets the needs of the program and the laboratory. If necessary, a request for procurement for a capability platform can also be delivered in FY06.

Along with a request for procurement, an early delivery system would be installed and integrated for initial applications and systems testing in FY07.

1.5.4.1.3 Q Maintenance Contract (LANL)

This project covers the Hewlett-Packard maintenance contract for the Q system.

The capabilities described here include Q system hardware/software support, maintaining a spare parts inventory, system/application support, and maintenance of third party software products.

The FY06 plan is to reduce the total cost of the Q system maintenance by reducing the overall hardware and software support requirements and reducing the amount of on-site analysts for the system. This will require a phased-in plan.

The maintenance support for the Q system will continue at a reduced cost in FY07.

1.5.4.1.4 Red Storm Capability Computing Platform (SNL)

Red Storm is a tightly coupled massively parallel processor with a little over 40 teraflops of peak processing capability. The machine uses AMD Opteron processors and a custom, very high performance 3D mesh communication network. Red Storm has a total of nearly 11,000 Opteron micro-processors, Red Storm has over 30 terabytes of memory and approximately 400 terabytes of high performance local disk that is split equally between classified and unclassified use.

The Red Storm computer system was designed to provide for a relatively easy upgrade path. The 3D mesh can be expanded to 32 K 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 PC. The memory is high volume commodity 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 Reliability, Availability, and Serviceability (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 that have from 2.0 to 4.0 gigabytes of dual data rate memory and 512 Service and I/O nodes each with 6 gigabytes of dual data rate memory. (The compute nodes in the normally classified section of Red Storm have 4.0 gigabytes of memory, the compute nodes in the center section of Red Storm have 3.0 gigabytes of memory, and the compute nodes in the normally unclassified section of Red Storm have 2.0 gigabytes of memory.) 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 light-weight kernel operating system on the compute nodes. The light-weight 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.

During FY06, Red Storm will provide capability computing for nuclear weapons applications. Red Storm has over 30 terabytes of memory and 10,368 compute processor that are connected through a very high performance network which will make it possible to run very large, complex, problems.

During FY06, Red Storm will transition from Limited Availability to full production use as a capability computing resource for the ASC Program. It is expected that Red Storm will be used to perform very important calculations for the SSP this year.

The Red Storm computer system was designed and constructed to allow for a processor upgrade. Sandia intends to consider as part of its overall strategy for capability and capacity computing an upgrade to Red Storm in late FY06 or early FY07.

Red Storm will be in full production throughout FY07.

WBS 1.5.4.2: Capacity Systems

This level 4 product provides capacity production platforms commensurate with projected user workloads. The scope of this product includes planning, research, development, procurement, hardware maintenance, testing, integration and deployment, and quality and reliability activities, as well as industrial and academic collaborations. Projects and technologies include the procurement and installation of capacity platforms.

Capacity Systems Deliverables for FY06

- Linux clusters will be procured to meet NNSA capacity computing needs.
- In FY06, the laboratories will continue to procure, install, and integrate capacity compute systems on the Scalable Unit model to meet programmatic requirements for resources into FY07 and beyond.
- The specific SNL deliverable is to provide capability computing for the Nuclear Weapons Program through the transition to production of the Red Storm computing system in FY06. Red Storm will be a shared capability computing resource for the NNSA tri-lab.

Strategy to Deliver Capacity Systems for FY06–FY07

- Leverage the extensive experience fielding world class Linux clusters within the tri-lab community.
    - By deploying a common hardware environment multiple times at all three sites over two years, it is anticipated that the time and cost associated with any one cluster will be greatly reduced. In addition, it is anticipated that purchasing a huge set of common hardware components will lead to lower cost through volume purchases.
- Provide quick expansion with production-ready systems, while meeting programmatic need for performance, capacity, and efficiency.
- Run Red Storm with typical minimum job-sizes of 3,000-4,000 processors (depending upon the section size).
    - This policy directive effectively establishes three classes of distributed memory systems for running our MPI applications (not counting advanced architecture systems): highest end capability platforms, mid-range capability platforms, and

turn-key commodity clusters with vendor provided/supported software stacks to help Sandia address its extensive 1-256 processor capacity production workload and provide cost-effective systems.

- Focus capacity system procurements on addressing our need to fill the mid-range capability gap with the expectation that the lower processor count workload will backfill on these same platforms or use other SNL institutional turn-key systems.

1.5.4.2.1 Tri-Lab Linux Capacity Cluster (LLNL)

A contract will be placed for a large amount of capacity computing resources to be delivered over the next two fiscal years. This tri-lab procurement will include options to procure a specific number of scalable units each quarter of the FY06 and through the third quarter of FY07 for a total of 32–64 scalable units over a total of seven quarters. The procurement will include level 3 support.

This contract will provide a substantial increase in capacity compute resources for NNSA at all three labs. These clusters will have a common architecture and will run Linux as the operating system.

In FY06, LLNL will deliver, install, and integrate the Scalable Units assigned to LLNL. We will ensure complete system delivery and ensure maintenance is included.

As part of the ASC platform strategy, additional Scalable Units will be delivered in FY07 to LLNL for capacity computing.

1.5.4.2.2 Capacity Systems Procurement (LANL)

Coordinate any and all issues with respect to the tri-lab capacity systems procurement. This covers all system hardware and software defined in the capacity systems procurement.

The capacity systems will provide computing cycles to the weapons program to meet capacity computing requirements. The system will be delivered as several separate Scalable Units that will be made available to the user community for production work. The procurement should include the Scalable Units, the interconnect, file systems, and the selected set of system software tools identified in the RFP.

In FY06, we will deliver and install the Scalable Units assigned to Los Alamos. Ensure complete system delivery and ensure maintenance is included.

As part of the ASC platform strategy, additional Scalable Units will be delivered in FY07 to Los Alamos for capacity computing.

1.5.4.2.3 Capacity Systems Integration (LANL)

The focus in this area is to take the delivered Scalable Units and integrate them into the Los Alamos computing environment for production work.

Completing the system integration defines the overall system environment delivered to end users for running application codes. Once completed, users can compile and run programs, use the system debugger, use the parallel file system, store files in archival storage, and use the scheduling system to input work to the system, among other things.

In FY06, we will integrate all hardware and software components to deliver a system environment to application users for programmatic work. Perform integrated quality assurance testing to ensure production readiness of systems.

The same activities will be required for any new capacity systems delivered in FY07.

1.5.4.2.4 Capacity System Procurement (SNL)

This project supports the planning to establish and manage request for proposals for capacity system procurements. This project will support Sandia's involvement in one or more of the four capacity system strategic options described above.

This project will draw on the expertise established with Sandia's institutional cluster procurements as well as the technical foundation that was leveraged to establish and foster a long-term collaboration with Dell and Intel for the Thunderbird cluster. The pursuit of a Red Storm option for Mid-range capability solutions will of course leverage considerations from Cray established by the 1.5.4.1 product.

In FY06, we will analyze the options for addressing Sandia's mid-range capability gap. Pursue the procurement option(s) that best address the strategic interests of Sandia and the ASC program. Since the ASC program will be pursuing an explicit capacity system platform strategy for FY06-07, this project will support capacity system procurements that will help Sandia provide its user community with Mid-range Capability computing resources to address problems in the regime of approximately 1,000 to approximately 4,000 processors.

FY07 will be the second year of the explicit ASC platform procurement cycle focused on capacity systems. FY07 procurements may reflect continuation strategy established in FY06.

1.5.4.2.5 Integration and Deployment of Scalability and Performance Enhancements that Allow Capacity Systems to Address Mid-Range Capability Problems (SNL)

Integration and Deployment of relevant capabilities from the Technology Development for Capability and Capacity Systems (SNL) project, and other sources, for example, the CSRFs project, MICS/OSCR projects, or LDRD projects. Example capabilities include, OpenIB, OpenMPI, Cheshire runtime, RAS subsystem, Open Catamount, and Lite Linux. The decision to "promote" these technology developments to the "production" software environment will be based on a systematic evaluation of the quantitative benefits to both Application and RAS performance. A formal process for test and evaluation will be used to demonstrate performance improvements at scale through dedicated system time. The demonstrated benefit should be shown from comparison to baseline performance provided by Reliability, Availability, and Serviceability Performance Metrics project.

This project provides focus on the decision point for when/how ASC technology developments are ready for integration into the production software environment.

In FY06, this project will support the test and evaluation of technical capabilities that are specifically targeted at improving the scalability and reliability of the Thunderbird cluster over the baseline performance of the Dell/Intel/Topspin commodity software stack. Capabilities that do not have a clear benefit will go back to the Application Performance Metrics project for further development. This project will also support the evaluation of tri-lab system software stacks that are proposed for deployment on the TLCC. This product is expected to integrate technical capabilities that will allow commodity clusters to scale up to 500-4,000 processor jobs.

In the FY07 timeframe, we expect to be ready to test and evaluate RAS sub-system capabilities developed in the Technology Development for Capability and Capacity Systems (SNL) project for large-scale capacity systems. Of course, the measurement of RAS performance metrics by the Development of Tools to Collect Standardized RAS

Metrics and Control Red Storm's Capability Usage Performance (SNL) project will be used to guide the determination of whether or not this capability would be ready for deployment into the production environment.

1.5.4.2.6 Application Performance and Reliability, Availability, and Serviceability Performance Metrics (SNL)

This project has two parts: the measurement and collection of standardized application performance metrics, and the measurement and collection of standardized RAS metrics for all our capacity systems. There should be a corresponding project under the capability systems product.

The Application Performance metrics portion of this project will provide the ability to assess machines that are being considered for purchase by Sandia, and will allow staff to determine the performance affects caused by system changes. This will be accomplished by monitoring how much different applications utilize the systems, using this information to develop a benchmark suite, and developing a database of benchmark results. The application benchmarks will be complemented with standard micro-benchmarks.

In FY06, we will begin monitoring application usage; establish a suite of application benchmarks starting with the ASC Red Storm 7X benchmarks, and selected micro-benchmarks; and establish preliminary benchmark suite and results for existing SNL capacity systems. Preliminary planned activities in FY07 include refining the application benchmark suite. We expect to add capabilities for automatic data collection, display and comparisons that will be developed by the ASC Programming Tools Project (SNL).

The RAS metrics portion of this project will provide the ability to establish baseline reliability performance for all our ASC capacity systems. A corresponding project will be used to collect similar RAS performance metrics for our capability systems. These long-term measurements will be used to assess the return on investment for future improvements in capacity system capabilities that may be considered, for example, RAS subsystem evaluation or various options for integrating fault tolerance.

In FY06, we will measure standardized RAS metrics on all our ASC capacity systems: Thunderbird Cluster, Red Squall. There may be interest in collecting RAS metrics on our institutional clusters as well, such as ICC, NWCC, Renegade/Rogue. We will establish baseline RAS performance for Sandia HPC resources. If there is interest at LANL and LLNL, we will establish collaborations to spread the adoption and collection of standardized RAS metrics. If they are not ready in FY06, by FY07 we expect to begin using standardized RAS metric collection tools developed in project Development of Tools to Collect Standardized RAS Metrics and Control Red Storm's Capability Usage Performance (SNL).

WBS 1.5.4.3: Advanced Systems

This level 4 product provides advanced architectures in response to programmatic, computing needs. The scope of this product includes strategic planning, research, development, procurement, testing, integration and deployment, as well as industrial and academic collaborations. Projects and technologies include strategic planning, performance modeling, benchmarking, and procurement and integration coordination. This product also provides market research, and the investigation of advanced architectural concepts and hardware (including node interconnects and machine area networks) via prototype development, deployment and testbed activities. Also included in this product are cost-effective computers designed to achieve extreme speeds in

addressing specific, stockpile-relevant issues through development of enhanced performance codes especially suited to run on the systems.

Advanced Systems Deliverables for FY06

- IBM will continue to support the BlueGene/L system for classified NNSA computing.
- Sandia will create a test bed to analyze and assess the performance of Processor-In-Memory architectures on several important applications.
- BlueGene/L will deliver nearly ten times the peak compute speed, in one-fifth the area, using a fraction of the electrical power of the largest supercomputers.

Strategy to Deliver Advanced Systems for FY06–FY07

- Partner with the National Security Agency (NSA) and IBM.

1.5.4.3.1 BlueGene (LLNL)

The Purple contract with IBM includes delivery and support of BlueGene/L, a next-generation massively parallel computing system designed to run a specific set of calculations for NNSA.

BlueGene/L is a scalable architecture in which the computational power of the machine can be expanded by adding more building blocks without introduction of bottlenecks as the machine scales up. BlueGene/L offers a theoretical peak computational rate of 360 teraflops per second through extreme scalability. With more than 65,536 dual processor nodes and 32 terabytes of total memory (16 x 240 bytes or 512 megabytes memory per node), BlueGene/L is expected to be the fastest supercomputer in the world when it becomes operational in 2005. To achieve this dramatic scale, BlueGene/L has three main communications networks: a 3D torus for nearest neighbor calculations on grids; a global tree network for broadcasts and reduction operations; and a barrier network for synchronizing the complex algorithms in scientific calculation envisioned for the machine.

In FY05, the BlueGene/L system will have been accepted and released for early science runs. In FY06 IBM will support the system at an acceptable level of stability and reliability. LLNL will collaborate with IBM in their support activities helping to identify and resolve issues, and will continue to work with IBM in the specifics of designing BlueGene/P, the next generation of the BlueGene system.

In FY07, we will continue on-going support of the BlueGene projects (BlueGene/L and BlueGene/P).

1.5.4.3.2 Cyclops Processor-in-Memory Supercomputer (SNL)

Cyclops is an advanced architecture supercomputer under development by IBM with funding from the NSA. Cyclops uses a Processor-In-Memory design that offers 1–2 orders of magnitude improved performance/cost ratio of over conventional microprocessor-based approaches. Cyclops is projected to be available in 4QCY05 at a cost of $15–$25M/petaflops. Basic analysis of Cyclops' architecture suggests it should offer this improvement for about half of Sandia's workload in both the 2005 and 2010 timeframes. The aim of this project is to acquire two racks of Cyclops hardware (30 Teraflops) and use it to run two Direct Simulation Monte Carlo (DSMC) applications.

This project would serve three purposes:

- Improved efficiency of neutron generator engineering. The neutron generator project reports an immediate need to shift from 2D to 3D DSMC simulations. This project would supply the computing platform.
- Demonstrate immediate ability of petaflops computing. DSMC for microelectromechanical systems (MEMS) design is an identified driver of petaflops acquisitions proposed for 2010. We will demonstrate the application on an affordable petaflops platform available in 2005.
- Demonstrating the viability of advanced architectures in the ASC context may motivate other groups to use Cyclops by shifting load from more expensive clusters/MPPs. This would both save money for supercomputer hardware and permit more effective deliverables based on simulation.

The Processor-In-Memory architecture approach has advantages on highly compute-intensive applications. The overall Cyclops architecture has remarkable similarities to Red Storm, including the 3D mesh, link bandwidth, memory per node, etc. However, a Cyclops node comprises 80 floating-point processors with 80 gigaflops peak throughput (20 × the 4 gigaflops of each Red Storm node). This makes Cyclops appropriate for applications that can effectively use dramatically more compute power per unit of memory.

Planned activities in FY06 include acquiring two racks of Cyclops hardware. Cyclops is an IBM research project funded by NSA. The terms of NSA's investment in this project require that the intellectual property be available to Government users. Sandia has been invited to participate in this project by attending reviews, sharing software, and acquiring hardware on the same terms as NSA. Cyclops is not an IBM product, so the procedure is to place several orders for parts and have the IBM Central Scientific Services organization assemble the system; this organization does not charge profit for government customers. Some systems software development will be required. Specifically, NSA has contracted with a startup for an operating system sufficient for NSA's needs. The terms of NSA's contract permit Sandia to have access to this software. However, DOE applications use different operating system services. A minimal set of these will need to be developed.

We will also port and/or develop two DSMC applications. Both neutron generator and MEMS engineering use of DSMC through the Icarus program. However, both groups agree that the current 2D Icarus needs to be rewritten to become 3D. The necessary 3D Icarus (which would presumably have a different name) will appropriate be written from scratch.

In FY07, without a follow-on project, the two-rack Cyclops purchased in FY06 is turned over to the neutron generator and MEMS groups. These groups would have 30 Teraflops to use until obsolescence for the cost of upkeep, increasing their engineering efficiency through greater use of simulation while simultaneously offloading more expensive supercomputers. In a proposed follow-on project, these and other groups see Cyclops as an option for increasing their use of simulation at the same or lower cost. These groups would purchase additional Cyclops hardware.

1.5.4.3.3 Supercomputer Network Development to Enable Petaflops Scale Capability Machines (SNL)

This project proposes to develop the network infrastructure that will be required for the next generation of capability supercomputers. The performance goals are aggressive: 30 gigabytes per second of bandwidth, 500 ns of MPI latency, and over 10 million messages per second of MPI message throughput. Message throughput is a network

characteristic that industry has shown little concern for, but it is critical for getting "usable bandwidth" from the network when applications use short messages. While message throughput is the most aggressive of the goals, it is unlikely that industry will achieve any of these goals in this time frame.

The proposed work is to create both the network interface and router chips to reach these levels of network performance. The overall project will include specifying the architecture for both of these chips as well as designing the two ASICs (network interface and router) that will be required to implement the network. The final year will include the fabrication of both chips to be ready to provide to a vendor. It is expected that a vendor partner would be engaged to build a system around these network chips.

The goal of this project is to provide network capabilities that will enable the creation of petaflops scale capability computers from commodity processors. It will deliver 30 gigabytes per second of bandwidth per direction per processor socket with 500 ns of latency through MPI and MPI message throughputs in excess of 10 million messages per second. This will enable petaflops scale capability systems to be built from well understood commodity processors at a scale that is well understood. This is in contrast with other approaches which propose higher risk specialized processors or extremely high degrees of parallelism.

Activities for FY06 will include specification of the network interface architecture and router requirements and development of the initial VHDL or Verilog code.

Preliminary planned activities in FY07 include completion of all VHDL/Verilog code and beginning of verification. We expect 50 percent verification completion by the end of the year.

1.5.4.3.4 Next Generation Capability System Development (SNL)

This project will involve the development of a next generation system architecture designed to scale to petaflops capability computing. The architecture will provide the balanced performance that is needed to support the complex physics and engineering codes that are the major application codes of the ASC program.

For large capability computer systems the overall system performance is primarily determined by the degree of parallel efficiency achieved. Parallel efficiency depends to a large extent on the system communication network performance. Communication network performance is primarily characterized by message throughput for small messages and by delivered bandwidth for medium to large messages.

Moving to petaflops scale computing also implies increasing the number of processors to the range of 50,000 to 100,000. Achieving good scalability of our mainline ASC application to this number of processors will be very challenging.

This work will produce a computer system architecture for a petaflops Capability Computer System.

In FY06, work for this project will be focused on the specification for the communications network design.

In FY07, the project will be expanded to the full system architecture for a next generation petaflops architecture.

WBS 1.5.4.4: System Software and Tools

This level 4 product provides the system software infrastructure, including the supporting operating system environments and the integrated tools to enable the development, optimization and efficient execution of application codes. The scope of this product includes planning, research, development, integration and initial deployment, continuing product support, and quality and reliability activities, as well as industrial and academic collaborations. Projects and technologies include system-level software addressing optimal delivery of system resources to end-users, such as schedulers, custom device drivers, resource allocation, optimized kernels, system management tools, compilers, debuggers, performance tuning tools, run-time libraries, math libraries, component frameworks, other emerging programming paradigms of importance to scientific code development and application performance analysis.

This product area supports important academic, industrial, and other DOE labs' contracts to meet users' system software and tools requirements from the tri-labs or a specific lab. There are two tri-lab academic contracts that will continue into FY06. The contract with the University of Oregon is the final part of a three-year project to provide enhancements to the tuning and analysis utilities performance tool to address the issues presented by the large ASC applications and scale of the ASC clusters. A second contract with the Universities of Wisconsin and Maryland is to address Dyninst testing and an open binary editing environment. A Dyninst test environment called ParseTest will be developed to support stress testing for multiple environments. Both of the contracts will terminate during FY06. At that time, a decision will be made about funding additional academic contracts in this area to address important research issues and continuing support for the training of students with skills important to maintaining the tools needed by ASC platforms.

In FY06 ASC will continue to collaborate with Argonne National Laboratory on the development of the message passing library MPICH2. This product won an R&D 100 award in FY05 and ANL will continue their work for support of ASC platforms, improvements to the library including work on performance, tool integration and I/O.

One industrial contract that this product area supports is the Open|SpeedShop (O|SS) Path Forward effort. This is a project with SGI to deliver an integrated suite of open source performance tools for the ASC Linux capacity systems. The architecture of the software is explicitly developed with expandability for future tools and experiments in mind. In addition, the design is such that is should be easily portable to other systems. The second industrial contract is with OpenWorks on extension of the open source Valgrind memory tool to the major ASC platforms. There are several project deliverables, including support for Purple and BlueGene/L, that will be completed in FY06.

System Software and Tools Deliverables for FY06

- For the Purple limited availability, this product will deliver acceptance testing, verify and support all aspects of the user software environment, and provide all of the resource management software (LCRM and SLURM) for the system and work with users in their efforts to get scalable performance on the systems.
- For the BlueGene/L availability, the list of product deliverables is similar, with increased emphasis on scalable performance and usage of tools and runtime libraries at processor counts.
- This product area is also responsible for the integration efforts of the DCE replacement security milestone.

- This product area will be involved in the tri-lab milestone to verify the user environment on Purple with special emphasis on the remote computing access to the system.
- SNL–specific deliverables for this product will include tools to measure our capability usage performance and to provide a means for prioritizing Capability jobs within our Red Storm resource management sub-system.

Strategy to Deliver System Software and Tools for FY06–FY07

- Focus on requirements from the ASC customers added together with the requirements that are derived from the platform strategy.
- Map the available resources against the requirements to deliver product results starts first with making the best possible use of the software provided and supported by platform partners.
- Provide the best tools and protect portability, there is a heavy focus on formal and defacto standards (for example, languages and communication libraries).
- Emphasize maturity and scale of the software for Purple and BlueGene/L, augmenting IBM software as needed, and in FY07, moving toward a software stack that provides more commonality between the tri-lab capacity systems, both from the user portability point of view and from the software development and support point of view.
- Learn from the BlueGene/L system what software requirements can be expected from future petaflops systems so that we can influence development early enough to have the software arrive with the systems.
- Establish standardized metrics for measuring RAS performance and develop tools that allow RAS performance measurements on all our ASC systems.

1.5.4.4.1 System Software Environment for Scalable Systems (LLNL)

This LLNL project provides system software components for all the major platforms at LLNL, research and planning for new systems and future environments, and collaborations with external sources such as the platform partners, especially IBM, and Linux vendors.

This project covers the system software components needed to augment Linux and required proprietary operating systems function in a manageable, secure, and scalable fashion needed for the LLNL platforms. Currently, this includes work on scalable system management tools, the security infrastructure to provide secure single-sign-on tri-lab access, and the resource management environment to queue and schedule code runs across the LLNL systems.

Primary LLNL activities in FY06 will focus on providing all capabilities of the project for the ASC Purple system and the ASC BlueGene/L system. Emphasis will be on completeness, manageability, and reliability of the system environment for Purple, leading up to the full tri-lab usage supporting the level 1 Purple general availability milestone. Emphasis for BlueGene/L is on providing a stable environment and learning how the system interfaces scale to the very large number of processors. Feedback on the limitations of this environment will be used to provide input into development activities needed to make future petaflops systems a reality. A third focus of activities in FY06 will address providing the operating system environment for any scalable units of the projected new capacity systems. Replacement of the security DCE software layer and

integration with future enterprise-wide security software is also a priority effort of this project.

Preliminary planned LLNL activities in FY07 will focus on taking the system components for each of the systems (Purple, BlueGene/L, new capacity) to the next level of maturity and scale. It is expected that there will be some activity around increased commonality of the tri-lab system software stack, increased emphasis on completeness of the Open Source environment and further integration with the enterprise security software. There will also be effort related to interaction with the ASC platform products (1.5.4.1, 1.5.4.2, 1.5.4.3) to research and plan for future platforms.

1.5.4.4.2 Code Development and Performance Environment for Scalable Systems (LLNL)

This LLNL project provides the Code Development Tools for all the major platforms at LLNL, supports user and code productivity through the tools environment, research and planning for new tools and future environments, and collaborations with external sources of tools such as the platform partners (especially IBM), independent software vendors (for example, Etnus and ParaTools), and academic sources of development tools. The project supports activities to apply these tools directly to user codes to understand and improve code performance and provide the customer-based feedback needed to plan future improvements to the environment. In addition, the project handles all bug reports, user trouble reports, and interactions with the software provider to fix software problems.

The tools covered by this project include, but are not limited to, compilers, debuggers, performance assessment tools and interfaces, memory tools, interfaces to the parallel environment, code analysis tools, and associated run time library work, with explicit focus on the development environment for the large scale parallel platforms. This project does not cover the development environment for workstations or other special purpose systems.

Primary LLNL activities in FY06 will focus on providing all capabilities of the project for the ASC Purple system and the ASC BlueGene/L system. Emphasis will be on completeness and reliability of the code development and performance environment for Purple, leading up to the full tri-lab environment supporting the level 1 Purple general availability milestone. Emphasis for BlueGene/L will be in providing a stable environment and learning how the environment/applications scale to the very large number of processors. Feedback on the limitations of this environment will be used to provide input into development activities needed to make future petaflops systems a reality. A third focus of activities in FY06 will address providing the expected environment for any scalable units of the projected new capacity systems. Underlying all of these activities will be direct customer support for the ASC code teams as well as development of new techniques for improving the robustness and performance of ASC codes on all platforms. User assistance, trouble reports, and interaction with vendors to improve or fix software products will continue to be an important aspect of LLNL service to the users

Preliminary planned LLNL activities in FY07 will focus on taking the code development and performance environment for each of the systems (Purple, BlueGene/L, new capacity) to the next level of maturity and scale. It is expected that there will be some activity around improving the commonality of the tri-lab code development environment software stack and increased emphasis on completeness of the open source environment. There will also be effort related to interaction with the ASC platform products (1.5.4.1, 1.5.4.2, 1.5.4.3) to research and plan for future platforms, both

capability and advanced architectures. All user and platform support activities will continue.

1.5.4.4.3 System Software and Tools Advanced Development (LANL)

This project produces production grade software for scalable Linux System management (Science Appliance), Scalable, Portable, Fault Tolerant MPI-2 Message Passing Library (Open MPI) with its supporting run-time environment (Open RTE), a parallel aware IDE for enhanced productivity (Eclipse), and an automated tracking and characterization system for end user simulations and their data generation process (Alexandria). This project covers the full software life cycle of these products, from requirements gathering to software maintenance.

Capabilities:

- Science Appliance: It (v9fs) provides fast, reliable, simple communications between cluster nodes, and will be the backbone of the newer Science Appliance software (Xcpu). This work is being done jointly with IBM.
- Open MPI: Provides a scalable, portable, high-performance, Heterogeneous, Fault-tolerant MPI-2 implementation. The implementation is highly configurable, using a Component Architecture approach to support a variety of implementations of a given feature within the same library, and is being developed as part of an international collaboration. This library provides support for messaging across multiple networks in a single job.
- Alexandria: An infrastructure for the collection of input and process information to determine the impact of software bugs and support reproducibility. An analysis tool to support profiling application deployment information at a global level across platforms and development tool usage.
- Eclipse: Provides an Open-Source, multi-platform, industry supported, parallel core set of integrated developer tools, including an editor with advanced features, debugging tools, build system and performance analysis tools.

Planned activities in FY06:

- Science Appliance: Verify v9fs functionality, extend Linux /proc to support Xcpu—a Linux Module version of BProc which does not require kernel patches—requirement, develop Xcpu, and work on scalability and reliability of this product.
- Open MPI: Add support for the MPI-2 one-sided and memory allocation API's, production grade port to the Purple and Red Storm platforms, InfiniBand specific collective optimization using the InfiniBand specific network features, latency and bandwidth performance optimizations, and continued production hardening of the code base.
- Alexandria: Provide an initial system release supporting characterization and analysis through call interception, characterization through parallel file signature generation, completion of un-optimized implementation of OO-database for data, and initial analysis tool development. Initial user (friendly) implementation across the simulation framework (all input processes that feed a simulation). Establish base infrastructure implementation, open / secure server implementations, and initial storage deployment.
- Eclipse: Improve functionality to support parallel job scheduling/resource allocation, and support for external runtimes and monitoring systems (for example, supermon). Improve parallel debugger user interface functionality, integrate of

parallel debug model with platform debug model, improve scalability/functionality of parallel debug infrastructure, and improve efficiency/functionality of data handling services. Develop services to support integration of performance and other tools, and develop common AST for C, C++, and Fortran, support for external generation of AST, and Fortran-specific tool support.

- All tools: Software release and regression testing, cross functional test code development, and documentation. Second line s/w support, including bug fixes, and full system debugging.

Preliminary planned activities in FY07 include Science Appliance (Production integration of Xcpu); Open MPI (optimizations for collective operations, ports to additional platforms and interconnects, OpenRTE productization as needed); Alexandria (development to expanded usage model to other areas other than simulation frameworks); and Eclipse (Enhanced debugger, remote job services, language support, and simplified deployment).

1.5.4.4.4 Performance Enhancements of ASC Weapons Performance Codes (LANL)

This project undertakes a systematic examination of the performance issues in the ASC code products. This includes characterization of the current state of code performance, analysis of the performance data, making recommendations on code improvement, and applying the state of the art tools and analysis to code optimization. This is an ongoing effort to aid the code teams and their users in making informed decisions regarding algorithms and compute platforms.

The project will be able to provide a basis for making informed decision in areas involving code optimization and performance prediction. This will allow developers of the codes to better direct their computer science resources, and will allow users of the codes to make informed estimates of the computer resources required to complete a proposed study.

In FY06, the project will concentrate on two goals: completing a baseline characterization of the computational performance of the main ASC weapons performance codes, and using the knowledge gained from those studies to recommend optimizations. Such recommendations will include estimates of the effort required to make any modifications proposed and the expected benefit. In addition, a baseline productivity of the end-to-end use of these codes will be performed. This will form the baseline for addressing productivity issues in the creation and use of these codes.

In FY07, based on the work in FY06, this project will design and implement one or more modifications to the ASC weapons performance codes with the goal of improving code performance. It will also provide access to training in optimization for the code developers, and repeat the performance assessment, using the process developed in FY06.

1.5.4.4.5 Application and System Performance Analysis (LANL)

The project concerns itself with the performance of large-scale systems and applications. The workload consists of realistic, full-blown applications both classified and unclassified, from the tri-lab community, with an emphasis on LANL's systems and applications. The machines under considerations are all platforms of interest to the ASC program, capacity, capability and advanced architectures.

In the project we develop methodologies for performance analysis, and analyze, measure, model and suggest solutions for optimizing performance of large-scale machines and applications of interest to the ASC program at large. We continue to develop and refine unique capabilities related to modeling of apps and systems. Our models are the tools of choice that we utilize for our work. They capture the workload (realistic apps) and we apply them to analyze and predict performance when changes are needed in the app or in the machine or to predict performance on architectures that don't exist. Through our work we offer insight into performance issues, answering authoritatively and quantitatively the "why" question related to performance findings. We have the capability of investigating "what if" type of scenarios, what the impact on performance would be from various changes in the app or system. We can "baseline" performance by quantitatively and accurately predicting what the performance of apps on large-scale machines should be. We explore the root causes when predicted performance is not achieved and suggest, and in many cases implement, changes in the system to optimize performance. We report, through publications in best scientific venues, and through technical reports on timely topics. The output from our work is widely utilized to guide decisions within ASC related to various strategies contemplated by the program. In addition, work in this area will support Advanced Architecture work.

In FY06 the project will develop performance models of Milagro (LANL), Alegra (Sandia), and of a LANL classified application. It will measure, model, and analyze the ASC capacity cluster solutions, as well as Purple and the full Red Storm system. It will, also, benchmark and analyze a variety of advanced architectures and vendor solutions for current and future architectures. The project will deliver on a performance analysis of the ASC capacity systems level 2 milestone, and several lower-level supporting milestones. Through quantitative performance analysis, we'll help guide decisions related to capacity cluster procurements and system software strategy for ASC.

In FY07 the project anticipates work on an level 2 milestone related to performance of all credible bids for the next ASC capability purchase.

1.5.4.4.6 Fault-Tolerant and High Performance System Software (LANL)

This project will develop system and user-level software and technologies to incorporate fault-tolerance features into current and future computer systems. In addition, functionality that enables better utilization of system resources to enhance application performance will be developed.

This project will continue to enhance critical system software components including Linux System management software (Science Appliance), Message Passing software (Open MPI), and file system software (PVFS2).

In FY06 work will done to improve overall system fault tolerance. This includes work on automatic (no application changes) recovery from Network Interface Card failures in Open MPI, initial work on MPI process migration in anticipation of failure, and file system fault tolerance using PVFS2 as the virtual layer to allow this. The process migration work includes changes to Open MPI to allow for changing the network addressing without any application code modifications (hooks are already in the base design and implementation), work in Open MPI's run-time layer (Open RTE) to collect run-time statistics and decide when failure is expected, incorporating the ability to freeze a running process and migrate it, notification to the running MPI processes that addressing has changed (mechanism implemented already), and modifications to PVFS2 to handle the new file descriptors that are created as a result of process migration. Work

to improve the system performance includes the implementation of the PVFS2 file system on top of a global file system to allow for caching at the PVFS2 level to allow for caching to improve file system I/O by properly aligning the data actually sent to disc, as well as buffering data for optimally sized writes. Btime will be integrated into the Science Appliance environment and integrated with the Cray enhancements to the Linux scheduler to reduce the O/S interference with the application, and keep it basically independent of the size of the job by ensuring the application process are schedule by the kernels to run at the same time. Finally, work will begin to understand the costs of scheduling a user-level process once an interrupt is received, with the aim of eventually reducing the interrupt costs to be bellow that of the network latency to make asynchronous message passing efficient, and to allow for effectively overlapping communications and computation.

In FY07 the plans are to finish prototype implementation of automated MPI process migration. Work is also planned to improve remote job execution, including investigation of process migration between clusters, pre-positioning remote data, and routing remote network traffic for job management and monitoring purposes. Work is also planned to improve the scalability of the system management tools.

1.5.4.4.7 Technology Development for Capability and Capacity Systems (SNL)

This project supports both capability and capacity system software development. The capability portion of this project has three primary elements: 1) Continued support for Red Storm Risk Mitigation activities, 2) Development of Virtual Node support in Catamount for dual-core Opterons, and 3) Coordination and Integration of Scalable I/O and Lustre capabilities developed by the 1.5.4.5 product area with the Lustre Parallel File system capabilities provided by Cray.

This project provided the technical foundation to meet the Red Storm Initial Operation level 2 milestone in 2QFY05. In FY06, we will provide system software support to transition Red Storm to General Availability and support evaluation of advanced interconnect technologies for next generation Capability Systems. If the planned processor upgrade to dual-core Opterons does not occur in FY06, by FY07 the upgrade will occur with a corresponding upgrade in memory. This project will provide the support within Catamount for dual-core Opterons and larger memory nodes.

The capacity portion of this project is focused on developing enhancements in application performance, scalability and reliability that will allow capacity systems to address our mid-range capability workload. This project will have several components: 1) Cheshire runtime for integration into large-scale clusters, 2) OpenIB support and extensions, for example, support for high performance interconnect capabilities, 3) PCI Express drivers for Open Catamount light weight kernel, 4) management and integration tools for capacity systems and 5) RAS sub-system capabilities.

In FY06, this project will develop capabilities that are specifically targeted at improving the scalability and reliability of the Thunderbird cluster over the baseline performance of the Dell/Intel/Topspin commodity software stack. Should the TLCC procurement take place in FY06, this project will define the system software stack that SNL will propose for deployment on the TLCC. A key focus area for this year is the development of a RAS subsystem capability for large-scale capacity systems.

In the FY07 timeframe we expect to have a system software stack that meets our scalability and reliability performance requirements that allow capacity systems meet Sandia's needs for our mid-range capability workload.

1.5.4.4.8 ASC Programming Tools Project (SNL)

This project is concerned with providing programmers with the required tools to aid them in making their code reliable and efficient. Programming tools for the ASC program have unique requirements including: coexistence with MPI, scalability to tens of thousands of processors, and operability on ASC platforms, which, in some cases, run operating systems unique to HPC platforms.

The sorts of tools required fall broadly into two categories, performance analysis tools and debugging tools. Performance analysis tools can be separated into tools for examining how well a program utilizes a processor and tools for examining how efficiently a program uses the communication network. Debugging tools can be divided into traditional debuggers, memory debugging tools, and code coverage tools. Traditional debuggers (for example, TotalView) permit programmers to step through the execution of a program and inspect data. Memory debugging tools (for example, Valgrind) provide more detailed information debuggers by catch illegal reads and writes earlier in program execution than traditional debuggers can. Code coverage tools (for example, Javelina) make sure all code is executed during regression testing to ensure that all potential bugs are exposed.

In FY06, the primary objective for this project is to establish, by supplementing vendor supplied tools and developing new functionality where needed, a complete suite of application performance analysis and debugging tools for Sandia application development environments. The SNL ASC Programming Tools Project is involved in the following activities to ensure that ASC programmers have the necessary tools to provide efficient and reliable programs:

- Participate in the oversight of tri-lab contracts for tool development. Contracts that are currently in place include: Intel (Intel Trace Collector), Etnus (TotalView), OpenWorks (Valgrind), and SGI (Open-Source Speedshop).
- Exploration of better ways to characterize application performance. This work is done primarily through our SNL developed tool: VProf.
- Selective deployment of preliminary tool releases to code teams for evaluation and testing. These tools are deployed on the ICC and information is made available to developers through the Tools Portal: http://tools.ca.sandia.gov.
- This work is done in close collaboration with LANL and LLNL to ensure that we can efficiently provide programming tools with little redundant effort.

In FY07, new versions of tools, including Open-Source Speedshop and Valgrind, will be tested and deployed on Sandia machines. Training in the use of these and other tools will be provided. Modules to assist users in understanding performance tools results will be developed for Open-Source Speedshop.

1.5.4.4.9 Development of Tools to Collect Standardized RAS Metrics and Control Red Storm's Capability Usage Performance (SNL)

This is a new project with two parts: to develop tools that will measure Red Storm and Sandia's capacity systems RAS performance, and to develop tools that will measure how Red Storm is meeting the ASC capability usage performance policy directive—80 percent of Red Storm's usage must be by jobs that use 40 percent or more of the available system nodes.

Tools are needed to measure our standardized RAS performance metrics in a manner that allows comparison across different systems. These tools will also be useful to

understand the cost/benefit of pursuing the development of active RAS sub-systems. These tools will also support the ability to establish a standardized set of RAS metrics that can be measured for all ASC systems.

Initial work has been carried out to develop standardized definitions for RAS metrics that can be applied to Sandia capability and capacity systems. The time-consuming part of implementing RAS metrics involves working with system administrators to annotate log-file anomalies. The development of tools to help automate the collection of RAS metrics will be required to increase acceptance and adoption of RAS performance requirements for both ASC and the HPC community at large.

A key goal for FY06 will be to review the current work on RAS metrics with the tri-lab ASC community and try to establish consensus on an ASC standard.

In FY07, longer term, we will know our goal has been met when HPC vendors are as interested in touting their RAS performance as their Linpack performance.

Tools are needed to measure our capability usage performance metric and provide resource management control to maintain or increase priority on Red Storm's capability workload. This effort will provide measurements of Red Storm's capability usage performance metric and develop at least a couple of PBS queuing policy implementations that can be used to foster Red Storm's ability to meet the ASC capability usage performance goals.

In FY06, this product will provide the ASC program with a measure of Red Storm's capability usage performance and a means for biasing the Red Storm workload to favor capability jobs.

Preliminary planned activities in FY07, if required, will include more proactive steps can be taken to prioritize capability jobs by limiting backfill, factoring job size and capability usage performance as considerations for establishing job priority.

WBS 1.5.4.5: Input/Output, Storage Systems, and Networking

This level 4 product provides I/O (input/output, or data transfer) storage infrastructure in balance with all platforms and consistent with integrated system architecture plans. The procurement of all supporting subsystems, and data transfer, storage systems and infrastructures occurs through this product. The scope of this product includes planning, research, development, procurement, hardware maintenance, integration and deployment, continuing product support, and quality and reliability activities, as well as industrial and academic collaborations. Projects and technologies include high-performance parallel file systems, hierarchical storage management systems, storage-area-networks, network-attached-storage (NAS), and HPSS or future hierarchical storage management system disks, tape, robotics, servers, and media. This product also includes relevant prototype deployment and testbed activities. Projects and technologies in the advanced networking and interconnect areas shall include networking and interconnect architectures, emerging networking hardware technologies and communication protocols, network performance/security monitoring/analysis tools, and high performance encryption and security technologies.

I/O, Storage Systems, and Networking Deliverables for FY06

- LLNL-specific I/O, storage systems, and networking deliverables for FY06 will provide appropriate throughput to/from storage and storage capacity, appropriate access to and capacity for global file systems, and appropriate inter-site access to resources via encrypted WANs.

- In FY06 SNL will provide I/O, storage, and local and WAN for the Red Storm computational, visualization, and data services resources. The file systems project will assist Cray with the deployment of the I/O library (SYSIO) and Lustre file system on Red Storm; and assist application and application library developers with performance optimization for the parallel file system and I/O libraries on Red Storm.
- The archive systems project will deliver upgraded version 6.2 HPSS systems, and migrate the data transfer agent to production on Red Storm.
- The advanced networking project will deliver a completed 25 GB/sec infrastructure for the classified Red Storm to the data services cluster; demonstrated Red Storm access at the committed rate of 100 megabytes per second from tri-labs via the DisCom network; a robust, integrated, tri-lab security infrastructure using Kerberos and LDAP services; an OpenIB open source InfiniBand software stack that meets ASC HPC performance requirements; and a number of analyses and reports on next-generation parallel file system and networking technologies for a petaflops computing environment.

Strategy to Deliver I/O, Storage Systems, and Networking for FY06–FY07

- Ensure that research efforts and architecture and procurement decisions for these subsystems are made with a complete understanding of vendors' R&D and product roadmap and pricing; a thorough characterization of the product performance, reliability, manageability, and interoperability through testing and analysis; sustaining key industrial and academic collaborations; and a balanced and integrated planning effort considering the requirements all resources and funding allocation.
- Work in close collaboration with commercial vendors and the HPC community, to influence technology maturation and leverage the investments of a very large community.

1.5.4.5.1 Archival Storage (LLNL)

The Archival Storage Project provides end-to-end long-term, reliable, high performance, archival storage services to ASC customers. This includes all development, deployment, and support of scalable archival storage software and interfaces for tri-lab ASC customers on the unclassified and classified networks. It also includes the selection, procurement, deployment, support, and maintenance of all archival storage hardware and storage media and the ongoing technology refresh and data stewardship necessary to safeguard and maintain the fruits of ASC platform and science investment.

The Archival Storage Project provides state-of-the-art archival storage of data for ASC customers at all three laboratories. The project develops, deploys and maintains the HPSS in concert with five DOE laboratories and IBM Global Services. HPSS provides a unique blend of scalable, parallel archival storage interfaces and services to customers running at all three ASC centers. Rather than constraining data transfer to the speed of a single storage device, HPSS is designed to distribute data across a configurable amount of storage units and to remove other limits to scaling including number of files, directories, concurrent users.

To supply the performance necessary to offload ASC platforms, and not hinder computation, a world-class array of storage hardware is deployed and supported underneath HPSS. This includes high performance disk arrays, tape subsystems, mover nodes, storage-area-networks, networks, robotics and petabytes of media. Together, this

hardware and software supports unlimited storage for an unlimited amount of time at speeds in excess of 1.5 gigabyte per second, as of FY05.

In FY06, the development arm of the project will focus on engineering HPSS Release 7.1 (R7.1), which will focus on greatly improving performance of both small and large files and transaction rates. Operationally, HPSS Release 6.2 (R6.2), which removes the dependence on DCE and provides full Linux support, will be deployed on both unclassified and classified networks through two carefully planned conversion efforts. The hardware and software required to provide support for Purple and BlueGene/L production operation will be deployed and supported.

In FY07, the development of HPSS R7.1 will be completed and the product will be released for deployment in ASC centers. The tri-lab requirements process for HPSS R8.1 will be launched. While fielding the required hardware in support of ASC platforms, the local HPSS teams will work to integrate HPSS with the centers' scalable global file system.

1.5.4.5.2 File Systems (LLNL)

The File Systems project provides for the development, testing (feature, capability, and performance), procurement, integration, and ongoing support of various file system technologies and interfaces necessary for the efficient and effective use of ASC high-performance platforms. Included is the continuing development and support of Lustre as a fully featured file system for the range of ASC capability and capacity platforms, the deployment and support of GPFS on the ASC IBM platforms (White and Purple), and the deployment and support of ubiquitous NAS services for home, project, and scratch space. A critical component addressed by the Scalable I/O effort (SIOP) is the testing, benchmarking, and support of various programming interfaces for parallel I/O.

This project deploys and supports large-scale, high-performance Lustre and GPFS file systems for ASC platforms as well as high-availability NAS file systems for home and project space, and scratch space for serial capacity clusters. Total disk capacity at the end of FY05 under Lustre is approximately 1.5 petabytes with the addition of BlueGene/L and 2.3 petabytes under GPFS with Purple. NAS services provides highly-available home and project space using the NFSv3 protocol that shared among all resources on each of the classified and unclassified networks to enable transparent file sharing between platforms. SIOP addresses the problem of I/O capability by supporting several standard programming interfaces for parallel I/O and by helping developers of applications and high-level I/O libraries use parallel I/O effectively as well as providing expertise in I/O and file system stability and reliability testing, and performance characterization.

The planned activities in FY06 are to deploy into production Lustre version 1.6 and the first instance of a shared Lustre file system on the classified network. We will complete through the HP/CFS PathForward Lustre development on clustered metadata, global namespace, security, and OpenIB deliverables as well as full regression testing of all features and functions developed as part of this effort. We will deploy large-scale Lustre (on BlueGene/L) and GPFS (on Purple) file systems and conduct tests to ensure that their stability, reliability, and performance characteristics meet expected metrics. We will begin testing and evaluation of NFSv4 for production use possibly replacing the current NFSv3-based NAS. Ongoing support of currently deployed NAS services and capabilities will continue. We will begin investigation and analysis of new technologies in the areas of NAS data redundancy (on center critical systems) and NAS backup technologies. We will accomplish NAS server consolidation where possible to reduce administration and maintenance.

Preliminary planned activities in FY07 include deploying into production Lustre version 2.0 resulting from the HP/CFS PathForward project; begin deploying NFSv4 as a replacement for current NFSv3-based NAS services; continued ongoing support of currently deployed NAS services and capabilities; and investigation and analysis expanding existing environments, based on center wide increases in compute capabilities.

1.5.4.5.3 Networking and Testbeds (LLNL)

The LLNL Networking and Testbeds project provides research, performance testing, capability testing, and analysis for the file system, network, and interconnect sub-systems in support of current and future systems and environments. This work relies heavily on an adequately provisioned testbed, skilled staff, and collaborations with vendors.

This project will test various hardware and software components to quantify the features, performance, reliability, security, and interoperability of the products and broader technology base. The information acquired as a result of this project will be used to help determine an integrated architecture and resultant procurements for these sub-systems.

In FY06, in support of the milestones—"Develop strategies for deploying and operating a petaflops-class compute resource by 2010," "Complete the hardware and software environment for BlueGene/L and Purple," and "Ready the Purple system for general availability"—and the tri-lab Linux capacity cluster, this project will perform research and testing for technologies and products pertaining to interconnects, local and WANs and IP NSA Type 1 encryptors, and file system servers, clients and disks. Results of these efforts will optimize the functionality, performance, reliability, manageability, and security of the I/O services supporting these computing systems.

Preliminary planned LLNL activities in FY07 will further leverage tri-lab activities in I/O related hardware and software, and seek to improve the reliability, performance and manageability of the I/O sub-systems in production. Additionally, this project will perform research and testing to determine what technologies and products should be considered for insertion into production to meet the growing I/O performance and capacity requirements.

1.5.4.5.4 Archival Storage (LANL)

This project provides end-to-end long-term, reliable, high performance archival storage services to ASC customers. This includes all development, deployment, and support of scalable archival storage software and interfaces for tri-lab ASC customers. This project is responsible for all hardware, software, and storage media provided to ASC customers to enable the storing of dozens of petabytes of ASC program data at rates of an order of magnitude greater than current commercial systems provide.

The Archival Storage Project provides state-of-the-art archival storage of data for ASC customers at all three laboratories. The project develops, deploys and maintains the HPSS in concert with five DOE laboratories and IBM Global Services. HPSS provides a unique blend of scalable, parallel archival storage interfaces and services to customers running at all three ASC centers. HPSS is designed to distribute user data across a configurable amount of storage devices to enable high performance data transfer as file sizes, and file system and network capabilities continue to increase. The project also develops, deploys and maintains the Parallel Storage Interface (PSI), which provides multi-node and other unique data transfer operations to LANL ASC users of HPSS. PSI

enables scalable high performance data transfer operations to or from HPSS given LANL's specific network, file system, and computational platform implementation.

In FY06 this project will deliver and deploy a new version of HPSS to eliminate dependency on DCE software, design, develop, document and test HPSS version 7.1 to improve small file performance with HPSS, and provide a new version of PSI to address FY05 user requirements as determined by the ACE requirements gathering process. It will deploy purchased storage technologies, provide on-going support of the production HPSS archive, and plan and implement remote area disaster protection of mission critical ASC user data. In addition the HPSS/PSI resource manager will be developed to increase HPSS availability while enabling necessary system maintenance operations.

In FY07 this project will initiate next generation archive planning. It will also support future HPSS development to meet user requirements, support the production HPSS archive, and deploy purchased storage technologies. It will continue to development, deploy and support the user interface to HPSS to meet the ongoing needs of the user community.

1.5.4.5.5 File Systems and Input/Output (LANL)

The File Systems and I/O Project provides end-to-end, high-performance networking and scalable I/O infrastructure for ASC program. It also delivers high bandwidth low latency interconnect technologies for the ASC compute platforms. The ASC program requires system and storage area network bandwidths at over 100 gigabytes per second, global file system I/O rates beyond 100 gigabytes per second, and latencies in the 1 microsecond range. All this performance must be provided in an integrated, usable, and secure way. Data transfer and storage bottlenecks are now a critical concern for current-generation, high-performance computing environments. Successfully meeting the ASC programmatic milestones requires carefully balanced environments in which the I/O infrastructure scales proportionally with increased ASCI platform capabilities and application data needs.

This project is a coordination point for planning of all online storage, network, and data movement activities within the ASC program at LANL. These capabilities include online file systems such as the NFS complex and local supercomputer file systems, GPFSs development, deployment and management, scalable I/O middleware development and support, interconnect technology development and deployment, and storage Area Networking development and deployment.

In FY06 this project will handle NFS support including planning for first generation scalable NFS and NFSv4 deployment, Panasas file system support, maintenance, regression testing, MPI-IO support, and enhancement for small and unaligned I/O, including development, testing, and deployment. In addition, it will deploy OpenMPI and OpenIB on new InfiniBand Clusters, implement the next phases of the PaScalBB to provide file system and archive bandwidth, and investigate alternative interconnects such as Quadrics, Myrinet, Infiniband, and 10 GigE.

In FY07 the project plans a study of possible next generation archival technologies and direct attached File Transfer Agents. It also plans to work on Panasas scalable metadata deployment and a demonstration of remote directory memory access (RDMA) data movement capability, deployment of a full collaborative caching layer in MPI-IO. It also plans to demonstrate the next generation InfiniBand technology, and deploy NFSv4.

1.5.4.5.6 File Systems (SNL)

The file systems project provides scalable I/O infrastructure for ASC and SSP computations such as coupled multi-physics simulations, and for shared use of resources such as distance computing on 10–100 teraflops systems. These often involve high fidelity, full system simulation capabilities. The project works with vendors and researchers to provide reliable, high-performance easily used scalable I/O libraries and file systems that make optimum use of disk I/O rates of 25 gigabytes per second and beyond. In addition, it educates users on how to ensure optimum I/O performance from their applications.

The scalable I/O libraries work contributes to the integration of current and future compute platforms, visualization rendering engines, and data management pre- and post-processor servers. To support advanced data management capabilities, the project works to ensure that higher-level I/O libraries effectively use the lower level software and capabilities. In particular, the layers of the tri-lab high-level I/O model (for example, SAF or UDM, HDF5, MPI-I/O, industry and research file systems) must work well together on all ASC platforms.

A number of different technologies are being developed. Specialized I/O libraries on Red Storm allow high performance access to I/O services from compute nodes running the Catamount lightweight kernel environment. On Linux platforms and nodes, a number of competing technologies capable of supporting network-attached high-performance parallel file systems, such as Lustre and Panasas, are being integrated and further developed to meet the demanding needs of the ASC HPC environment.

The ASC computing environment is slowly moving from closely coupled storage and compute architectures to scalable, secure, shareable storage, separate from and shared among multiple compute platforms, as the ASC user moves from model pre-processing to simulation to analysis and visualization. A number of candidate future technologies are being developed in this project and others to enable this common high-performance storage vision.

In FY06, a critical activity will be performance and reliability testing of parallel file systems (Lustre File System and Panasas File System) and intermediate I/O libraries (MPI-IO and parallel HDF5) from vendors and researchers. The project provides feedback to those vendors and researchers to assist them in improving their product for Sandia's environment. Another critical activity is assisting application and application library developers with performance optimization for the parallel file systems and I/O libraries on HPC platforms. The project will continue research in parallel file systems (such as Lustre, Panasas, Terragrid and GPFS), working with vendors and researchers, for the future generation of petaflops systems. These research areas include: Parallel NFS (PNFS); integration of Northwestern's I/O library research into MPI-IO; monitoring development work on HDF5 and MPI-IO libraries to focus on ASC needs; influencing POSIX standards to create a better interface for parallel I/O; and the use of PVFS2 as a research parallel file system to guide next-generation research and development.

In FY07, it is expected that most of the FY06 research and development of parallel file systems and I/O libraries will yield candidate technologies for future petaflops systems. These technologies, coupled with advances in network transport services, such as RDMA and service guarantees, will create new opportunities to push the state-of-the-art in I/O.

1.5.4.5.7 Archive Systems (SNL)

The archive systems project provides economic storage for extremely large sets of data produced by ASC computational users. The current archive system of choice in the tri-lab environment is the HPSS. HPSS is a hierarchical storage manager comprised of disk cache and tape storage systems that provides end-to-end long-term, reliable, high performance, archival storage services to ASC customers. This includes all development and deployment of scalable archival storage software and interfaces for tri-lab ASC customers on the Secure Restricted Network (SRN) and Secure Classified Network (SCN).

HPSS provides state-of-the-art archival storage of data for ASC customers at all three laboratories. The Project develops and deploys the HPSS in concert with five DOE laboratories and IBM Global Services. HPSS provides a unique blend of scalable, parallel archival storage interfaces and services to customers running at all three ASC centers. Rather than constraining data transfer to the speed of a single storage device, HPSS is designed to distribute data across a configurable amount of storage units and to remove other limits to scaling including number of files, directories, and concurrent users.

In order to supply the performance necessary to offload ASC platforms, and not hinder computation, a world-class array of storage hardware is deployed and supported underneath HPSS. This includes high performance disk arrays, tape subsystems, mover nodes, storage-area-networks, networks, robotics, and petabytes of media. Together, this hardware and software supports unlimited storage for an unlimited amount of time at speeds in excess of 1.5 gigabytes per second (as of FY05).

Planned activities in FY06 include performing final testing of HPSS version 6.2 and providing for general availability and deployment of this release (removing a dependency on DCE and providing full Linux support). The tri-labs and IBM Houston will focus on engineering HPSS release 7.1 by defining requirements. For Red Storm the Transfer Agent will be migrated to production.

Preliminary Planned Activities in FY07 include design, coding, testing, and deploying version 7.1 on all HPSS systems; and work with the tri-labs and IBM Houston to define version 8.1 requirements.

1.5.4.5.8 Advanced Networking (SNL)

The advanced networking project provides key foundational network and communication related technologies and services to enable the seamless integration of file systems, archives systems, and ASC compute resources from the user's desktop to the most powerful capability platforms like Red Storm.

Currently, the advanced networking project is composed of five main thrusts:

- High-performance protocols and transport technologies to access network-attached storage in the local and wide areas.
- The continued development of a robust, high performance network infrastructure from the system to the wide area that is capable of providing secure communications with well-understood service level characteristics for different traffic classes.
- A security infrastructure to provide essential authentication and authorization services to the tri-lab community.
- The development of open source networking and communication software to meet the most demanding performance requirements of the ASC program while leveraging the development investment of the entire HPC community.

- The development of algorithms and data analysis tools for monitoring the performance of ASC applications and services.

This project is focused on the development of advanced network hardware and software capabilities from optimizing the Red Storm interconnect to connectivity between Red Storm and RoSE resources to access via the tri-lab DisCom WAN. With a broad range of the latest network technologies such as IP encryption, 10 gigabytes per second ethernet, InfiniBand, high-speed firewalls, service level guarantees, etc., this project provides a robust, high performance network infrastructure spanning latencies from a couple of microseconds to tens of milliseconds. This network infrastructure requires status and monitoring, and predictive modeling and simulation tools to efficiently and proactively provision, configure, and diagnose problems with the network at any level.

The security infrastructure capabilities include a Kerberos-based authentication service, lightweight directory access protocol (LDAP)-based directory services to be used for storing authorization data, and administrative tools and services to support the infrastructure over the tri-lab network environment.

The open source thrust enables ASC applications to more effectively utilize, both capacity and capability resources. This work can be leveraged across institutions and computing platforms. This project works closely with the open source software community and Linux distributors to incorporate HPC requirements into their software support models.

On of the key tri-lab open source efforts is focused on the development and delivery of a common InfiniBand software stack, capable of meeting ASC performance and stability requirements for capacity and capability systems, through the OpenIB InfiniBand Alliance. Through this activity the tri-lab community has taken a leadership position by funding HPC-specific development with a key InfiniBand vendor, Voltaire, and its subcontractors, Cisco (Topspin) and Intel.

For the OpenIB effort, FY06 planned activities include further hardening of the rapidly maturing second generation "gen2" code base on large-scale systems of many hundreds to thousands of InfiniBand nodes, as well as new development in a number of areas. These areas include extensive diagnostic support at all levels of the "stack," support for multi-path and traffic prioritization (such as, virtual lane to service level mappings), support for machine booting over InfiniBand, new upper level protocol development, as well as support for several new network adapters (HCAs).

In general, the set of planned project activities in FY06 is quite large and varied. The activities themselves range from next-generation technology deployment to exploratory, advanced development to address anticipated HPC performance and scalability needs. In terms of deployment, a robust, integrated tri-lab security infrastructure based upon Kerberos and LDAP will be finished in FY06. In the Red Storm environment, a 25 gigabyte per second network infrastructure between the classified Red Storm and data services cluster will be completed. In terms of advanced development, some representative activities include the investigation of next-generation, high speed security devices; the engineering of guaranteed levels of network service in the tri-lab environment; tool development for the real-time analysis of network state and its effects on application performance; the evaluation and development of RDMA transports from system area to WAN applications; and software development to enable the highest levels of inter-process communication.

Likewise, given the challenge of maintaining a balanced computing infrastructure in a constantly evolving environment, the range of FY07 activities is anticipated to be as large and varied as it is in FY06. It is anticipated that new technologies will be

investigated and developed to meet the ever-growing need for high performance networking at all levels of the ASC computing infrastructure.

1.5.4.5.9 Applications in Support of Manufacturing Production and Connectivity (Y-12)

This project will support the utilization of ASC codes and computing resources to solve production manufacturing problems through modeling and simulation. The project will include determination of optimal methods for connecting to ASC computing resources and job submission, execution and visualization.

FY06 planned activities include integrate Y-12 account management system with ASC account requests; evaluate file transfer methods; develop network infrastructure plan to support large file transfer; utilize remote ASC resource for Manufacturing Casting Problem solution; and participate in Nuclear Weapons Complex ASC activities.

Expected deliverables include file transfer method for large files; documentation for network infrastructure upgrade; and results from Manufacturing Casting Problem solution.

Preliminary planned activities in FY07 include participate in evaluation of GigE encryptors; continue utilization of ASC resource for Production Manufacturing problems; develop plan to integrate Y-12 compute/visualization resource with ASC environment; and participate in Nuclear Weapons Complex ASC activities.

WBS 1.5.4.6: Pre- and Post-Processing Environments

This level 4 area provides integrated environments to support end-user simulation set up, and post-processing visualization, data analysis and data management. The scope of this product includes planning, research, development, integration and deployment, continuing customer/product support, and quality and reliability activities, as well as industrial and academic collaborations. Projects and technologies include tools for optimized problem set-up and meshing, metadata and scientific data management, and application-specific and general-purpose visualization, analysis, and comparison. Research includes innovative data access methods and visualization of massive, complex data. Special focus will be placed on tools for improving end-user productivity. Also included are procurement, deployment, and support of office and collaborative space visualization displays, mechanisms for image data delivery, and custom graphics rendering hardware.

Pre- and Post-Processing Deliverables for FY06

- Products and tools necessary to meet the LLNL FY06 Level 2 milestone "Deploy Next-generation Data and Visualization Capabilities for BlueGene/L and Purple Environments."
- Contributions to the deployment of a Sandia-usable ASC Purple environment; prototype tools and/or techniques with applicability to V&V; general availability of Red Storm environment infrastructure; and initial design through analysis (DTA) environment release on Sandia's SCN.

Strategy to Deliver Pre- and Post-Processing for FY06–FY07

- Coordinate efforts of four projects: Scientific Visualization, Scientific Data Management, Displays and Image Delivery, and Systems and Services Integration.

- The tri-labs jointly support certain academic and industrial contracts for this product area (in addition to any lab-specific contracts). Academic partners currently include: University of Utah, for work relating to large data visualization and volume rendering; and Brown University, for work relating to immersive environments and advanced user interfaces. Key industrial partners are: Computational Engineering International, for customized development and support of the proprietary, production EnSight visualization tool suite; and Kitware, for customized development and support of the open source ParaView/Visualization Tool Kit system, which provides a foundation for active collaboration, prototyping and possible rapid delivery of advanced capabilities.

1.5.4.6.1 Scientific Visualization (LLNL)

The Scientific Visualization Project is tasked with providing high-end rendering, compositing, and analysis capabilities for all levels of scientific simulation within the Defense and Nuclear Technologies (DNT) Directorate at LLNL. This can be broken down into three activities: computer graphics research, long-term exploration into data management and rendering techniques; custom visualization application development, providing tools that complement the scientists' existing toolset to provide expanded capability; and visualization theater and collaborative-space support infrastructure development. LLNL has ongoing academic research collaborations with UC Davis (Dr. Ken Joy), Georgia Tech (Dr. Jack Rossignac), and Duke University (Dr. Herbert Edelsbrunner). LLNL also has an industrial development collaboration with Tungsten Graphics for improved network drivers, compositing, and better support for display lists and tiled stereo projection.

The team members of this project have extensive experience handling data processing needs of DNT users. Our researchers are world-renowned for their expertise with data and image compression, including on-the-fly compression of very large datasets; work on multi-resolution streaming architectures for data processing and visualization; topological "summary" techniques for scientific datasets; and view-dependent rendering and data management techniques. We have extensive experience with parallel rendering techniques, both for tiled displays and compositing architectures. The team exploits the latest capabilities of clustering hardware, graphics processing unit advances, and parallel storage systems. Our team also develops and maintains the software infrastructure that supports our five Powerwalls. This software controls the video switching infrastructure, interfaces with our institutional job control system, and launches software services to provide distributed rendering capabilities to our visualization theaters.

There are several projects started in FY05 that will be extended in FY06. These include enhancing our simulated radiography work to support scattering, improving our hardware-accelerated compositing work in the VisIt tool, continued development of the Chromium Render Server for remote desktop and tiled wall delivery, refinement of the high-dimensional analysis capabilities in VisIt, and extending our topology infrastructure to support new data analysis capabilities. We will continue to work toward delivering capabilities within VisIt to leverage its large installed user base. New activities that we will embark on in FY06 include integration of the multi-resolution capabilities of the ViSUS architecture into the VisIt visualization system and extension of the rendering capabilities of VisIt to include other technologies such as Chromium and/or ICE-T.

In FY07, hardware dedicated to compositing will likely available as commodity components, possibly as cell processors. We hope to leverage such technology to provide a generalized rendering and compositing infrastructure for LLNL. In addition,

we hope to deploy the Chromium Render Server remote rendering system to address requirements-driven DNT needs.

1.5.4.6.2 Scientific Data Management (LLNL)

The Scientific Data Management Project is focused on providing users with better ways to generate, organize, search, access, extract, compare, track, and archive large-scale scientific data. This is achieved through two major themes: metadata and data applications for enhancing data access and organization, and data discovery techniques and tools to represent, explore and extract pertinent information. The metadata and data tools effort at LLNL develops production tools that provide solutions for everyday data management needs, from organization to movement to sharing. Its goal is to present the user with an easy-to-use, consistent interface to data, regardless of location, and to automate and simplify repetitive tasks. Data discovery develops scalable algorithms for the interactive exploration of large, complex, multi-dimensional scientific data. It applies and extends ideas from data mining and pattern recognition in order to improve the way in which scientists extract useful information from data.

The data and metadata tools team has expertise in data transport protocols, graphical user interfaces, web technologies, data representation, and advanced system architectures. This team developed the Hopper file management tool and the SimTracker simulation data management tool. Hopper features a sophisticated software infrastructure allowing seamless interaction with many file archival and transfer protocols, allowing the user to enjoy the same user interface no matter where the data resides or where Hopper is running. Hopper provides advanced data operations including synchronization, access checking, and searching by attribute and content. SimTracker provides a web-based view of a user's simulations, with powerful capabilities for archiving, documenting, and sharing the data within a workgroup. Integration of a comparison framework allows the user to easily invoke comparisons of simulations, while access to external analysis tools is facilitated through the SimTracker web interface. The data discovery effort focuses on the Sapphire data mining project, which has expertise in data mining, image analysis, video tracking, statistical techniques, and pattern recognition. The algorithms (some of these have been issued patents) and software in Sapphire are used for the comparison of simulations to experiments, the analysis of experimental images to extract statistics for use in building models, and feature extraction and tracking in data from high fidelity simulations of fluid mix problems, utilizing Sapphire capabilities in pattern recognition, advanced image processing, noise removal, feature extraction and feature tracking.

FY06 activities in metadata and data tools will focus on addressing key user requirements identified in the past year. These include: the ability to create standalone transfer operations from which the graphical user interface can be disconnected and later reconnected; persistent operations capable of handling system and network interruptions; and a command line mechanism that allows power users and simulation codes to utilize Hopper's advanced data transfer and connection infrastructure. For SimTracker, the focus area will be providing a convenient way to create new simulation summaries from online and archived data repositories. Sapphire will continue its activities in data analysis, addressing problems of interest to DNT scientists. Specifically, it will continue the comparisons of simulations to experiments, the analysis of experimental images, and the analysis of high-fidelity simulation data for use in building models.

For Hopper in FY07, we plan to provide transfer verification, regardless of transfer type, assuring that each file was copied with no loss of data. This includes using verification techniques provided by the transport mechanism as well as externally applied

techniques. In addition, we plan to provide application programmer interfaces for other languages to allow use of Hopper's data transfer and connection infrastructure by other applications. In Sapphire, we plan to continue analysis of experimental and simulation data as requested by DNT scientists.

1.5.4.6.3 Displays and Image Delivery (LLNL)

The Display and Image Delivery Project's systems include a broad array of high resolution and high performance display devices and tiled-display arrays for individual user offices and collaborative use areas, together with the associated delivery systems for connecting these to visualization platforms that are remote from them. Also included within the scope of this project are the necessary switching systems and control devices for these displays and visual arrays.

The display and image delivery systems permit DNT scientists and code developers to exploit the power and performance of data analysis and visualization servers for understanding and exploiting their simulation results graphically with high-resolution displays. Both classified and unclassified Powerwalls and collaborative facilities are provided, and are co-located with these individuals.

FY06 activities will include upgrading and improving existing capabilities, investigating and evaluating new capabilities, and providing ongoing support and improved usability. Upgrades and new improvements include deploying tiled displays for the B-453 Visualization Developer Drop-In Center, deploying displays for the B-453 classified collaborative facility, procuring and deploying stereo-capable projection and image delivery system for the B-132 Assessment Theater presentation projector, upgrading image delivery system to support deployment of new visualization platform for driving B-132 Powerwall, and improving stereo capabilities of B-453 Powerwalls with support for deployment of stereo-capable graphics cards that properly handle synchronization, enhancing usability of display equipment in collaborative facilities and theaters with new or improved control panel interfaces. Investigation and evaluation activities include investigating technologies and designs for a B-111 VWC PowerWall upgrade, evaluating alternative or improved keyboard and mouse remote delivery architectures and products (for example, USB-based), evaluating improved image delivery technologies, and evaluating new display products. Support, maintenance and usability activities include providing support hardware and configurations for enhancements to the Telepath resource management system, providing maintenance, improved usability, incremental functionality enhancements, and user assistance for all Powerwalls, other collaborative facilities and user office display systems.

Planned FY07 activities are to procure and deploy a long-needed, but delayed B-111 VWC Powerwall projector upgrade, investigate providing enhanced capabilities to other older visualization facilities as needed, evaluate improved image delivery technologies and display products, deploy improved image delivery technologies as needed, design, procure and deploy alternative or improved keyboard and mouse remote delivery products, provide maintenance, improved usability, incremental functionality enhancements, and user assistance for all Powerwalls, other collaborative facilities and user office display systems.

1.5.4.6.4 Systems and Services Integration (LLNL)

The Systems and Services Integration Project is focused on two main areas: visualization servers and operational support of the Pre- and Post-Processing product resources for ASC computing customers. The server effort includes architectural evaluations and planning, testbed prototypes, component and system testing, and computer security

planning and execution, in addition to the deployment, system administration, system debugging, and maintenance of visualization servers. Operational support includes managing the use of five Powerwall facilities and the associated servers, running video production labs, and applying and consulting on software including resource management tools, movie players, animation and visualization packages. The project also includes liaison activities between ASC customers and Pre- and Post-Processing projects, ensuring that tools and capabilities are meeting user requirements and that they are easy to use.

The project has expertise in systems administration, software design and development, a broad range of visualization hardware and software tools and techniques, windowing systems, graphics processing units, video production, computer animation and 3D modeling, user interfaces, and software quality assurance. Hardware capabilities include five production visualization servers that have a variety of central processing units, interconnects, graphics cards, and disks. The Linux clusters are connected to a Lustre file system and video display infrastructure that drives Powerwalls and smaller displays. The project maintains both an unclassified and classified video production lab, each of which includes desktop systems with video editing software and an assortment of video peripherals. Video production software includes 3D modeling and animation packages, compositors, and related tools. We install, maintain, and consult on a wide variety of software tools (including EnSight, VisIt, IDL, Tecplot, AVS, and NCAR). We consult with users on our tools including movie players (Blockbuster, xmovie), visualization resource management software (telepath), software to run tiled displays as one logical display (DMX), and other tools (ViSUS, TeraScale Browser, and Hopper). The project supports demonstrations on the PowerWall, and we have the capability to visualize simulation data and create movies to be shown on Powerwalls or laptops. We also create DVDs and videotapes as needed in addition to supporting live demos.

FY06 activities include production-level integration of a new visualization server to support BlueGene/L. We will conduct architectural evaluations of cluster technologies, followed by planning, procurement, and deployment of clusters to run the 15-tile display in the classified theater in B-132 and a development cluster on the open side. We will address what hardware architecture can best drive the office displays in Building 132 through a prototyping effort. We will continue to maintain all of the visualization servers, and we will move toward retirement of the remaining large classified SGI systems. Priorities include applying visualization tools and techniques to the large data sets that will be generated on BlueGene/L and Purple. We will continue to provide consulting and support for graphics and video production, and we will keep the production graphics software environment current and consistent.

Planned FY07 activities will include continuing to support visualization on the BlueGene/L visualization server and other platforms. We will continue to conduct ongoing architectural evaluations and perform architectural planning for future systems. We will continue to provide consulting and support services in graphics and video production, and we will continue to keep our production graphics software environment current and consistent on the high-performance platforms, including the compute servers.

1.5.4.6.5 Production Visualization (LANL)

Visualization and visual analysis are essential tools needed by code teams and designers in understanding the terabytes of data that are generated in a single simulation run. The Production Visualization Project provides visualization services from the machine to the desktop for users in the ASC program. Most importantly, people funded by Production Visualization work with code teams and designers to visualize their datasets, train them

so that they can visualize their own datasets, assist them in using the large facilities, and assist in giving briefings in the facilities to high-level visitors. Software currently supported at full strength by the Production Visualization Project includes EnSight, EnLiten, EnVideo, Vista, PoP and GMV. This project also supports and maintains the large facilities, including the new CAVE, the PowerWall Theater and the collaboratories. It maintains the visualization infrastructure, which delivers video from the machines to the users' desktops. Finally, it assists in the process of bringing new machines up by troubleshooting graphics systems on these machines, by performing the visualization software integration tasks needed, and by installing and maintaining critical visualization software on ASC machines.

This project is the place where all client-oriented visualization work takes place in the ASC program at LANL. Capabilities include:

- Custom visualizations for Code Teams A and B, ESA Division and RRW
- Expert knowledge of visualization software, such as EnSight, EnLiten, Vista
- Development and support of PoP and GMV
- Support of the large facilities, such the CAVE and the PWT, including assistance, training and developing new tools to work with these facilities
- Briefing support
- Deployment and maintenance of Viz Corridor software, such as Matrix

In FY06 this project will continue support of Code Team A and B, ESA Division, and RRW. It will provide outreach to users to encourage use of the large facilities, and provide support for briefings at these facilities. It will continue the support of Viz Corridor infrastructure, and assist in standing up of ViewMaster—LANL's distributed memory visualization cluster, and remote visualization capabilities for Purple. Finally, it will provide oversight of EnSight development and maintenance contracts, and of the facilities maintenance contracts.

In FY'07 this project will continue to support the Code Teams A and B, ESA Division, and RRW. It will continue to assist in standing up remote visualization portions of Purple, provide visualization support for briefing, and continue to provide outreach to users to encourage of the large facilities.

1.5.4.6.6 Pre-Production Post-Processing (LANL)

Visualization provides the analyst with the means to assess the quality of their simulations and to determine the correctness and sensitivity of their results. This task is dedicated to supporting that mission by finding the most expedient way to deliver useful information to the scientists. We will achieve this goal by proceeding along two parallel tracks: one, a systems approach that exploits technologies in graphics, networking, and systems architecture; and the other, a user/desktop tool foundry to support scientific decision making. As the systems and tools mature, they will be deployed to the users and incorporated into the production environment.

This project has the expertise in developing and deploying state of the art visualization capabilities to meet the needs of analyzing very large local and remote data sets, as well as series of similar data. This work is used in state-of-the-art facilities including stereo display capable flat multi-panel tile displays, three-dimensional immersive environments, and desktop systems.

In FY06 this project will integrate the distributed memory visualization and rendering cluster, ViewMaster, into LANL's production theater and PowerWall environment,

while fully deploying the fully distributed memory client from Computational Engineering International. This project will, also, continue to track and test new visualization technologies, as they become available, to see how they meet the stated ASC needs. Finally, this project will develop prototypes of visualization and analysis tools using ParaView. These will include simplified and automatic comparative visualization through linked panels, statistical measures within data and between distinct realizations of simulation, and improved tool suite for dealing with time varying data beyond animation and keyframe blending.

In FY07 this project will continue to deploy new visualization and rendering capabilities, as needed. It will continue evaluation of promising technologies that will significantly increase user ability to interact with large data sets in analytical fashion, in variety of environments from desk side to theater to remote system. It will also pursue the development of tools and the integration of powerful techniques to convert large data into verifiable and statistically meaningful information.

1.5.4.6.7 Scientific Visualization (SNL)

The Scientific Visualization project researches, develops, deploys, and supports software that, together with associated infrastructure, delivers a visualization environment in support of ASC platforms and applications. This project develops visualization capabilities to meet the most difficult post-processing challenges facing the ASC community, while also ensuring the availability and support of an appropriate suite of tools, software components and systems that enable effective analysis of simulation results by ASC-environment customers.

A major thrust for this project has been the development of scalable visualization software that makes effective use of the aggregate power of cluster-based platforms. In the past year, the Sandia visualization group has deployed, to our knowledge, the world's highest-performing scalable visualization system. The project employs the open source ParaView/Visualization Tool Kit framework as a mechanism for development and rapid deployment of advanced capabilities within Sandia—it is with enhancements to ParaView that Sandia has achieved the performance result referenced above. Aside from scalability and high performance, ParaView is being leveraged to deliver custom features such as volume rendering for highly unstructured mesh data, which mesh-form is uniquely prevalent in Sandia's computational engineering codes amongst the tri-labs, and the correct visualization of high-order unstructured elements. Computational Engineering International's EnSight suite of tools, a proprietary commercial tool set which has been enhanced in partnership with this project, is provided for baseline relatively full-featured production use. Certain other software is developed and/or provided as needed, such as utilities for high-resolution movie generation and playback on tiled displays, to enable use of shared visualization facilities. Tools are designed and implemented to enable access to high performance resources as needed, to enable use of the highly distributed ASC environment (including across the tri-labs), and to enable use from or directly on the desktop. The project provides testing, benchmarking, installation, and end-user support for its full suite of tools and the project is working with other elements of the Pre and Post Processing Environment product to deliver an integrated DTA capability.

Planned activities in FY06 are support the deployment of the tri-lab ASC Purple user environment; provide direct support for Red Storm environment users; support the application of visualization tools for V&V through the development of a simulated radiograph tool; support strategic planning efforts targeted at the eventual delivery of a petaflops computing environment; development, deployment and support of visualization capabilities.

Preliminary planned activities in FY07 include development and support of visualization tools; continued development of customized/targeted interfaces; continued Red Storm user support; continued participation in the development of an improved DTA environment; and direct Sandia user support, as needed, of the ASC Purple user environment.

1.5.4.6.8 Scientific Data Management (SNL)

The Scientific Data Management effort provides users with better ways to generate, organize, search, access, extract, compare, track, and archive large scale scientific data. This is achieved through three thematic aspects: (1) metadata and data tools (MDT) for enhancing data access and organization, (2) 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.

At Sandia, the Metadata and Data Tools effort provides easy to use components for processing and analyzing simulation data. These components ease large data movement, management, and manipulation. Data Discovery is developing a collection of techniques and tools for the detection, representation and extraction of information from simulation data. These tools scale to terabyte data, make use of ASC's visualization techniques, and are independent of specific simulation codes.

Specifically, the MDT effort at Sandia provides desktop tools for large data movement and management. Examples are dsacp (large data movement between HPC systems and HPSS archive), zephyr copy (also known as zcp, large data movement between HPC systems), and dsabrowse (browse and manage the HPSS namespace). MDT also provides tools for data manipulation. The primary tool is dstk, a Python based interactive program that permits data derivation, subsetting, extraction, output, and plotting.

Tools in the data discovery suite include the ParaView attribute editor add-on (for marking regions of interest for computer learning, and useful for data cleaning and labeling in general), infrastructure software for rapid, robust pattern recognition in terascale data, the ParaView Lookmarks add-on (which permits rapid screening of computer detected regions of interest, as well as marking and returning to points of personal interest), and the FCLib feature characterization software library (for building custom automatic characterizations of regions of interest that eliminate the tedious parts of post-processing analysis).

In FY06, in the MDT context, work will focus on DSTK support for the Verification Software Toolkit (VST). VST is aimed primarily at code studies that involve sequences of meshes and time-steps where the studies focus on the numerical solution as a function of mesh and time-step size, such as, the VST will address mesh and temporal resolution studies. This will involve designing the DSTK integration with VST, and implementing DSTK support for VST code and solution verification, including observed order of accuracy and error estimation. Other related MDT work will include DSA and DSTK usability enhancements and product support, continued development of parallel tools using the DSTK infrastructure, and performance enhancements for DSA tools. Those enhancements will involve integration of the HPSS multi-node server using Parallel File Transfer Protocol, improved small file performance, integration with Hopper, and integration with the DTA application controller. One Data Discovery activity will be the use of the FCLib feature characterization library, by both developers and analysts, to build useful custom characterizations. Feedback from that process will improve FCLib and result in version 2.0. Pattern recognition research will tackle the problem of bypassing gather/scatter while retaining accurate results. We will also refactor the

current pattern recognition implementation to support SAF, to improve the parallel implementation, and to integrate with other DD tools. Finally, we will also pursue a contact with Computational Engineering International to replicate lookmark and attribute editor functionality in the EnSight viz tool.

In FY07, in the MDT arena, we will provide DSTK support for VST pre-processing verification (including mesh manipulation), further develop parallel tools using the DSTK infrastructure, and continue to provide DSA and DSTK usability enhancements and product support. In the DD context, we will re-implement appropriate parts of the AVATAR Tools suite to provide massive data pattern recognition capabilities on the desktop, not just on the large ASC machines. We will also integrate the Lookmark and FCLib capabilities to provide a simple data comparison tool that will operate across distinct meshes.

1.5.4.6.9 Display Environments (SNL)

This project is responsible for design and development, procurement and deployment, initial operations, technical oversight, and continuing critical maintenance of Data Analysis & Visualization (DAV) advanced display environments -- including high-resolution displays in shared visualization facilities and the related audiovisual infrastructure. Integral to this effort is the design, procurement, and deployment of advanced display systems and their interface to the DAV compute infrastructure. There will be significant FY06 emphasis on integration with Red Storm environment high performance resources (in both of the unclassified and classified networks). Shared visualization facilities must be engineered to serve as a user output interface for presentation, data analysis & visualization of data produced in the complete ASC computational environment.

The core competencies of this project include the design and development, procurement and deployment, initial operations, technical oversight, and continuing critical maintenance of the data analysis and visualization environments—including high-resolution displays and the related audiovisual infrastructure. These facilities strive to provide a user-friendly environment for effective data discovery, analysis, and immersion as well presentation and collaboration.

The following activities are planned for FY06: Microsystems and Engineering Sciences Applications (MESA) Microlab Design & Education Center: Deployment and Initial Operations; MESA Weapons Integration Facility (WIF-C and WIF-U): Design process begins; existing DAV Facilities; ongoing operations/maintenance/support; and Technical Network Infrastructure (Fiber/image distribution infrastructure (for example dark fiber, image delivery) must grow in support of the Red Storm environment and multiple visualization facilities serving as scientific visualization output environments.

Preliminary planned activities in FY07 include MESA Weapons Integration Facility (WIF-C and WIF-U): Design completion, deployment, and initial operations; existing DAV Facilities: Ongoing operations/maintenance/support; and continuing deployment of Technical Network Infrastructure.

1.5.4.6.10 Visualization Server Deployment (SNL)

The Visualization Server Deployment projects will develop, deploy and operate terascale servers that will interactively analyze, visualize, store and archive output from the largest scientific computers: Sandia's capacity-computing clusters, Red Storm, ASC-Purple and beyond.

Capabilities of this project include highly interactive data analysis, visualization; integrated Archival Storage with HPSS; shareable, high-performance Institutional File System; and RoSE Clusters can provide Visual Computing capabilities which complement batch computing capabilities.

Planned activities in FY06 include production-quality operation of Red RoSE (classified data/visualization cluster); production-quality operation of Feynman & Black RoSE (unclassified data/visualization cluster); institutional File System Deployment; and test cluster & test suite deployment.

Preliminary planned activities in FY07 include production-quality operation of Red Storm visualization services.

1.5.4.6.11 Design through Analysis Realization Team (SNL)

The Design through Analysis Realization Team (DART) project provides a finite element analysis environment that enables analysts to significantly reduce the time required to complete the DTA process. DART is focused both on the development of specific tools to help the analyst with individual steps in the DTA process as well as integrating technologies to make those tools work well together. To reduce analysis time, DART technologies focus on three general areas of opportunity: reducing the time required to traverse individual process steps, reducing the fraction of rework required during subsequent visits to process steps, and reducing the likelihood of backward process iteration.

DART will deploy an SNL analysis environment on both the SRN and SCN that supports analysis tool interoperability and reduces overall engineering time for the design-through-analysis process. Tool interoperability will be guided by the Analysis Process Coordinator and will be enabled by a metadata construct that each of the design-through-analysis tools supports. In addition to guiding the analysis process, the Analysis Process Coordinator will provide the analysts with means to view and organize analysis artifacts as well as a means to archive and retrieve them. Simulation runs will be submitted and monitored by the ASETS job submission tool, which will provide support for a subset of ASC applications and platforms that will be determined based on user priorities. Additional capability will be provided for managing families of related analyses, specifically by implementing a data passing mechanism with DAKOTA to support the use of DDACE for running predetermined sets of simulations. The Analyst Home Page will provide a one-stop-shop for analyst information needs. An adaptive partitioning scheme will be developed and ultimately deployed through the Zoltan library to improve the performance of simulations on parallel compute platforms.

In FY06, DART will upgrade the initial limited capability environment released on the SRN in FY05. Specifically, the Analysis Process Coordinator will include enhanced capabilities, ASETS will support a broader selection of ASC applications and platforms, and an initial Analysis Family Management capability for predetermined design parameter sets will be released. The environment will also support richer metadata content for enhanced tool interoperability. In addition to the SRN environment upgrade, an initial limited capability environment will be released on the SCN. An adaptive partitioning scheme and associated metrics will be developed, initially for structured mesh simulations.

In FY07, DART will upgrade the initial limited capability environment released on the SCN in FY06. At the end of FY07, the SCN deployment of the DART environment will provide the same basic capability as the SRN release. In addition, the SRN environment will support a basic data passing mechanism to support simple automated optimization analyses through DAKOTA.

1.5.4.6.12 Model Generation and Manipulation (SNL)

The Model Generation and Manipulation project comprises development of several individual tools, including CUBIT, SIMBA, and Materials WISDM. CUBIT provides a wide variety subtools that support geometric manipulation to prepare a model for meshing and for creating the meshes themselves. SIMBA provides subtools for modifying existing meshes, augmenting them with additional information, managing collections of model artifacts, and producing input decks for many ASC applications. Materials WISDM is a materials information system and data manager.

The Model Generation and Manipulation project will provide analysts with advanced capabilities for creating and manipulating simulation models. These tools will focus on design solid model generation, analysis solid model generation from the design solid model, mesh generation for several analysis types, manipulation of the mesh, assignment of additional mesh information, management of model artifact sets, input deck generation, and identification of materials properties and constitutive model parameters. Additional tools will address specific geometry manipulation problems identified in the DART System Analysis study as well as on identifying and correcting DTA process problems as early as possible in the process. The latter effort focuses on reducing process iterations that do not add overall value, but contribute to long analysis times.

In FY06, the Model Generation and Manipulation project will enhance the individual tool capabilities. Specifically, CUBIT will release an interoperable virtual geometry capability that will complement the Power Geometry tool released in FY05. SIMBA will complete a restructuring of its user model based on feedback from the analyst community. This restructuring effort promises to improve ease-of-use and draw additional users. Materials WISDM will establish a more complete database of useful material information. In addition, Materials WISDM will deploy on the SCN in FY06. Additional effort will be expended to address opportunities identified in the DART System Analysis: reduction of geometric manipulation time and model verification (the early identification and correction of process problems).

In FY07, the Model Generation and Manipulation project will focus on the development of tools to address additional DTA process improvement opportunities identified in the DART System Analysis.

WBS 1.5.5: Facility Operations and User Support

WBS 1.5.5.1: Facilities, Operations, and Communications

This level 4 product provides necessary physical facility and operational support for reliable production computing and storage environments. The scope of this product includes planning, integration and deployment, continuing product support, software license and maintenance fees, procurement of operational equipment and media, quality and reliability activities and collaborations. This product also covers physical space, power and other utility infrastructure, and LAN/WAN networking for local and remote access, as well as requisite system administration, cyber-security and operations services for ongoing support and addressing system problems.

Facilities, Operations, and Communications Deliverables for FY06

- System administration and 24/7 operational support of ASC platforms; necessary software and hardware maintenance, license fees, and development and support contracts; efficient and secure infrastructure services to support the deployment and operation of ASC platforms; facilities, power, and other utilities and services sufficient to support the large-scale ASC computational environment; operational support of networks for the unclassified and classified facilities; and operational support for the DisCom and SecureNet WANs.
- Continuous and reliable operation and support of production computing systems and all required infrastructure to support these systems, including primarily networking and facilities.
- Successful operation of the Red Storm system, initially as a Limited Availability Platform and later in the year transitioning to a General Availability Platform.
- KCP will continue an effort to build up the hardware resources, system administration expertise, systems integration, and remote computing capabilities to provide current generation ASC code support to KCP's finite element analysis engineers.

Strategy to Deliver Facilities, Operations, and Communications for FY06–FY07

- Focus on the end product to users: an integrated production environment that reliably provides computing resources that meet performance and availability needs of the users.
- Hold Cray, Inc. to its contract to maintain and operate the Red Storm platform for five years following acceptance of the system by Sandia.
- Leverage Readiness initiatives to participate in extensive collaboration with the design laboratories. These collaborations will provide the ability to support KCP's unique manufacturing-oriented analysis job profile, including local capabilities for urgent, unclassified, limited resource needs as well as remote capabilities for larger, manufacturing research investigations.

1.5.5.1.1 System Administration and Operations (LLNL)

The System Administration and Operations project provides for the ongoing system administration and computer operations functions for the successful management and support of the ASC platforms and computing environment. Includes laboratory-maintained hardware support capabilities.

Capabilities include highly skilled system administration to ensure installation, integration, and ongoing support of ASC platforms including operating system and software configuration; feature, functionality, and security patches; troubleshooting, analysis, and diagnosis. This project also includes 24/7 operational monitoring capability for unclassified and classified computing environments consisting of large-scale computing platforms, infrastructure components, and networks. For laboratory-maintained systems, this project provides hardware maintenance capabilities including component inventory and replacement.

In FY06, we plan to complete integration and initiate ongoing support activities for BlueGene/L and Purple. We will continue to train and develop staff in laboratory-maintained hardware support.

Preliminary planned activities for FY07 include integration and ongoing support of projected TLCC capacity systems, and planning and preparation for next generation peta-scale computing platforms.

1.5.5.1.2 Software and Hardware Maintenance, Licenses, and Contracts (LLNL)

This project provides for vendor-provided hardware and software maintenance, support, licenses, and development contracts.

Capabilities include negotiated hardware and software maintenance and license contracts to ensure a robust ASC computing environment and to protect the computational investment of the NNSA. Targeted development contracts to enhance the capabilities of specific software components are also included.

Planned activities in FY06 include ongoing vendor support for designated platforms.

Preliminary planned activities for FY07 include ongoing vendor support for designated platforms.

1.5.5.1.3 Computing Environment Security and Infrastructure (LLNL)

The Computing Environment Security and Infrastructure project provides for computing environment infrastructure services, software, servers, workstations, and desktop systems necessary for the efficient, effective, and secure operation and support of large-scale ASC platforms.

Capabilities include ongoing integration, development, and support on unclassified and classified networks of robust infrastructure environments to support large-scale ASC platforms including but not limited to name and time services, backups, staff productivity tools (for example, e-mail and messaging), cyber security tools and technologies.

Planned activities in FY06 include continued ongoing support of currently deployed services and capabilities. Investigation and analysis of new technologies for the possible replacement of existing technologies will also continue.

Preliminary planned activities for FY07 include continued ongoing support of currently deployed services and capabilities. Activities also include investigation and analysis of new technologies for the possible replacement of existing technologies.

1.5.5.1.4 Facilities Infrastructure and Power (LLNL)

The Facilities Infrastructure and Power project provides for the necessary physical facilities, utilities, and power capabilities to support staff and the ASC computing environment.

Capabilities include adequate raised floor space, cooling facilities, and power to site large-scale ASC platforms. In addition, needed office, meeting room, and auxiliary space to enable a highly motivated and effective staff is part of this project.

Planned activities in FY06 include ongoing maintenance and support of existing computational and staff facilities, and analysis of future ASC computing requirements to anticipate the needed modification and/or expansion of facilities to be able to site next generation ASC platforms.

Preliminary planned activities in FY07 include ongoing maintenance and support of existing computational and staff facilities, and analysis of future ASC computing

requirements to anticipate the needed modification and/or expansion of facilities to be able to site next generation ASC platforms.

1.5.5.1.5 Classified and Unclassified Facility Networks (LLNL)

The Classified and Unclassified Facility Networks project provides the architecture design, planning, procurement, deployment and operational support of the classified and unclassified facility networks.

Capabilities include a thorough understanding of the resource deployment roadmap is acquired by participating in ongoing facility-wide planning efforts that includes the archival storage, visualization, platforms, capacity computing and file systems. Network design, procurements and deployments are updated and scheduled to accommodate these plans and ensure the network connectivity, performance, reliability, security and operational support is available for the facilities to meet the requirements of all subsystems is also part of this project.

In FY06, we will complete the integrated planning process so the networking requirements are understood, particularly to meet our level 2 milestones and accommodate major deployments such as BlueGene/L, Purple, visualization servers, and the Lustre file system.

Planning for the FY07 facility networks is an ongoing process and will be similar to other years. The actual network activities are dependent on the requirements. It is expected that in FY07 requirements for a substantial, high-performance 10 gigabit ethernet core will be a significant activity for this project.

1.5.5.1.6 Wide-Area Classified Networks (LLNL)

The Wide-Area Classified Networks project provides the architecture design, planning, procurement, deployment and operational support of the classified wide-area networks, namely the DisCom WAN and the SecureNet WAN.

Capabilities include ongoing discussions with the tri-lab community are critical to this project to ensure that the network requirements for those remote users and facilities are mutually agreed upon and understood. This project must also plan far in advance to ensure the required NSA Type 1 encryption products are available, since these products are not commercial and have a long R&D and product development lead time. Operational support of these wide-area networks also requires effective and regular communication with and cooperation between the tri-lab network support teams. These activities will help ensure the proper planning occurs for the WANs, and the operational support is effective for the broader tri-lab user community.

For FY06, the LLNL-SNL DisCom WAN link must be rebid. This will be completed in FY06 and will include options to increase the bandwidth if required. To benefit from network product developments the NSA Type 1 Encryptors for the DisCom WAN will migrate from ATM to IP encryptors. Ongoing activities strive for improved reliability, responsiveness to problems, and application performance.

Preliminary planned activities in FY07 strive for on-going improved reliability, responsiveness to problems, and application performance. With new platforms expected at LLNL and SNL, the DisCom WAN bandwidth may be inadequate to meet the tri-lab user requirements. This would require an upgrade to the network components and encryptors to provide this bandwidth.

1.5.5.1.7 Requirements and Planning (LANL)

This project includes planning activities for computing operations, collection and statistical evaluation of user requirements for computing resources, development of new metrics and data collection, and the project management of the tri-lab Workload Characterization Project.

The primary capability of this function is to collect and understand user requirements for production computing resources and quality of service, and to develop new metrics and data collection and analysis techniques to assist these purposes.

In FY06, this project will continue to interact with the user community and their program and line management to understand and document their computing needs and plan to meet those needs with current systems. The project will also provide input on user requirements for computing resources to strategic planning functions for capability and capacity systems as required by those projects. The focus in FY06 will be to improve the quality and reliability of the requirements collected through various means, including comparison to historical data. This project includes the project management of the tri-lab Workload Characterization Project to collect and report specific data on the use of the machines across the tri-lab arena, for comparison to stated requirements. FY06 activities will also include the planning and development of new metrics and/or measures for continuous improvement in quality of production services.

In FY07, we will continue to contribute to improvements in the quality and reliability of computing requirements collection and analysis, both at LANL and in the tri-lab arena.

1.5.5.1.8 Ongoing Network Operations (LANL)

Ongoing Network Operations encompass all aspects of the network infrastructure that support ASC computing in the classified and, to some extent the unclassified arena. This includes directly attached networks to HPC systems (machine area network), network backbones, the user's local area network, and the WAN connecting the three laboratories.

The network aspect of Production Computing provides the network technical expertise and operation required to support 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 WAN through which LANL users can access White at Livermore, Red Storm at SNL, and Purple and BlueGene/L at Livermore when those systems are available. Network services in the classified partition are required to promote and maintain an environment that is acceptable to users in order to complete their assignments. Increased availability and security require 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. Increased bandwidth over the WAN is being planned for anticipated requirements from LANL users of the new remote systems. 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 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 WAN, and the high-performance parallel interface/gigabit and ten gigabit 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.

- WAN operation and support: In close cooperation with LLNL and SNL, operate and maintain the 2.5 gigabits per second WAN. Deploy new technologies to increase bandwidth and reliability where warranted. Deploy new Internet Protocol (IP) encryptors to position WAN growth and control costs. Plan for bandwidth growth from two to four times current bandwidth if use by LANL designers warrants such growth. In addition, new vendor offerings such as GeoMax from Qwest have provided cost savings of up to 40 percent for the WAN link from LANL to SNL.
- Work closely with the Integrated Cyber Security Initiative (ICSI) project to deploy the new Enterprise Secure Network (ESN) which will not only include SecureNet operations but will also address directory, email, and other network services currently running locally at each site or over SecureNet. Plan for a demonstration of the new ESN working with an ASC application by April 2006.

The network LAN/MAN/WAN operation and maintenance requires the skills of network engineers and technicians knowledgeable in all aspects of network technology. These skills have been developed over the past 25 years at LANL. LANL network engineers participated in the first national gigabit test beds in the early 1990s and developed the first standards based gigabit network technology and deployed IP based networks throughout the Lab in the late 1980's and moving this technology to the HPC arena in the 1990s.

Planned activities in FY06 include continued operation and maintenance of the LAN/MAN/WAN infrastructure that in the past was covered by Production Computing Network Support and the DisCom WAN project. The LAN/MAN planned activities are to complete deployment of 10GigE technology in high traffic areas and provide network expertise in the deployment of the PaScalBB (Parallel, Scalable, BackBone for a GPFS) effort. In the WAN area new IP encryptors will be deployed to position the WAN for future growth if and when necessary. Cost of the WAN is expected to drop as long distance data links are becoming more affordable.

For FY07 the activities will include continued operation and maintenance of the LAN/MAN/WAN infrastructure. We also anticipate more integration with the ESN deployment. For the WAN, we expect to see the first deployment of 10 gigabit encryptors.

1.5.5.1.9 Infrastructure Integration (LANL)

Infrastructure Integration encompasses the entire network infrastructure upgrades need to support integration of new HPC computing platforms planned for FY06 and FY07. This includes designing, procuring, and installing network switches and routers needed to support the new HPC platforms and provide increasing bandwidth to HPSS, VIZ systems, and customer workstations. Will include integration of the network components into the HPC computing platforms and storage systems. This project will also include integrating new switches/routers into our network monitoring platforms and training operational personnel to monitor and troubleshoot the new systems.

Network engineers and technicians knowledgeable in all aspects of network technology including HPC platform operating systems and storage systems.

In FY06, we will develop PaScalBB networks to support new HPC clusters in both the Yellow and Red networks. Upgrade network infrastructure to increase bandwidth to HPSS, VIZ platforms, and customer workstations. Install new backbone routers that

support single and multiple 10 GigE trunks between HPC platforms and customer LANs.

Preliminary planned activities in FY07 include developing plans to support the needs of petaflops HPC platforms.

1.5.5.1.10 Ongoing Systems Operations (LANL)

This project includes all services for computational systems operated by Los Alamos for the purpose of developing and running user codes. These services include system configuration, computer security, resource management, system administration, system operation and monitoring, and customer-driven system software development. 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 collaborate with systems research, development, and integration efforts in the Simulation and Computer Science program element to usher new technology into production. Thrust areas include:

- Computer system support. Conduct daily system administration and continual monitoring of production systems and infrastructure servers. 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. Maintain security plans and tests for existing systems and create plans as required for new production resources.
- Scheduling environment daily management. Provide daily administration, monitoring, and problem resolution of software subsystems used in resource scheduling, including accounting and reliability 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.
- System Operations: Ongoing operations currently requires staff to provide around-the-clock operations and monitoring of the scientific computing resources including high-performance computers, such as ASC Q and Lightning, and data storage and retrieval systems such as the HPSS. System operators monitor all components 24/7 and take corrective action and/or escalate problems to others who can effect corrective actions.
- System Self Maintenance: Replace failing field replaceable units in selected systems on a 24/7 service basis. Repair field replaceable units and test to maintain a stock of reliable spare field replaceable units. Return failed components to suppliers as required. Maintain adequate stock of spare parts based on past and projected future component failure rates.

This project utilizes the skill, experience and talents of professional teams of system administrators, operators, and other skilled technical resources. These resources utilize automated tools and documented procedures to administer, maintain, schedule and operate all HPC systems and components. This includes all components of the production computing environment, including compute engines, networks, fileservers, archival storage systems, the facilities they reside in and utilities they are dependent upon, and all required software on these systems.

Planned activities in FY06 include prepare to support the new Linux capacity systems in production; plan for and execute the retirement of systems that have reached end of life;

continue to provide system support, operations and management of all ASC production assets; study the feasibility of reduced staff ("lights out") computer operations; implement additional formal and informal customer satisfaction metrics and measurement techniques; and expand self maintenance to additional systems and components.

Preliminary planned activities in FY07 include prepare new Linux capacity systems for production and support them in production environment; continue to provide system support, operations and management; and implement a reduced staff ("lights out") computer operations model.

1.5.5.1.11 Systems and Network Maintenance (LANL)

This project obtains hardware and software support services for all production ASC systems and network assets operated by Los Alamos. Support services include vendor on-site hardware and software support contacts; contracts for parts sparing and logistics for self maintained equipment; software licenses, annual software maintenance and support fees; and contracts for telephone support and other remote hardware and software support requirements.

Two main activities are the initial procurement of services for new production resources, and the renewal of existing maintenance and support contracts, normally on an annual basis. This project also produces and maintains budgetary planning data and earned value reporting on hardware and software maintenance commitments and projects.

This project is a coordination point for all maintenance contracts for system and network hardware and software. Customers include ongoing operations and integration teams, projects and groups. Interfaces include third party vendors and suppliers and the Los Alamos supply chain and accounting organizations. This project, in coordination with supply chain, negotiates new and renewal contract pricing and terms and conditions. It maintains databases of contractual expiration dates and ensures that renewals are initiated and completed in a timely way so that lapses in support and disruptions in services do not occur. Orders, both original and renewal, are tracked as they proceed through procurement and fulfillment.

Planned activities in FY06 include refine order entry and tracking capabilities including interfaces with customers, supply chain, program management, and accounting; forge even stronger relationships and understanding with customers and external interfaces; develop methods and procedures to ensure the capture of maintenance requirements for all new production resources well in advance of their required date; procure and ensure fulfillment of all maintenance services required by existing and new systems in FY06; and plan for all maintenance services required in FY07 and beyond.

Preliminary planned activities in FY07 include procure and ensure fulfillment of all maintenance services required by existing and new systems in FY07 and plan for all maintenance serves required in FY08 and beyond.

1.5.5.1.12 Systems and Network Equipment (LANL)

This project ensures the procurement of systems and networking equipment required for support of ongoing production systems. In addition procurements of related software support and third party labor are coordinated and executed through this project. This project also produces and maintains budgetary planning data and earned value reporting on systems and networking equipment procurement activities.

This project is a coordination point for system and network equipment and related software procurements. Customers include ongoing operations and integration teams,

projects, and groups. Interfaces include third party vendors and suppliers and the Los Alamos supply chain and accounting organizations. This project, in coordination with supply chain, negotiates purchase pricing and terms and conditions. Procurements are tracked as they proceed through procurement and fulfillment.

Planned activities in FY06 include refine order entry and tracking capabilities including interfaces with customers, supply chain, program management, and accounting; develop even stronger relationships and understanding with customers and external interfaces; develop methods and procedures to ensure the identification of requirements for all new production systems and network equipment well in advance; procure and ensure delivery of all systems and network equipment required by existing and new systems in FY06; and plan for all equipment required in FY07 and beyond.

Preliminary planned activities in FY07 include procure and ensure delivery of equipment required in FY07 and plan for all equipment required in FY08 and beyond.

1.5.5.1.13 Ongoing Facilities (LANL)

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

The SCC, LDCC, and CCF 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 the SSP. 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 SSP. 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.

The computer facilities were established to house large, mission-critical computer systems (such as, the Q system) in support of the SSP and other research efforts. This project provides the ability to ensure the continued operation of current computing systems and support infrastructure as required to meet programmatic computing needs. A part of this function is ensuring that facility site preparations have been made and design of electrical and cooling requirements have been met for computer systems planned by the Division.

Planned activities in FY06 include the following:

- Prepare site to support new systems. The project includes site preparation for computer installations and design of electrical and cooling requirements for computer systems planned by the Division (such as, electrical, cable trays, cooling, design, etc.). This is in support of the platform acquisition that will bring over 500 Teraflops computing resources into the tri-lab computing centers. Additional facilities upgrades will be needed in the LDCC to support future growth in the unclassified computing systems.
- Ongoing Operations. This project ensures the continued operation of current computing systems and support infrastructure as required to meet programmatic

computing needs. This minimizes interruption to the operation of systems and optimizes the performance, reliability, and availability from end-to-end (HPC system to the user's desktop). This includes all components of the production computing environment, including compute engines, networks, fileservers, archival storage systems, the facilities they reside in and utilities they are dependent upon, and all required software on these systems, as well as user support and assistance in making effective utilization of these resources. On call support is provided on a 24/7 schedule to ensure continued operations of electrical and mechanical systems.

In FY07, planned activities include maintenance and support for ongoing operations including site preparations for future computer systems.

1.5.5.1.14 Facilities Upgrade Project (LANL)

The project will provide an additional computing power capability as required to support future systems by the end of FY06. The project will consist of the installation of capital construction equipment as needed, possibly including but not limited to Rotary UPS units, new electrical substations and switchboards and a number of Power Distribution Units chillers, cooling towers, and air handling units on the computer floor of the SCC.

With execution of this project the total overall computing power capability will be increased as required to support planned future systems. This power capability will provide enough power to stay ahead of computer projections with planned computer installations. With final design completed in FY05, construction will be performed in FY06. The contractor should be complete with the project in approximately six months and operational acceptance finalized by the end of the fiscal year.

1.5.5.1.15 Cyber Security Operations (SNL)

This project provides the cyber security support for the ASC Program, including development, deployment and management of cyber security components related to authentication, authorization and remote access. The project also has responsibility for accreditation of SecureNet.

The Cyber Security Project is focused on providing the authentication and authorization services used by applications for the purposes of remote access and data movement across ASC sites. This project and its deliverables are important for meeting an FY06 level 2 milestone to replace the tri-labs DCE security infrastructure. An important aspect of this is maintaining the accreditation of SecureNet, and establishing a working relationship with the ICSI program.

Planned activities in FY06 include activities related to the FY06 level 2 milestone for the replacement of the tri-labs DCE security infrastructure; place into a production state the DCE replacement Kerberos authentication servers; integrate authorization services with the ICSI Directory Service; perform a Tri-labs demonstration of applications utilizing replacement technologies; continue software support for Kerberos based applications; deploy NFS V4 server for pilot as a DFS replacement; provide the Security Officer for SecureNet; and maintain accreditation of SecureNet.

Preliminary planned activities in FY07 include production NFS V4 services across the tri-labs and integration of ICSI need-to-know services with high-performance computing applications.

1.5.5.1.16 Power, Physical Security, and Facilities Support Personnel (SNL)

This project funds the power and space bills for all ASC scientific computing, storage, visualization and infrastructure support activities carried out in the central computing facilities at Sandia National Labs in Albuquerque.

The planning, physical access control, cyber security compliance and coordination with corporate facility and building managers necessary for the continuous operation of the scientific computing infrastructure constitute this project's capabilities. Funds provided by this project pay for electricity, computing floor space, 24x7 operational personnel who monitor the networks, computer services, building environments and provide appropriate response to error conditions.

Planned Activities in FY06 include maintain operational stability of the CCF (Building 880 Computing Annex), and the Super-Computing Annex (SCA, Building 725) in Area I of Sandia Albuquerque; prepare a multi-year plan for infrastructure upgrades and improvements to existing facilities to replace aging and inefficient cooling and power distribution technologies; and renovate and redeploy the computing floor space freed up due to the retirement of the ASC Capability Platform ASCI Red.

Preliminary planned activities in FY07 include prepare for possible infrastructure additions to power and cooling plant in response to expanded SCA facility and future ASC Capability or Capacity platforms and support Core Network renovations in the Open and Restricted Networks moving to 10 GigE backbone capabilities throughout the main campus.

1.5.5.1.17 Tri-Lab Dedicated Wide Area Network Monitoring and Operations (SNL)

This project manages the day-to-day operation of the WAN interconnecting the tri-lab Classified computing environments.

The project will enhance the distance computing and machine network infrastructure, monitoring and reporting to improve network availability and user support and improve the network architectures for sharing the tri-lab resources. The project will place emphasis on finding innovative ways to continue to provide required services while enhancing efficiency. The project will provide status, performance and configuration of resources to support end users and the operational customer, as well as metrics for management reporting and planning purposes.

Planned activities in FY06 include collaborate with other ASC programs elements to provide an updated Usage Model for Purple; determine Purple status and monitoring Requirements; integration of Purple into current DisCom status and monitoring tools; integration of DisCom WAN monitoring of connections to Purple; determine User Perspective Tests that will be run from SNL to Purple; determine enhanced integration of Red Storm into CEMS at Sandia; determine integration of HPC Environment into CEMS at Sandia; determine additional reporting (including metrics) from available data; operational Support of WAN and Distance Computing; update tri-lab Services offered via SARAPE; perform the network engineering necessary to provide SNL access to BlueGene/L and Purple as they become available; procure a replacement service for the current AT&T network link between SNL/NM and LLNL/CA and make it operational. Develop a cutover plan to implement the new service and move production traffic to the new service before the AT&T contract expires on January 31, 2006; and utilizing CEM and other capabilities, continue to improve the real-time monitoring and management of

the DisCom environment and generate enhanced status reports and other performance metrics.

Preliminary planned activities in FY07 include integration of the next Computational Super Computer in the DisCom Status and Monitoring; ee-evaluation of requirements for User Perspective Monitoring, Status and Reports of HPC Environment; integrate 10 gigabytes per second encryptors into the WAN if required to support applications; and incorporate new ASC resources into the DisCom WAN as they are installed.

1.5.5.1.18 Sandia Production Systems, Albuquerque, New Mexico (SNL)

This project coordinates and manages all the activities within the computing centers that support daily operations and scheduling of ASC capability and capacity computing systems and pre- and post-processing platforms and the several hierarchical storage systems providing long-term storage of scientific data.

Capabilities for this project include the following: Host the tri-lab Expedited Priority Run sessions for Red Storm. Negotiate system-dedicated time, operating system upgrade schedules, and facilitate problem identification and resolution across the tri-lab user community. Manage account granting process user requests appropriate to the ASC priorities and system status of Limited or General Availability. The end-to-end computational process requires a variety of pre-processing and post-processing capabilities and a variety of communications, storage, archive and infrastructure support systems. This project provides funding to manage the operation of the various commercial systems supporting ASC – from the deployment, testing, and integration of systems into the user environment, to the continuing maintenance and management of systems in production operation. And, most importantly, the project provides for the team of skilled and experienced technical staff that administers the complex HPC environment and supports system users.

Planned activities in FY06 include the following: Support ASC Milestone computing needs of Sandia, Los Alamos and Livermore customers. Continue to improve collection and dissemination of knowledge and user experiences on Red Storm via the Collaborative Learning, Information and Knowledge tool. Track and resolve all error conditions encountered by customers and administrators in cooperation with Cray, Inc. and other system providers. Conduct monthly user seminars to disseminate "best practices," advertise system schedules and provide a face-to-face feedback mechanism in addition to on-line contact methods. Collect, analyze and distribute system utilization metrics and modify operational parameters to improve customer satisfaction. Proceed with an orderly migration of the HPSS systems from Release 5.1 to Release 6.2, and realign the existing IBM storage subsystems following the retirement from service of ASCI Red.

Preliminary planned activities in FY07 include provide additional assistance in porting codes and improving computational performance, scalability and I/O usability of the Red Storm platform and plan for system component upgrades and/or integration of additional system components.

1.5.5.1.19 Sandia Production Systems, Livermore, California (SNL)

This project provides production computing, visualization and storage infrastructure, and supporting staff at the Sandia California site. The compute resources supported are used corporate wide, while the visualization and storage are generally for use by users running at the local site.

Production Systems, CA provides funding for (1) the maintenance and support of the California production NWCC; (2) maintaining resources to visualize data produced on NWCC, Red Storm, and ASC White; and (3) support of the local data storage (NFS, HPSS, StorageTek) available to analysis users in California. Our ultimate goal is to provide operation of stable, powerful, efficient, accessible, and easily useable computation and visualization systems services for the California CSSE community in both SRN and SCN environments and for both R&D and production use.

Planned activities in FY06 include continue support of all California production computing, visualization, and storage infrastructure; improve visualization cluster usage in combination with deployment of a user environment common with the NWCC systems; increase size of available storage and functionality of archival systems; technology refresh of visualization servers through acquisition of large memory Linux machines; and develop/write facility refresh plan for California Computing Center.

Preliminary planned activities in FY07 include acquisition and deployment of production centralized cluster/heterogeneous file system and deploy and support FY07 TLCC in production mode.

1.5.5.1.20 Red Storm and High Performance Computing Network Deployment (SNL)

This project will provide the high performance network environment to interconnect all of Sandia's local supercomputing resources.

The latest technologies (for example, 10 G Ethernet, IP encryption, high-speed firewalls, and parallel data movement applications) will be validated and deployed to provide the required level of performance and reliability for the current major supercomputing resources. These performance requirements range from 25 gigabytes per second for Red Storm to 1 gigabits per second for login and other services.

Planned activities in FY06 include complete the installation of the 25 gigabytes per second infrastructure for the Classified Red Storm to the Data Services cluster; tune the classified and unclassified Red Storm/Data Services network systems to achieve maximum network performance; and work with the parallel data movement application teams to optimize the performance and functionality of user data transfers in the Red Storm/Data Services environment.

Preliminary planned activities in FY07 include support expected expansions of Red Storm and capacity cluster performance requirements.

1.5.5.1.21 Kansas City Plant Facility and Operations Support (KCP)

The Kansas City Plant (KCP) Facility and Operations Support project provides support for transition of KCP simulation environment to local and remote use of the SIERRA code framework.

This project will provide the capability to apply ASC mechanical engineering and physics codes (specifically SIERRA) to the evaluation of production processes to the Nuclear Weapons Complex stockpile, both current builds and any readiness and enhanced surveillance issues that may occur.

Planned activities in FY06 include collaborating with design agencies to establish local and remote computing resources and support.

In FY07, we will complete the transition of production computing capabilities to support of SIERRA applications.

WBS 1.5.5.2: User Support Services

This level 4 product provides users with a suite of services enabling effective use of ASC tri-lab computing resources. The scope of this product includes planning, development, integration and deployment, continuing product support, and quality and reliability activities collaborations. Projects and technologies include computer center hotline and help-desk services, account management, web-based system documentation, system status information tools, user training, trouble-ticketing systems, and application analyst support.

User Support Services Deliverables for FY06

- Product services for several level 2 milestones including Purple limited availability, BlueGene/L availability, and tri-lab Purple environment.
- This product's deliverables include user assistance and consulting via help desk and in person consultation; preparation and presentation of appropriate training sessions and documentation for LANL and tri-lab customers; coordination of account management activities within the Los Alamos customer base and among tri-lab users and affiliates; problem identification, resolution and tracking; maintenance of historical records of problems and their resolution; reports on metrics such as system utilization and reliability (reliability metrics include interrupt and repair data from the individual components to complete systems); planning and user support for commercial production software tools; and direct end-user and application development support for effectively utilizing systems.
- Contribute to the HPC Consortium Community particularly for sharing common information such as training.

Strategy to Deliver User Support Services for FY06–FY07

- Maintain a well-trained and motivated workforce capable of providing user support services for Purple and BlueGene/L systems.
- Focus on customer requirements for access and effective use of all ASC systems, take responsibility for direct customer service to local and remote users, and take responsibility for usage statistics and administrative interface for external users such as ASC Alliances.
- Achieve continuous improvement in the quality of user support and user satisfaction with these services through the use of appropriate metrics and user feedback mechanisms.
- Utilize quality software engineering design that is well planned and managed. We will be expeditious, incorporating code reuse when possible.

1.5.5.2.1 Hotlines and System Support (LLNL)

The Hotlines and System Support project provides users with a suite of services enabling effective use of ASC tri-lab computing resources.

This project includes computer center hotline and help-desk services, account management, web-based system documentation, system status information tools, user training, trouble-ticketing systems, and application analyst support.

Planned activities in FY06 include supporting ASC tri-lab systems in the following areas: provide daily technical consulting and user support services; respond to customer calls to resolve questions about systems use or status; provide account management activities and system event scheduling including technical bulletin publishing; administer and

maintain Remedy for problem reporting and tracking; continue development of the LCAMS product to improve efficiency and accountability of account management activities and policy implementation; and develop and maintain web pages, documentation, and training as needed.

For FY07, we expect to continue to provide the same activities and services described for FY06.

1.5.5.2.2 Integrated Computing Network Consulting, Training and Documentation, and External Computing Support (LANL)

This project is comprised of three teams: the Integrated Computing Network consulting office, responsible for direct customer service to local and remote users of LANL ASC resources, the training and documentation team, responsible for the development and delivery of documentation and training materials for LANL ASC 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. Thrust areas consist of:

- User support services. Daily technical consulting and user support services. The Integrated Computing Network 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. They 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 data regarding machine usage, machine availability, and mean-time-to-failure as needed by various interested parties and make that data accessible.
- Develop and deliver documentation and training.

This project is staffed by teams of skilled and experienced consultants, trainers, documenters and statistical professionals. This staff, coupled with a set of procedures and tools deliver user support services including help desk, account management, documentation and training. They also maintain statistics on system utilization and reliability.

Planned activities in FY06 include perform ongoing user support for users of LANL's ASC computing resources; expand class offerings particularly in the use and support of Linux capacity systems and Panasas based file systems; expand online documentation in both breath and depth; deploy new trouble tracking systems in the open and secure; deploy enhanced HPC statistical reports and infrastructure; re-architect the accounts system; and further refinement and development of ongoing customer satisfaction surveys to quickly identify and deal with any future shortcomings.

Preliminary planned activities in FY07 include performing ongoing user support for users of LANL's ASC computing resources, and continuing to improve the quality of support for productive use of the computing services.

1.5.5.2.3 Ongoing User Services (LANL)

This project has two main focus areas grouped under the umbrella of User Services. The first focus is to support the production environments by ensuring that tools needed by users are available and working on production platforms. Tools in this context include compilers, debugging tools, and performance and profiling tools. To do this we research, develop, and deploy reliable, available, and scalable capabilities in commercial and custom software development. The essential elements must be identified and advanced to minimize cost, enable similar environments across like platforms, and enable developers to successfully develop, debug, and analyze applications. Specific activities include: interact with vendors and other third party tool providers to negotiate requirements, licenses and product issues; work with the project lead for Systems and Network Maintenance to budget for tool contracts and to forecast new requirements; test tools on new computing resources before they go into production use; establish acceptance/regression test suite for tools; assist users in applying tools to their problems; continue development of a comprehensive tools strategy, base on LANL needs and in concert with the tri-lab tool workshops; and participate in planning and assessing tools environments for future ASC systems.

The second focus is on application development and end user in-person support. This involves technical consulting and collaborations with customers on issues related to the application code development environment and use on production systems, including documentation and training. The goal is to engage users directly to understand problems and issues and assist in their solution. The staff fulfilling this focus area also serve as a two-way conduit for communication of requirements, issues, and information between users and all the ASC teams that support them.

Planned activities in FY06 include assisting users via direct support and with tools as the number and use of Linux capacity computing platforms grows and moves from 32-bit to 64-bit operation; providing support for the 64-bit production development environment on Lightning and new capacity clusters and establishing a focused approach to supporting users; ensuring that an acceptance/regression test suite process is initiated for tool acceptance prior to production implementation; to provide technical consulting and collaborations with customers on issues related to the application code development environment on production systems; and to manage requests for and installations of third-party software on the production systems.

Planned activities in FY07 include planning for software tools required for future systems, and continuing to improve the quality of support for productive use of the computing services.

1.5.5.2.4 Red Storm Customer Care (SNL)

Classroom instruction provided through Cray, Inc. and augmented by local experts. Web based training will provide overviews and baseline education about the Red Storm system and access methods. In an effort to cultivate a shared wisdom community we provide the Collaborative Learning, Information and Knowledge tool to gather, share and maintain HPC user knowledge. SARAPE provides remote users with the ability to request account access for NNSA wide platforms, engineering applications and network access. We will continue significant investigations of application code performance on specific architectures (specifically, Red Storm) and prepare general models to predict the behavior of codes on new architectures. Implement and support a Software Quality Environment for applications developers, systems administrators and operating systems developers. This activity is in cooperation with the system level metrics gathering work identified in the Systems Software and Tools product area (1.5.4.4).

Capabilities for this project include the following: Statistics gathering through interview and review of access logs to determine the use of the services that provide customer support. Continue to provide methods for administrators to verify status of support and for all users to collaborate within secured access environment. Provide SARAPE web based request access to all ASC platforms within the tri-lab arena to all customers of these platforms. Administer software quality platforms to minimize disruptions to production platforms and support application development regression tests and quality processes. Identify to what extent real application performance correlates to the performance of select application kernel benchmarks. Use models to identify the limiting features of codes and platforms. Collect production based workloads to support software quality practices for system software.

Planned activities in FY06 include using a well defined statistical analysis design to gather data at 1 month from release of Red Storm and six months following release to compare to determine growth direction, capability and requirements. The primary activity will be to employ the ability for consultants to provide user support solely from within the email environment while having the code append history to database objects. Document the SARAPE process and work with the Sandia Infrastructure Support group to possibly transfer responsibility. Develop and expand Access Grid training capability and work with the other labs to develop a training "library" to allow for reuse of training material and sharing of tools among the labs. Expand coverage of research to additional codes exhibiting varied computational and I/O characteristics. Initiate the Software Quality Environment with appropriate development platforms as determined by application development teams at Sandia.

Preliminary planned activities in FY07 include a review of data that will determine these activities, including an ongoing metrics gathering and evaluation plan.

WBS 1.5.5.3: Collaborations

This level 4 product provides collaboration with external agencies on specific high-performance computing projects. The scope of this product includes planning, development, integration and deployment, continuing product support, and quality and reliability activities collaborations. This product also includes any programmatic support across the entire ASC program and studies, either by internal or external groups, that enable the program to improve its planning and execution of the its mission.

Collaborations Deliverables for FY06

- LLNL will manage tri-lab contracts and procurements, support tri-lab meetings and conferences, prepare and release ASC documents, and continue with earned value management of the Purple contract.
- Sandia will explore possible cooperative work with the SC05 ASC Research Exhibit and the FY06 Principle Investigators meeting.

Strategy to Deliver Collaborations for FY06–FY07

- Encourage a strong relationship with the US academic community and NNS for the benefit of ASC. We are also committed to excellent service to the tri-lab community in our joint activities.
- Support SC05 Research Booth.

1.5.5.3.1 Program Support (LLNL)

The Program Support project provides service to the ASC program. These services include document management, technical writing and editing, procurement and contracting, project management, and meeting support. These services are in support of both LLNL-only and tri-lab activities.

In FY06, this project will support preparation and release of technical reports, publicity media, and tri-lab documents such as FY07 Implementation and SuperComputing publicity. Procurement activities will include management of existing tri-lab contracts and negotiating and executing new contracts. Project management support will be provided for earned value management of the Purple project. Meeting support will be needed for the FY06 principle investigator's meeting, SC06, predictive simulation workshops, and other meetings.

In FY07, we plan to continue FY06 activities.

1.5.5.3.2 University Outreach (LLNL)

The University Outreach project is the focal point for the ASC Program to engage the U.S. academic community, facilitating scientific exchanges between laboratory and academic researchers and developing the next generation of scientists.

In FY06, the ASC program will partner with universities and research centers, gaining access to the most current advances in applied sciences, computer science and scientific computing. These partnerships also permit the ASC program to influence the direction and focus of applied research activities in areas of relevance to the program. The ASC program will support the High Performance Computer Science Graduate Fellowship and the summer and visitor programs. Through these activities, the ASC program trains and recruits the next generation of applied and computer scientists. Visits to the Laboratory and participation of laboratory researchers involve these young researchers in problems aligned with programmatic interest

In FY07, we plan to continue FY06 activities.

1.5.5.3.3 One Program/Three Labs (SNL)

One Program/Three Labs 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.

One Program/Three Labs supports expenses incurred by the laboratories to meet management expenses for the Alliance program for laboratory/Alliance center meetings, cross-Center meetings and workshops, and NNSA and tri-lab Sponsor Team reviews.

Planned activities in FY06 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; and SAIC contract to provide various administration support.

FY07 activities will continue to be a tri-lab program management effort.

V. ASC Level 1 and 2 Milestones

Table V-1. Quick Look: Level 1 Milestone Dependencies

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
349	Deliver advanced ASC physics and engineering simulation capabilities to support the W76 and the W80 LEP/certification.	1	2006	Jun-06	ASC/Integrated Codes	HQ, LLNL, LANL, SNL	Enhanced predictive capability, DSW Deliverables, Increasingly productive environment	Yes	LANL-VV-06-01, LANL-IC-06-01, LANL-IC-06-02	Yes	359 (M44)
350	Proved a 100 teraflops platform environment supporting to the tri-laboratory DSW and Campaign simulation experiments.	1	2007	Dec-06	ASC	HQ, LLNL	Enhanced predictive capability, DSW Deliverables, Increasingly productive environment	Yes	461, 464, 1348, LL-CSSE-06-02, LL-CSSE-06-04, LL-CSSE-06-05, CSSE-07-03	Yes	359 (and many more)
359	Complete modern baseline of all enduring stockpile systems with ASC codes.	1	2009	Sep-09	ASC/Integrated Codes	HQ, LLNL, LANL, SNL	DSW Deliverables		349		

Table V-2. Quick Look: Level 2 Milestone Dependencies for FY06[6]

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
1	Code B release to support RRW	2		Sep-06	ASC/Integrated Codes	LANL	Enhanced predictive capability	Yes	L3, L4, L5 milestones	Yes	M28, M36, M38, 359 (M44)
2	Code B release to support RRW and W76	2		Mar-06	ASC/Integrated Codes	LANL	Enhanced predictive capability	Yes	L3, L4, & L5 milestones	Yes	M28, 349 (M33), M36, M38, 359 (M44)
3	Code A release to support RRW and W76	2		Jun-06	ASC/Integrated Codes	LANL	Enhanced predictive capability	Yes	L3, L4, L5 milestones	Yes	M28, 349 (M33), M36, M38, 359 (M44)
4	Code A release to support RRW and W76	2		Sep-06	ASC/Integrated Codes	LANL	Enhanced predictive capability	Yes	L3, L4, L5 milestones	Yes	M28, M36, M38, 359 (M44)
5	Plutonium science for W88	2		Sep-06	ASC/Physics and Engineering Models	LANL	Enhanced predictive capability	Yes	L3, L4, L5 milestones	Yes	M38, 359 (M44)
6	Multiphase EOS capability	2		Sep-06	ASC/Physics and Engineering Models	LANL	Enhanced predictive capability	Yes	L3, L4, L5 milestones	Yes	M36, M38, 359 (M44)
7	Pilot Demonstration of UQ in 5 Areas of Physics and Engineering	2		Sep-06	ASC/Physics and Engineering Models	LANL	Enhanced predictive capability	Yes	L3, L4, L5 milestones	Yes	M36, M38, 359 (M44)
8	Secondary V&V Assessment Supporting W76-1 LEP Certification (Intermediate)	2		Sep-06	ASC/Verification & Validation	LANL	Enhanced predictive capability	Yes	L3, L4, L5 milestones	Yes	LANL-IC-06-04

[6] Factors such as FY06 Congressional Appropriations, NNSA/DP directives, and National Security considerations may necessitate a change in the current milestone set.

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
9	Primary V&V Assessment Supporting Code Capabilities for Primary Burn	2		Jun-06	ASC/Verification & Validation	LANL	Enhanced predictive capability	Yes	LANL-IC-06-01	Yes	LANL-IC-06-03
10	Validation assessment capability for simulation of engineering shock transmission through nonlinear materials	2		Jun-06	ASC/Verification & Validation	LANL	Enhanced predictive capability	Yes	L3, L4, L5 milestones	Yes	M36, 359 (M44)
11	Define and baseline end-to-end productivity measures for use of code projects A and B products	2		Jun-06	ASC/Computational Systems and Software Environment	LANL	Increasingly productive environment	Yes	LANL-IC-06-01, LANL-IC-06-02	Yes	359 (M44)
12	Performance prediction study of representative ASC application workload based on candidate capacity hardware platforms	2		Sep-06	ASC/Computational Systems and Software Environment	LANL	Increasingly productive environment	Yes	LANL-IC-06-01, LANL-IC-06-02	Yes	M36, M38, 359 (M44)
13	Characterize code project A and code project B on capacity production systems	2		Sep-06	ASC/Computational Systems and Software Environment	LANL	Increasingly productive environment	Yes	LANL-IC-06-01, LANL-IC-06-02	Yes	M36, M38, 359 (M44)
14	Capacity computing systems integration using revised software stack and code developer acceptance	2		Sep-06	ASC/Computational Systems and Software Environment	LANL	DSW Deliverables	Yes	L3, L4, L5 milestones	Yes	M36, M38, 359 (M44)
15	Computer Center Infrastructure upgraded to support growth in computing systems.	2		Sep-06	ASC/Facility Operations and User Support	LANL	Enhanced predictive capability	Yes	L3, L4, L5 milestones	Yes	359 (M44)
16	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	2	06	Mar-06	ASC/Integrated Codes	LLNL	Enhanced predictive capability				

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
17	Apply enhanced 3D secondary simulation capability to calculations required for the W80 LEP/certification	2	06	Sep-06	ASC/Integrated Codes	LLNL	Enhanced predictive capability DSW deliverables				
18	Implement and demonstrate a parallel 2D capability in an existing 3D secondary performance code	2	06	Dec-05	ASC/Integrated Codes	LLNL	Enhanced predictive capability				
19	Enhance capabilities of nuclear weapon simulation codes to support current and planned design efforts	2	06	Jun-06	ASC/Integrated Codes	LLNL	Enhanced predictive capability				
20	Explore and assess new opportunities to enhance the predictive capability of primary performance and safety codes for future stockpile activities	2	06	Sep-06	ASC/Integrated Codes	LLNL	Enhanced predictive capability				
21	Next-generation Pu multiphase EOS delivered for QMU and stockpile certification	2	06	Sep-06	ASC/Physics and Engineering Models	LLNL	Enhanced predictive capability				
22	Hydro-nuclear Global Sensitivity Analysis of Selected Nuclear Events	2	06	Sep-04	ASC/Verification & Validation	LLNL	Enhanced predictive capability				
23	Boost Physics Global Sensitivity Analysis of Selected Nuclear Events	2	06	Jun-06	ASC/Verification & Validation	LLNL	Enhanced predictive capability				
24	Application of Multi-Variate Adaptive Response Surface and Adaptive Latin Hypercube Analysis Methods to Selected Issues in W-80 Performance	2	06	Sep-04	ASC/Verification & Validation	LLNL	Enhanced predictive capability				

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
25	Deploy Next-Generation Data and Visualization Capabilities for BlueGene/L and Purple Environments	2	06	Jun-06	ASC/Computational Systems and Software Environment	LLNL	Increasingly productive environment				
26	Purple System Ready for Limited Production	2	06	Jun-06	ASC/Computational Systems and Software Environment	LLNL	Increasingly productive environment	Yes	461, 1348	Yes	350, LL-CSUE-07-02, LL-CSUE-07-03
27	Algorithms for error-corrected reliability analysis in risk-informed design	2	06	Sep-06	ASC/Integrated Codes	SNL	Enhanced predictive capability				
28	Apply coupled mechanical-electrostatics analysis capability to microsystem device.	2	06	Sep-06	ASC/Integrated Codes	SNL	DSW deliverables				
29	Simulate W76-1 electronic systems performance in combined thermal and hostile environments.	2	06	Sep-06	ASC/Integrated Codes	SNL	Enhanced predictive capability				
30	Demonstrate robust PRESTO simulation capability for B61 impacts, W76 abnormal mechanical environments & SGT accidents.	2	06	Sep-06	ASC/Integrated Codes	SNL	Enhanced predictive capability				
31	Demonstrate the calculation of current-voltage curves (collector and base currents) for an npn silicon bipolar junction transitor using two-dimensional CHARON simulations, and incorporating a finite set of defects and defect annealing in the simulations.	2	06	Jun-06	ASC/Physics and Engineering Models	SNL	Enhanced predictive capability				

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
32	Develop and demonstrate a predictive computational capability for polymers in confined geometries that connects changes in polymer mechanical performance to slow chemical reactions of aging.	2	06	Sep-06	ASC/Physics and Engineering Models	SNL	Enhanced predictive capability				
33	Apply a validation process for determining adequacy of AF&F response predictions in a full-system blast test	2	06	Sep-06	ASC/Verification and Validation	SNL	DSW deliverables				
34	Perform system-level Uncertainty Quantification and sensitivity analysis for abnormal thermal environments.	2	06	Jun-06	ASC/Verification and Validation	SNL	DSW deliverables				
43	Perform integral-level validation of fire model predictions of heat flux to a weapon in a hydrocarbon fuel fire.	2	06	Sep-06	ASC/Verification and Validation	SNL	DSW deliverables				
35	Provide the networking and I/O technology road map to support a petaflops computing environment and the conversion of the existing service to a new provider	2	06	Sep-06	ASC/Computational Systems and Software Environment	SNL	Increasingly productive environment				
36	Develop a high-level interprocessor communication network for petaflops computing.	2	06	Sep-06	ASC/Computational Systems and Software Environment	SNL	Increasingly productive environment				
37	Tri-lab verification methodology	2	06	Sep-04	ASC/Verification and Validation	LLNL, LANL, SNL	DSW deliverables				

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
39	Deploy Security Infrastructure for ASC Tri-Lab	2	06	Jun-06	ASC/Computational Systems and Software Environment	LLNL, LANL, SNL	Increasingly productive environment				
41	BlueGene/L Simulations Informing Pit Lifetime Estimates	2	06	Sep-06	ASC/Physics and Engineering Models	LLNL, LANL	Enhanced predictive capability	Yes	LL-CSSE-06-03		
42	Deploy Purple Tri-Lab User Environment	2	06	Sep-06	ASC/Computational Systems and Software Environment	LLNL, LANL, SNL	Increasingly productive environment	Yes	LL-CSUE-06-04	Yes	350

Table V-3. Quick Look: *Preliminary* Level 2 Milestone Dependencies for FY07

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
LL-IC-07-01	Develop enhanced capabilities in a multidimensional (1D,2D,3D) effects code to support current and planned effects modeling efforts	2	07	FY07-Q4	ASC/Integrated Codes	LLNL	Enhanced predictive capability DSW deliverables				
LL-IC-07-02	Demonstrate a dynamic P&M model capability with multi-physics coupling in a performance code	2		FY07-Q3	ASC/Integrated Codes	LLNL	Enhanced predictive capability				
LL-IC-07-03	Complete initial 2D mesh generation capability	2		FY07-Q2	ASC/Integrated Codes	LLNL	Enhanced predictive capability				
LL-IC-07-04	Enhance capabilities of nuclear weapon simulation codes to support current and planned design efforts	2		FY06-Q3	ASC/Integrated Codes	LLNL	Enhanced predictive capability DSW deliverables				
LL-IC-07-05	Explore and assess new opportunities to enhance the predictive capability of primary performance and safety codes for future stockpile activities	2		FY06-Q4	ASC/Integrated Codes	LLNL	Enhanced predictive capability				
LL-PEM-07-01	Advanced HE reactive flow model for scaled hydrodynamic studies.	2		FY07-Q1	ASC/Physics and Engineering Models	LLNL	Enhanced predictive capability				
LL-PEM-07-02	Produce and provide advanced assessment of a complex physics model using the full compliment of verification and validation tools and techniques available.	2		FY07-Q3	ASC/Physics and Engineering Models	LLNL	Enhanced predictive capability				

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
LL-CSSE -07-01	Develop strategies for deploying and operating a petaflops class compute resource by 2010	2	07		ASC/Computational Systems and Software Environment	LLNL					
LL-CSSE-07-02	Complete the hardware and software environment for BlueGene/L and Purple	2	07		ASC/Computational Systems and Software Environment	LLNL		Yes	LL-CSUE-06-04, LL-CSUE 06-03		
LL-CSSE-07-03	Ready the Purple system for General Availability	2	07		ASC/Computational Systems and Software Environment	LLNL		Yes	LL-CSUE-06-04	Yes	350
LANL-CSSE-07-01	Plan for Next Generation Capability System Architecture and Design, Based on Tri-Lab Application Drivers and Requirements	2	07		ASC/Computational Systems and Software Environment	LANL					
LANL-FOUS-07-01	Capacity Computing Systems Using Revised Software Stack, Designer Tested and Ready for Production Use	2	07		ASC/Computational Systems and Software Environment	LANL					
SNL-IC-07-01	Deliver fully integrated solver capability in Trilinos Release 7	2	07	Q4	ASC/Integrated Codes	SNL	Enhanced predictive capability				
SNL-IC-07-02	Allegro High Energy Density Capability	2	07	Q4	ASC/Integrated Codes	SNL	Enhanced predictive capability				
SNL-IC-07-03	PREMO vortex-fin interaction capability	2	07	Q4	ASC/Integrated Codes	SNL	Enhanced predictive capability				
SNL-IC-07-04	ARIA level set capabilities	2	07	Q4	ASC/Integrated Codes	SNL	Enhanced predictive capability				
SNL-IC-07-05	Combined cable SGEMP, box IEMP, and cavity SGEMP capability	2	07	Q4	ASC/Integrated Codes	SNL	Enhanced predictive capability				

Milestone ID	Milestone Title	Level	FY	Completion Date	DOE Program/Subprogram(s)	Site(s)	ASC Category	Depends on another Milestone	Milestone ID	Has another Milestone depending on it	Milestone ID
SNL-PEM-07-06	Fluid-Structure Interaction Subgrid models for Microsystems To Predict Damping-Type Models for Use In Structure Dynamics Code	2	07	Q4	ASC/Physics and Engineering Models	SNL	DSW deliverables				
SNL-PEM-07-07	A Physics-Based Methodology for Calculating Properties of Radiation-Induced Defects	2	07	Q4	ASC/Physics and Engineering Models	SNL	Enhanced predictive capability				
SNL-VV-07-08	Develop A Tri-Lab QMU Methodology and Implementation Plan	2	07	Q4	ASC/Verification and Validation	SNL	DSW deliverables				
SNL-CSSE-07-09	Deliver techniques and methodologies developed under DVS to support verification and validation	2	07	Q4	ASC/Computational Systems and Software Environment	SNL	Increasingly productive environment				

Detailed Milestone Descriptions for FY06

Milestone (ID#): Define and baseline end-to-end productivity measures for use of code projects A and B (#11)
Level: 2
Fiscal Year: FY06
DOE Area/Campaign: ASC
Completion Date: June 30, 2006
ASC nWBS Subprogram: Computational Systems and Software Environment
Participating Sites: LANL
Description: he principal goal of this Milestone is to engineer a means to compress the end-to-end execution of Directed Stockpile Work, in pursuit of making the Laboratory more timely and responsive to dynamic national need without sacrificing quality or precision. In industrial terms, its goal is to instill a method of continuous process improvement initially through the application of productivity measures made upon ASC code projects, with the intent to extend such measures across the LANL Stockpile Program complex.
Completion Criteria: The Project shall result in the definition, trial, and evaluation of a method of assessing productivity and productivity improvement applicable to the execution of ASC tasking. A governing metric will be the sense of progress gained (explicit performance measure as-yet TBD) towards implementing an infrastructure responsive to dynamic stockpile certification issues.
Customer: Line Organizations, DoD
Milestone Certification Method: A Final Review will be conducted and its results documented. Formal documentation, such as a report or a set of viewgraphs with a written summary, will be prepared as a record of milestone completion.
Supporting Resources: FTE's: 2.5; Purchases: none; Service contracts: none; Computing hardware: desktop tools; Computing cycles: none
Codes/Simulation Tools Employed: No Weapons Complex simulation runs will be initiated by this Project.
Contribution to the ASC Program: By deliberately and successfully engineering a "responsive infrastructure" requirement into the ASC Program, the ASC Program's value to DOE Defense Programs and to the LANL Weapons Program will be significantly increased. The over-arching goal of this Milestone is to enable continuous process improvement in the context of Directed Stockpile Work. Specifically, the ASC Program will be positioned to bring robust and more-timely value into settling significant Stockpile issues, which directly translates into an enhanced national strategic posture in a dangerous world.
Contribution to Stockpile Stewardship:

No.	Risk Description	Risk Assessment (low, medium, high)		
		Consequence	Likelihood	Exposure

Milestone (ID#): Performance prediction study of representative ASC application workload based on candidate capacity hardware platforms (#12)				
Level: 2				
Fiscal Year: FY06				
DOE Area/Campaign: ASC				
Completion Date: Jun-06				
ASC nWBS Subprogram: Computational Systems and Software Environment				
Participating Sites: LANL				
Description: Complete a formal systematic performance study of candidate compute architectures considered for the anticipated next ASC capacity platform procurement against a tri-Lab application workload. We anticipate that Partisn, Sage, CTH, and UMT2K will be included. The spectrum of architectures under consideration will include all credible bids in the procurement process. The study will use validated application models to rank the proposals based on achievable/sustained performance on the realistic workload considered. For a subset of the bids, we will perform point-design studies, to assess the impact of various proposed changes in the configuration on application performance. The software stack from each of the three Labs will be utilized in the analysis.				
Completion Criteria: The milestone will be complete when the ranking for a system and application performance standpoint of all credible bids will be done. This includes the point-design studies mentioned in the Milestone Description.				
Customer: The client is the ASC program (S&CS, Platforms, and HQ) which are keenly interested in ensuring that the next procurement exhibits superior performance characteristics for the ASC applications.				
Milestone Certification Method: To certify the completion of this milestone, a formal review will be conducted, and formal documentation will be submitted documenting the milestone work.				
Supporting Resources:				
Codes/Simulation Tools Employed: Sage, Partisn, UMT2K and CTH, at a minimum will be employed. In reality, we expect that a larger suite of apps will be considered. PAL developed models of these applications will be employed.				
Contribution to the ASC Program:				
Contribution to Stockpile Stewardship: text				
No.	**Risk Description**	**Risk Assessment (low, medium, high)**		
		Consequence	**Likelihood**	**Exposure**

Milestone (ID#): Characterize code project A and code project B on capacity production systems (#13)				
Level: 2				
Fiscal Year: 2006				
DOE Area/Campaign: ASC				
Completion Date: September 30, 2006				
ASC nWBS Subprogram: Computational Systems and Software Environment				
Participating Sites: LANL				
Description: As the ASC codes become the main line for design activities at LANL, and as ASC activities move from capability to capacity, two things will become more important. First, design activities will require the ability to predict the compute resources (central processing units and time) required to complete a given calculation. Second, as the capability of the codes matures, their performance and optimization will become increasingly critical to the success of their users. To aid in the efficient use of capacity systems, and to move toward a more systematic approach to code performance, codes from code Project A and code project B will be ported to run on the new ASC Linux capacity hardware. A set of baseline performance measurements will be collected on a set of full application simulations running on approximately 64, 128, 256, and 512 processors. Simulation time, memory requirements, MPI messaging patterns, and I/O patterns will be collected and analyzed. These will serve as reference points for future performance optimization work.				
Completion Criteria: Existence of instrumented versions of the products of the Code Projects A and B Existence of documentation reflecting code developer and user approval of the set of problems on interest for each code product instrumented				
Customer:				
Milestone Certification Method:				
Supporting Resources:				
Codes/Simulation Tools Employed:				
Contribution to the ASC Program:				
Contribution to Stockpile Stewardship:				
No.	**Risk Description**	**Risk Assessment (low, medium, high)**		
		Consequence	**Likelihood**	**Exposure**
1				
2				
3				

Milestone (ID#): Capacity computing systems integration using revised software stack and code developer acceptance (#14)
Level: 2
Fiscal Year: FY06
DOE Area/Campaign: ASC
Completion Date: Sep. 30, 2006
ASC nWBS Subprogram: 1.5.4 Computational Systems and User Environments
Participating Sites: LANL
Description: Capacity computing systems integration complete and system is operational for identified application codes. In response to programmatic requirements for increased capacity computing cycles in FY06, major deliveries of Linux Capacity units are anticipated. This milestone ensures the integration of an operational systems software stack over the hardware procured in FY06. This systems software stack will include at a minimum the operating system, the message passing interface, the resource management system, the file system, and the core set of tools and applications needed for code development (debuggers, compilers, etc.).
Completion Criteria: The LANL system software stack will be tested on actual hardware procured in FY06 for full integrated functionality. Successful milestone completion will also include testing by selected code development projects for the necessary functionality to perform code development work. The milestone will be considered to be complete when a new capacity Linux system procured in FY06 has integrated the LANL software stack and has been demonstrated to be ready for compilation and code development of the major ASC applications.
Customer: Other ASC Programs, including 1.5.1 Integrated Codes, 1.5.2 Physics and Engineering Models, and 1.5.3 Verification and Validation; DSW Programs for Weapons Certification efforts, SFIs, etc.
Milestone Certification Method: 1 - A program review is conducted and its results are documented. 2 - Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion.
Supporting Resources: Supporting resources for the milestone include 5.5 FTEs dedicated to systems and networking integration. Funding will be needed for the capital procurement of capacity systems and supporting infrastructure hardware.
Codes/Simulation Tools Employed: The subprogram 1.5.4 Computational Systems and Software Environments will provide functional elements of the Software Stack as required, tested and ready for integration on hardware procured through the 1.5.4 subprogram.

Contribution to the ASC Program: The ASC Program provides the tools, applications, and computing resources to the Weapons Programs to meet simulation and modeling requirements for predictive science capabilities in support of stockpile stewardship. The Program has demonstrated requirements for increased computing resources in the level 1 milestone #1411, "Document the requirements to move beyond 100TF compute platforms to petaflops," completed Dec. 2004. As an outcome of this level 1 milestone, a tri-lab Platform Acquisition Timeline was formulated to meet the requirements established to achieve Weapons Programs objectives. This level 2 milestone is one step in the ASC Program meeting its obligation to provide capacity computing resources as outlined in this timeline.

Contribution to Stockpile Stewardship: The Stockpile Stewardship effort uses the compute resources provided through ASC for weapons simulations in support of weapons certification, resolution of Significant Findings Investigations, safety studies and analysis, and other stockpile maintenance related needs.

No.	Risk Description	Risk Assessment (low, medium, high)		
		Consequence	Likelihood	Exposure
1	Procurement Schedule delay	High	Low-medium	High
2	Software Stack functionality; reduced functionality	Medium	Low	Medium

Milestone (ID#): Computer center infrastructure upgraded to support growth in computing systems (#15)
Level: 2
Fiscal Year: FY06
DOE Area/Campaign: ASC
Completion Date: Sep. 30, 2006
ASC nWBS Subprogram: 1.5.5 Facility Operations and User Support
Participating Sites: LANL
Description: Note: Completion of the FY06 SCC Project is contingent upon receiving the necessary funding for this project. A platform acquisition timeline has been planned that will bring over 500 Teraflops peak new computing resources into the tri-lab computing centers between FY07 and FY08 (307.1TF of capacity cycles, and 282.8TF of capability cycles). Facility and networking infrastructure upgrades have lead times that necessitate preparations in FY06 in order to support this influx of new computing in this time frame. This milestone is aimed at preparing the LANL computing center to play its role in supporting the complex-wide computing growth in FY07-FY08. In the facilities arena, the FY06 SCC Infrastructure Project is the next in a series of power/cooling infrastructure upgrades for the SCC. These upgrades provide the equipment to receive the raw power as it is delivered to the building and distribute and deliver this power to the machine room for use by systems. The previous phase of upgrades provided a total-to-date computer power capability of 7.2 MW. The FY06 SCC Infrastructure Project will consist of the electrical and mechanical equipment necessary to provide an increase in this capability as required to support future systems. The design phase of the project will determine the specific technical requirements to produce this capability. Once design is complete and a project cost estimate is generated a construction contractor will be procured and specific schedule milestones will be finalized and measured. Also, in order to support the planned computing resources additional networking infrastructure will be required. This will be needed to support the GPFS as well as the archival storage and scientific visualization delivery. Increased deployment of ten gigabit Ethernet routers and switches will provide the increased bandwidth capability to meet this requirement
Completion Criteria: Power infrastructure capable of supporting the new computing resources is the criteria for the power upgrade. Data transfer rates from the computing resources to the global file system and archival storage that meet system requirements will be the completion criteria for the network upgrade.

Customer: This work is in direct support of Weapons Program predictive science through computer simulation and modeling for stockpile stewardship. ASC and DSW Nuclear Weapons Programs are the Program Office level clients/customers for this milestone. Our primary customers for the completion of the milestone include the Computing and Communications Division, the Production Computing and Infrastructure Program Manager, as well as all code developers and weapons designers and engineers who are users of the high-performance computers (X-Division, ESA Division, T-Division, CCS-Division, and their counterparts in the tri-lab arena). CCN-18 provides the utility upgrades, maintenance and support for high-performance computer systems, and CCN-5 provides the networking upgrades, maintenance, support, and ongoing operation. This includes ensuring that electrical, mechanical, and networking systems supporting the computers are operational 24 hours a day, seven days a week.

Milestone Certification Method:

1 - A program review is conducted and its results are documented.

2 - Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion.

Supporting Resources: TBD

Codes/Simulation Tools Employed: N/A

Contribution to the ASC Program: These infrastructure upgrades are critical to the operation of increased compute capacity. The power upgrade impact is needed to support adequate computing resources to meet ASC deliverables. The network upgrade is needed to make sure the data transfers to the global file system and archival storage system are adequate to insure optimum use of the computing resources.

Contribution to Stockpile Stewardship: These infrastructure upgrades are critical to the operation of increased compute capacity. The power upgrade impact is needed to support adequate computing resources to meet Stockpile Stewardship deliverables. The network upgrade is needed to make sure the data transfers to the global file system and archival storage system are adequate to insure optimum use of the computing resources.

No.	Risk Description	Risk Assessment (low, medium, high)		
		Consequence	Likelihood	Exposure
1	Capital Funding Absence	High	High	High
2	Design Delays/Failure	Low	High	Medium
3	GFE RUPS Schedule Delays	Medium	High	High
4	Contractor Procurement Delay	High	High	High
5	Electrical Equipment Delays	High	High	High

Milestone (ID#): Deploy Next-Generation Data and Visualization Capabilities for BlueGene/L and Purple Environments (#25)
Level: 2
Fiscal Year: FY06
DOE Area/Campaign: ASC
Completion Date: FY06-Q3
ASC nWBS Subprogram: Computational Systems and Software Environment
Participating Sites: LLNL
Description: The unprecedented capabilities of BlueGene/L and Purple, as well as their unique system characteristics, require next-generation data and visualization tools, running on next-generation server and image delivery infrastructures (existing data and visualization capabilities are commensurate with present capability and capacity machines). As a result of meeting this milestone, users will be provided measurably enhanced data management and visualization functionality, sized to meet the exceedingly powerful BlueGene/L and Purple environments. Milestone deliverables include: deployment of a large 256-node cluster-based visualization server utilizing next-generation interconnects, processors, and graphics cards; hardware-accelerated parallel rendering and compositing technologies supported within the VisIt tool; new releases to extend user features of the Hopper file management tool and Telepath resource session orchestration tools; high-resolution digital image delivery to new collaborative-use areas; and improved I/O and visualization for BlueGene/L applications through the ViSUS software infrastructure. Successful deployment of next-generation capabilities requires close and ongoing interaction with key customers to help ensure that delivered functionality meets user requirements for increasingly productive environments. Enhanced data management and visualization for BlueGene/L and Purple data requires determination of necessary scaling, specific improvements, and newly needed capabilities based on the size and power of BlueGene/L and Purple. Success also requires close interaction and integration with other product areas of Computational Systems and User Environments, as well as Facility Operations and User Support.
Completion Criteria: Successful installation, integration, deployment, and customer use of the new Gauss visualization cluster in support of BlueGene/L. Formal release(s) of VisIt that incorporate hardware-accelerated parallel rendering and compositing, together with measurements that demonstrate higher rendering and compositing rates than previous tools. Formal release(s) of Hopper and Telepath that incorporate new user requested or BlueGene/L- or Purple- required data and resource management functionality. Successful installation, integration, deployment, and customer use of new collaborative space displays, using digital image delivery technology, and BlueGene/L or Purple generated visualization data. Demonstrated efficiency improvements for use of hardware resources, and reduction in the overall time required for the design, simulation, and visualization cycle using new high-performance I/O and visualization techniques such as ViSUS and IDX.
Customer: LLNL stockpile stewardship scientists and engineers.

Milestone Certification Method:

1 - A program review is conducted and its results are documented.

2 - Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion.

Supporting Resources: Projects from the Pre and Post Processing Environments product.

Codes/Simulation Tools Employed: N/A

Contribution to the ASC Program: A powerful computational infrastructure is a key enabling technology for the ASC Program. Pre- and Post-Processing Environments that allow data to be efficiently generated, managed, stored, visualized and analyzed is a mandatory component of this computational infrastructure. Appropriately sized, and appropriately-powerful, data and visualization capabilities are required for ASC scientists to understand, and to convey to others, the results of their physics calculations performed on new platforms such as BlueGene/L and Purple.

Contribution to Stockpile Stewardship: Both the enhancement of predictive capability and the meeting of DSW simulation deliverables demand ever more powerful platforms such as BlueGene/L and Purple, together with appropriately balanced data generation, data management, and data visualization capabilities. Completion of this milestone supports overall stockpile stewardship goals by applying advanced data and visualization capabilities toward an overall integrated intellectual framework to analyze and understand SSP data.

No.	Risk Description	Risk Assessment (low, medium, high)		
		Consequence	Likelihood	Exposure
1				
2				

Milestone (ID#): Purple System Ready for Limited Production (#26)
Level: 2
Fiscal Year: FY06
DOE Area/Campaign: ASC
Completion Date: FY06-Q3
ASC nWBS Subprogram: Computational Systems and Software Environment
Participating Sites: LLNL
Description: 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 suitably stable for applications usage. When this milestone is complete, the system will begin providing useful computing cycles for production needs of NNSA. Deployment of the Purple system requires integration and interface between all parts of the ASC computing organization at LLNL as well as interfaces with ASC code developers at LLNL. Close integration of efforts between 1.5.5 Facility Operations and User Support, 1.5.4 Computational Systems and Software Environment, and IBM is required to assure that the computing environment needed by ACS codes is available and functional on the system. Training of system and network administrations, operators, maintenance personnel, and user support personnel has been completed.
Completion Criteria: Successful completion of the exit criteria for the Purple SWL test and LLNL accepts the vendor's (IBM) plan to remedy any deficiencies. Functional, performance, and reliability requirements specified in the SOW have been met or appropriate remediation agreed to. A programmatically relevant classified production simulation run has completed – demonstrating that the system is ready and approved for NNSA classified production use.
Customer: Tri-lab stockpile stewardship scientists and engineers.
Milestone Certification Method: 1 - A program review is conducted and its results are documented. 2 - Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion.
Supporting Resources: Multiple projects from both the Computational Systems and Software Environment subprogram and the Facility Operations, and User Support subprogram.
Codes/Simulation Tools Employed: N/A
Contribution to the ASC Program: Purple provides the tri-lab computational system for development of the full system simulations. It also represents a major deliverable defined at the beginning of the ASC program and has external visibility.
Contribution to Stockpile Stewardship: The Purple system will provide the major source of tri-lab capability computing for the large simulations needed by DSW for LEP and SFI calculations. Purple will also be a source for capacity computing until adequate alternative capacity computing resources can be deployed.

No.	Risk Description	Risk Assessment (low, medium, high)		
		Consequence	Likelihood	Exposure
1	IBM HW/SW not sufficiently reliable to release system for LA	Moderate	Very low	Low
2	LLNL SW and operational deployment not sufficiently reliable to release system for LA	Moderate	Very low	Low

Milestone (ID#): Provide the networking and I/O technology road map to support a petaflops computing environment and the conversion of the existing service to a new provider (#35)
Level: 2
Fiscal Year: FY06
DOE Area/Campaign: ASC
Completion Date: 9/30/06
ASC nWBS Subprogram: Computational Systems & Software Engineering
Participating Sites: SNL
Description: Projects and technologies in the advanced networking and interconnect areas shall include networking and interconnect architectures, emerging networking hardware technologies and communication protocols, network performance/security monitoring/analysis tools and high performance encryption and security technologies. a number of analyses reports on next-generation networking technologies for a petaflops computing environment. The ASC computing environment faces many challenges of performance and robustness at pioneering scales of compute nodes and raw network performance. The advanced networking project provides key foundational network and communication related technologies and services to enable the seamless integration of the many elements of a system such as file systems, archives systems, and ASC compute resources from the user's desktop to the most powerful capability platforms. Currently, the advanced networking project is composed of five main thrusts: 1) high-performance protocols and transport technologies to access network-attached storage in the local and wide areas; 2) the continued development of a robust, high performance network infrastructure from the system to the wide area that is capable of providing secure communications with well-understood service level characteristics for different traffic classes; 3) a security infrastructure to provide essential authentication and authorization services to the tri-lab community; 4) the development of open source networking and communication software to meet the most demanding performance requirements of the ASC program while leveraging the development investment of the entire HPC community; and 5) the development of algorithms and data analysis tools for monitoring the performance of ASC applications and services. The required extensions of technologies listed above will provide the foundation for the development and implementation of an environment that will support a petaflops computing environment. This effort will provide the systems level technology road maps in the areas of network architectures, network topologies, networking protocols, networking switches and routers and the monitoring strategies to successfully implement and operate the required HPC infrastructure. In addition, this effort will insure the conversion of the current WAN service to another provider during FY06.
Completion Criteria: The successful deployment and operation of a new provider for the current WAN and the delivery of technology roadmaps and the analysis reports of the infrastructure elements required to implement and support a Petaflops computing environment.
Customer: Capability platform systems developers and systems operations personnel.

Milestone Certification Method:

1. The test and operations reports for the acceptance of the new WAN service provider.

2. The delivery of professional documentation, such as reports and/or viewgraphs with a written summary as a record of milestone completion.

3. Conduct peer reviews (external if possible).

Supporting Resources: OPNET modeling and simulation tools and a number of compute cycles to develop and run the network models and simulations.

Codes/Simulation Tools Employed: N/A

Contribution to the ASC Program: The required networking technical knowledge and understanding to guide the development and deployment of the next generation environment to support the next generation platform.

Contribution to Stockpile Stewardship: This effort will enable the deployment of the next generation computing platform that supports the execution of more accurate and complete models and simulations of our systems.

No.	Risk Description	Risk Assessment (low, medium, high)		
		Consequence	Likelihood	Exposure
1	Industry development and deployment schedules may not align with the ASC platform schedule.	Medium	Medium	Medium
2	Required FTE's are not available	Low	Low	Medium

Milestone (ID#): Develop a high-level interprocessor communication network for petaflops computing (#36)
Level: 2
Fiscal Year: FY06
DOE Area/Campaign: ASC
Completion Date: 9/30/06
ASC nWBS Subprogram: Computational Systems & Software Engineering
Participating Sites: SNL
Description: The interconnection network between processors in a supercomputer is one of the fundamental building blocks in massively scalable systems. To deliver general purpose petaflops scale computing, the network will need to deliver 30 gigabytes per second (per direction), 500 ns MPI latency, and 15 million messages per second of throughput. A high-level network architecture will be developed to deliver this level of performance for deployment in petaflops scale computers. The architecture will address network issues from the connection to the primary processor to the network interface architecture to the end-to-end reliability issue to the router architecture and topology to connect the nodes. The effort will include preliminary simulation studies to validate architectural design choices.
Completion Criteria: A full specification of the high-level architecture including a specification of both the network interface and router that will be capable of delivering the performance needed for petaflops scale computing will be completed. The architecture specification will include functional diagrams illustrating the basic components required in both the network interface and router and their interconnection. The functional behavior of each block will be fully described along with the interaction between blocks.
Customer: ASC as a procurer of systems leveraging the network technology. The analyst community as a user of those systems. The HPC industry as builders of the systems using the technology.
Milestone Certification Method: 1 - A program review is conducted and its results are documented. 2 - Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion.
Supporting Resources: FTE Funding will be required to support the design effort. Compute cycles will be required for preliminary simulation studies of network features.
Codes/Simulation Tools Employed: Computer system and hardware simulation applications. ASC applications to provide input to drive network design choices.
Contribution to the ASC Program: The ASC program is responsible for providing scalable computing resources to solve the most challenging problems in the weapons program. Recent studies indicate the need for petaflops scale computing and this effort is the first step in delivering the interconnection network that will be needed to support it.

Contribution to Stockpile Stewardship: Stockpile Stewardship relies on scalable computing resources provided through ASC for weapons simulations in support of the Stockpile Stewardship mission. The scalability of these resources depends on high performance networking capabilities.				
No.	**Risk Description**	**Risk Assessment (low, medium, high)**		
		Consequence	**Likelihood**	**Exposure**
1	The MPI bandwidth, latency, and message throughput objectives may not be achievable given the limitations of technology in the timeframe where petaflops scale computing is expected. The risk has been mitigated by preliminary analysis that indicates technology can definitely approach these objectives.	Low	medium	medium

Milestone (ID#): Deploy Security Infrastructure for ASC Tri-Lab (#39)
Level: 2
Fiscal Year: FY06
DOE Area/Campaign: ASC
Completion Date: FY06-Q3
ASC nWBS Subprogram: Computational Systems and Software Engineering
Participating Sites: LANL, LLNL, SNL
Description: 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. The deployment of the tri-lab security infrastructure will require integration and cooperation between the Computational Systems and User Environment at LLNL, LANL, and SNL. Tri-lab personnel will also work closely with developers of inter-site application and Nuclear Weapons Complex plant sites to ensure successful adoption of the new security infrastructure. Further, close interaction with ICSI is essential to ensure the ICSI ESN directory service can be utilized for inter-site authorization.
LANL Work Scope: **LLNL Work Scope**: **SNL Work Scope**:
LANL Completion Criteria: **LLNL and SNL Completion Criteria:** Demonstrate that SNL, LLNL, and LANL users can successfully authenticate and access major ASC classified production resources at LANL, LLNL and SNL using the account managed by the new Kerberos authentication service. Demonstrate that SNL, LLNL, and LANL users can successfully authenticate and access major ASC classified production resources using credentials associated with their account managed by the Kerberos authentication service at their respective sites. Demonstrate that SNL users can successfully authenticate and access a generally available web-based SNL inter-site application, where usage customization or an authorization decision involves the application accessing the ICSI directory for user attributes.
Customer: All users of SNL, LLNL, and LANL computer systems.
Milestone Certification Method: 2 – Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion. 3 – The "handoff" of the developed capability (product) to a nuclear weapons stockpile customer is documented.
Supporting Resources: Multiple projects from both the Computational Systems and Software Environment subprogram and the Facility Operations and User Support subprogram.

Codes/Simulation Tools Employed: N/A				
Contribution to the ASC Program: Update to the mandated security infrastructure software for all systems. Supports single system authentication to computational resources across the tri-lab complex.				
Contribution to Stockpile Stewardship: Update to the mandated security infrastructure software for all systems. Supports single system authentication to computational resources across the tri-lab complex.				
No.	**Risk Description**	**Risk Assessment (low, medium, high)**		
		Consequence	**Likelihood**	**Exposure**
1	ICSI fails to deliver functional directory service	Low	Low	low

Milestone (ID#): Deploy Purple Tri-Lab User Environment (#42)
Level: 2
Fiscal Year: FY06
DOE Area/Campaign: ASC
Completion Date: FY06-Q4
ASC nWBS Subprogram: Computational Systems and Software Environment
Participating Sites: LANL, LLNL, SNL
Description: Demonstrate a user environment that provides application development and execution, data analysis and visualization, and distance computing in accordance with ASC Purple and application requirements as defined in the Purple Usage Model. The CSSE, and FOUS ASC subprograms will build on the limited environment deployed in Q3 to deliver both a local and distance-computing environment for a tri-lab limited user base. Deploy initial Purple production environment needed by SNL and LANL application codes targeted to run on Purple. This milestone will be done in conjunction with the LLNL Purple Limited Availability milestone, extending appropriate access and software to meet the needs of remote users from SNL and LANL. This will include limited 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 SNL and LANL. This milestone is complete when the required SNL and LANL application code services are deployed in a limited availability mode and the targeted SNL and LANL application codes have successfully run in production mode on Purple.
LANL Work Scope: **LLNL Work Scope**: **SNL Work Scope**:
LANL Completion Criteria: Designers accept environment: the designers in X-Division will be the users of the codes on Purple, hence they will need to be able to say if the environment is acceptable for their use. Successful completion of capability calculation on Purple using Code Project A code products. "Successful" here means that the results agree with those previously obtained on existing platforms, and are approved by the relevant designers and V&V people. Successful completion of capability calculation on Purple using Code Project B code products. "Successful" here means that the results agree with those previously obtained on existing platforms, and are approved by the relevant designers and V&V people. A documented level of use of Purple by the LANL design community for the type of work intended for Purple. **LLNL Completion Criteria:** 1) Purple Usage Model documented; 2) Mapping of ACE requirements to Purple Environment documented and demonstrated; 3) Web documentation, including usage policies complete and available remotely; 4) (draft) something about a LLNL code capability run; 5) demonstrate full functionality of Ensight and VisIt visualization tools on Purple; 6) demonstrate file transport between Purple GPFS system and remote site file systems and archives at rates that meet or exceed those available on ASC White 7) demonstrate the build environment for the principle ASC codes from LLNL 1.5.1.1 Modern Multi-physics Codes. **SNL Completion Criteria:** The following objective success criteria have been defined for

the milestone: ensure SNL access to Purple (accounts, passwords, authentication); ensure SNL access to tools and documentation for management of the work environment (user group management, recommended environment variables); data transfer (Purple–SNL network architecture, tools for transferring files); assist SNL application library developers in making effective use of the file systems and I/O libraries on Purple; assist with I/O performance tuning of SNL tools and libraries (SEACAS, SIERRA, SAF); assist SNL application code developers, as needed, in making effective use of third-party libraries and utilities, debugging and correctness testing, performance measurement, analysis, and tuning on Purple; and assist SNL analysts, as needed, in processing simulation output (data analysis and visualization) using Purple.

Customer: Tri-lab stockpile stewardship scientists and engineers. Stakeholders include NNSA/HQ, ASC managers at SNL, and stockpile stewardship scientists and engineers.

Milestone Certification Method:

1 - A program review is conducted and its results are documented

2 – Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion.

3 – The "handoff" of the developed capability (product) to a nuclear weapons stockpile customer is documented.

Supporting Resources: Multiple projects from both the CSSE subprogram and the Facility Operations, and User Support subprogram.

Codes/Simulation Tools Employed: N/A

Contribution to the ASC Program: The results of this milestone will assure that the Purple system can be accessed and used by ASC customers from LANL and SNL, as well as LLNL. Purple provides the tri-lab computational system for development of the full system simulations. It also represents a major deliverable defined at the beginning of the ASC program and has external visibility.

Contribution to Stockpile Stewardship: The results of this milestone will assure that the Purple system can be accessed and used by DSW customers from LANL and SNL, as well as LLNL. The Purple system will provide the major source of tri-lab capability computing for the large simulations needed by DSW for LEP and SFI calculations. Purple will also be a source for capacity computing until adequate alternative capacity computing resources can be deployed.

No.	Risk Description	Risk Assessment (low, medium, high)		
		Consequence	Likelihood	Exposure
1	User environment software doesn't meet application requirements	Low	Low	Low
2	Tri-lab classified network access and security infrastructure not reliable for remote use	Low	Low	Low
3	Resources for this milestone, from the Computational Systems and Software Environment subprogram, will also be working on taking Red Storm from Limited to General Availability.	Medium	Medium	Medium

Milestone Descriptions for Preliminary FY07

Milestone (ID#): Develop strategies for deploying and operating a petaflops-class compute resource (LL-CSSE-07-01)
Level: 2
Fiscal Year: FY07
DOE Area/Campaign: ASC
Completion Date: FY07-Q1
ASC nWBS Subprogram: Computational Systems and Software Environment
Description: Petaflops computing will require a robust software and hardware environment that does not exist today. We will develop the requirements for such software and hardware using our experience with using the BlueGene/L system. Performance and reliability at the scale for such high-end computing will be our key goals for this environment. From these requirements we will develop strategies for each major component of the environment.

Milestone (ID#): Deploy the Purple system for General Availability (LL-CSSE-07-02)
Level: 2
Fiscal Year: FY07
DOE Area/Campaign: ASC
Completion Date: FY07-Q2
ASC nWBS Subprogram: Facility Operations and User Support
Description: When Purple is placed in the limited availability status it will be made available to a large, but controlled, set of users and have a functional hardware and software user environment. However functionality will be missing. We will complete the environment by deploying the missing capabilities. We will upgrade the data analysis servers, and provide sufficient archival bandwidth and capacity. We will complete the system software and the software development environment and ensure that it is stable and reliable. User documentation will be complete and accurate and training modules made available. A system for ensuring program directed scheduling will have been put into operation.

Milestone (ID#): Models and data supporting RRW
Level: 2
Fiscal Year: FY07

Milestone (ID#): Plutonium material/EOS theory and modeling advances
Level: 2
Fiscal Year: FY07

Milestone (ID#): Boost predictive theory advances
Level: 2
Fiscal Year: FY07

Milestone (ID#): Models and data supporting RRW
Level: 2
Fiscal Year: FY07

Milestone (ID#): Plutonium material/EOS theory and modeling advances
Level: 2
Fiscal Year: FY07

Milestone (ID#): Boost predictive theory advances
Level: 2
Fiscal Year: FY07

Milestone (ID#): Deliver techniques and methodologies developed under DVS to support verification and validation. (SNL-CSSE-07-01)
Level: 2
Fiscal Year: FY07
DOE Area/Campaign: ASC
Completion Date: 9/30/07
ASC nWBS Subprogram: Computational Systems & Software Engineering
Description: As V&V gains importance throughout the ASC program, an increasing emphasis is being placed on the development and delivery of data and visualization tools that support the needs of V&V. We will test prototypes and evaluate approaches in the FY06 time frame, with the intent of targeting delivery of selected techniques and methodologies in FY07. We are expecting to partner with V&V and/or key application milestones that are linked to V&V deliverables.

VI. ASC Integration

In the tables below, ASC program management has described how the subprograms contribute to a milestone or another deliverable of any of the subprograms, products, or external programs for a given subprogram. Included in the descriptions is whether or not a delay would impact a planned deliverable or subprogram, product, or external program. If the table cell is blank, the product does not affect any deliverables.

Table VI-1. All Subprograms as Related to Integrated Codes

	Integrated Codes (Modern, Multi Physics Codes; Legacy Codes; Engineering Codes; Focused Research, Innovation, and Collaboration; and Emerging and Specialized Codes)
Integrated Codes	
LLNL	MMPC acts as the vehicle, which integrates the work from many other products to provide the complexes weapons physics simulation tools. Legacy Codes act a touchstone with the past and serve as a first check for the ability of MMPC to simulate UGTs. FRIC provides libraries (especially solvers) and other algorithms that are used by MMPC and Emerging and Specialized Codes. Emerging and Specialized Codes provide MMPC with nascent codes as they reach a sufficient level of maturity.
LANL	Theory and experiment developed in the Science Campaigns come together the MMPC, which provide DSW with the simulation tools required for weapons certification, assessment, surety, SFI resolution, and design feasibility. Legacy codes are historical UGT calibration tools that provide a benchmark for the MMPC, with that benchmark being a rudimentary predictive simulation capability with uncertainties greater than those deemed acceptable by the MMPC. FIRC Provides for higher-risk, exploratory research (Weapons-Supported Research) necessary to pursue high-payoff numerical algorithm innovations. Deliverables include more robust and accurate algorithms for MMPC in the area of shock physics, transport, linear and nonlinear solvers, and coupled multi-physics. Provides an analysis tool for the design of casting/welding operations in the nuclear weapons complex, setup tools for providing mesh geometry and initial and boundary condition information for the MMPC, and energy diagnostic tools for post-processing the MMPC output in weapons effects studies. The casting simulation tool contributes reusable software components (solvers, parallel communication, etc.) for all of IC Products.

	Integrated Codes (Modern, Multi Physics Codes; Legacy Codes; Engineering Codes; Focused Research, Innovation, and Collaboration; and Emerging and Specialized Codes)
SNL	FRIC Provides the libraries and frameworks, including solvers, optimization other algorithms that are used by integrated codes at SNL, particularly engineering codes.
Physics and Engineering Models	
LLNL	Improved models of physical behavior—including, strength, equation of state, nuclear reactions, opacity, high explosive performance, and advanced hydrodynamic behavior—are delivered for use in the modern multi-physics codes, leading towards the goal of improved predictive capability using science based models. Contributes to FY06 L1 and L2 IC milestones, and a proposed FY07 L2 milestone. Delays in this product impact the progress in improving the predictive capability of the integrated codes. Model Implementation facilitates the delivery of an effective capability within the modern multi-physics codes, moving forward with improved predictivity. New model implementations are achieved through close collaboration between the integrated code developers and the developers of the new physics models. In some cases the ASC integrated codes are utilized as the development test-bed for new models. Contributes to FY06 L1 and L2 IC milestones, and a proposed FY07 L2 milestone. Delays in this product impact the progress in improving the predictive capability of the integrated codes. This activity provides new material and physics models for integration in the MMPC and possibly ESC and legacy codes. Fundamental Physics Codes and Application delivers codes that provide opacity data that is directly inserted into integrated code simulations. Contributes to FY06 and FY07 L2 IC milestones. Delays in this product impact the progress in improving the predictive capability of the integrated codes through accuracy of simulations and increased uncertainties. Material Data Libraries delivers updated libraries of properties of programmatic materials for various physics packages, including equation of state, opacity, and nuclear reactions, to the integrated codes. Library maintainers work closely with the integrated code developers to insure effective data access through the library APIs. Contributes to FY06 L1 and L2 IC milestones. Delays in this product impact the accuracy of simulated predictions, increasing uncertainty, and delaying DSW applications. This activity provides new material data libraries for integration in the MMPC and possibly ESC and legacy codes.
LANL	Theoretical Models and Experimental Integration Provides for development of fundamental, first-principles theory in area of nuclear and atomic physics, equations of state, high explosives, materials response and damage, turbulence and mix, thermonuclear burn, and engineering analysis. Also provides for higher-risk, exploratory research (Weapons-Supported Research) necessary to pursue high-payoff weapons physics innovations. These theoretical developments drive the improved models instantiated in the Model Implementation Products that are delivered into the MMPC. Implements (in software libraries) new and improved models developed in the Theoretical Models and Experimental Integration Product for the MMPC and legacy codes in area of materials response and damage, equations of state, turbulence and mix, thermonuclear burn, and engineering analysis. Fundamental Physics Codes and Application Develops, maintains, evolves, and applies codes whose algorithms represent high-fidelity solutions to fundamental,

	Integrated Codes (Modern, Multi Physics Codes; Legacy Codes; Engineering Codes; Focused Research, Innovation, and Collaboration; and Emerging and Specialized Codes)
	first-principles formulations for nuclear and atomic physics, equations of state, materials response, high explosives, turbulence and mix, and thermonuclear burn. These codes are the vehicle by which new, postulated theories developed in the Theoretical Models and Experimental Integration Product are verified and validated. Successfully validated theories are delivered as new models and materials libraries to the MMPC. Material Data Libraries Integrates and tests software libraries and databases into the IC Sub-Program (primarily the MMPC product) that instantiate nuclear and atomic physics data, equations of state, and high explosive and foam materials response.
SNL	Model implementation provides science-based sub-grid and constitutive models for the ASC Engineering Codes. This activity requires tight integration between project leads and code PIs.
Verification and Validation	
LLNL	Establishes the validity of the models and code functionality required to assess Performance. May confirm the adequacy, or otherwise, of developments in the MMPC, ESC or Legacy codes and hence may provide new requirements. V&V Methods supports all aspects of software quality assurance for the Integrated Codes as well as the development of mathematical methods for assessing Uncertainty Quantification of the outputs of the Integrated Codes. Specialized V&V Assessments are used to make targeted assessment of code performance against specific stockpile weapons systems or families of systems. Data Validation and Archiving is used to support the variety of databases that the Integrated Codes access to perform their function. This activity may provide improved experimental data with which to aid the validation of models in MMPC, ESC or legacy codes.
LANL	Develops fundamental V&V and QMU methodologies and test suites to be used in periodic formal and quantitative assessments of codes primarily released in the MMPC Product area. The test suites are archived, assessments are documented, and methodologies are delivered as standard tools. Also supports software quality assurance activities for all codes developed in the IC Sub-Program. Develops and conducts, for performance codes in the MMPC Product area, test suites, sensitivity analyses, uncertainty quantification, single- and multi-effects physics validation, and verification studies. These assessments, which are conducted and documented regularly, are part of an evolutionary delivery life cycle in which primary performance simulation requirements are progressively elaborated. Develops and conducts, for selected SNL and LLNL engineering codes delivered in the IC Sub-Program, test suites, sensitivity analyses, uncertainty quantification, single- and multi-effects physics validation, and verification studies. These assessments, which are conducted and documented regularly, are part of an evolutionary delivery life cycle in which engineering simulation requirements are progressively elaborated. Performs focused V&V assessments of specific physics or combinations of physics of interest to the IC Sub-Program, such as astrophysical applications (for radiation hydrodynamics) and output diagnostics (for transport). Establish requirements and deliver the software and hardware infrastructure for maintaining

	Integrated Codes (Modern, Multi Physics Codes; Legacy Codes; Engineering Codes; Focused Research, Innovation, and Collaboration; and Emerging and Specialized Codes)
	archival databases needed to support V&V assessments of codes in the IC Sub-Program. These databases include (but are not limited to) data generated in small-scale and integral experiments as well as UGT events.
SNL	The Engineering Codes and Legacy Code CTH rely on verification methodologies developed in the V&V Methods product to execute software quality practices. Methodologies for verification, validation, UQ and Sensitivity analyses are used extensively through V&V applications and all L1 and L2 milestones to which the V&V program contributes. Directly supports L1 milestones and supporting L2 milestones; Directly supports Alegra-HEDP Z-Pinch milestone.
Computational Systems and Software Environment	
LLNL	Contributes the required computational resources to enable the development, test, and usage of the 3D and full systems physics for the large codes. A delay in delivery of capability systems impacts the resources available to the entire tri-lab program, making it more difficult to provide the Integrated code capabilities. Contributes the required computational resources for code development and production parameter studies using the products of the Integrated Codes. Delay or inadequate capacity system resources slow down the progress of this area. Contributes to the resources needed for research in preparing for future petascale calculations needed by the program in about 2010. Contributes the software environment needed to operate the computational resources for the development, test, and production usage of the new codes. A delay in delivery of system software and tools impacts the resources available to the entire tri-lab program, making it more difficult to use the computational resources effectively. User productivity and time-to-solution is impacted. Contributes the files systems and storage systems needed to operate the computational resources for the development, test, and production usage of the codes. A disruption or delay in delivery of these systems may make the computational resources needed by Integrated codes unusable. A disruption or delay of the networking developments may impact the remote usage of the capability systems by the Integrated Code efforts at the other laboratories. The Post Processing product contributes to the understanding of the results of the Integrated Codes. For the large codes on the large systems, the volume of data produced is frequently too great to make judgment about the quality of the result without visual processing of the results. Delay in deliverables from this product impacts productivity of the Integrated Code efforts.
LANL	Ensures the hardware and software maintenance, reliability, availability, and security of LANL capability platforms (currently the Q platform) for reliable execution of MMPC codes during the simulation of high-fidelity, 3D, full physics scenarios. Procures, integrates, and maintains the capacity computing resources required for development of codes in the IC Sub-Program and their end use application for DSW, certification, assessment, and SFI resolution. Perform R&D work with selected computer vendors in the design and demonstration of next-generation (>3-5 years away) computing platforms whose characteristics are tuned for more efficient execution performance of codes in the MMPC Product area.

	Integrated Codes (Modern, Multi Physics Codes; Legacy Codes; Engineering Codes; Focused Research, Innovation, and Collaboration; and Emerging and Specialized Codes)
	Provide a reliable and resilient system software environment for codes in the IC Sub-Program by focusing on Linux software stack extensions (Science Appliance), efficient and portable MPI, useful IDEs (Eclipse environment), code coverage tools (Alexandria), process migration, scalable run-time, and network device failover. Understand, predict, and improve performance of IC codes on these computer systems through performance modeling and analysis. Provide, support, and evolve the hardware and software necessary to meet the run-time and archival output requirements for codes in the IC Sub-Program.
SNL	Robust operating systems are required for Engineering Codes and Legacy Codes to run reliably on capability platforms. Robust operating systems are required for Engineering Codes and Legacy Codes to run reliably on capacity platforms. Sufficient computing capacity is required to meet the user demand for simulations with Engineering Codes and Legacy Codes. Provides the computing systems focused on the mid-range capability gap (workloads in the range of approximately 500-4,000 processors). Supports both production computing workload and application/algorithm development resources. May also provide resources for jobs below 500 processors. Robust operating systems that run predictably on various platforms are required for V&V assessments and applications requiring capacity computing. Sufficient user capacity required to meet needs of V&V and applications, especially those requiring QMU. Provides the system software for both Capability and Capacity Systems the will be used by Integrated Codes workload. This Product also provides the code development tools to support both Application and Algorithm development. Provides and supports critical infrastructure required for code development and production simulations. In FY06, this product is completing the production deployment of file systems, storage and networking for the Red Storm general availability computing environment; developing the next generation security infrastructure in support of tri-lab computing; and laying the groundwork in the form of a roadmap to deliver petaflops computing. SNL: Fast creation of meshes and input files for Engineering Codes and Legacy Codes are required for efficient and effective simulations with these codes. Visualization capabilities on both the desktop and other platforms are needed to interpret results from Engineering Codes and Legacy Codes.
Facility Operations and User Support	
LLNL	This product is required for all production operation of the computational resources needed by this subprogram, including tri-lab system access. Contributes the user support needed to access and operate the computational resources for the development, test, and production usage of the integrated codes. A disruption or delay in delivery of user support impacts the resources available to the entire tri-lab program, making it more difficult to use the computational resources effectively. User productivity and time-to-solution is impacted.

	Integrated Codes (Modern, Multi Physics Codes; Legacy Codes; Engineering Codes; Focused Research, Innovation, and Collaboration; and Emerging and Specialized Codes)
LANL	Deliver systems and network operations and maintenance and facilities maintenance and upgrades for all capacity and capability computing platforms used by codes in the IC Sub-Program. Provide on-call experts for timely consultation with end users and developers of codes in the IC Sub-Program experiencing software and hardware problems on all computing platforms.

Table VI-2. All Subprograms as Related to Physics and Engineering Models

	Physics and Engineering Models (Theoretical Models and Experimental Integration; Model Implementation; Fundamental Physics Codes and Application; Material Data Libraries)
Integrated Codes	
LLNL	Supplies requirements and feedback to PEM regarding Material Data Libraries and models.
LANL	Supply requirements and feedback to the PEM Sub-Program through (integral, regression, unit) testing and end use on the accuracy and robustness of delivered and integrated material data libraries and models for material response, turbulence, burn, and high explosive behavior. Supply requirements and feedback to the PEM Sub-Program through (integral, regression, unit) testing on the impacts of new material data libraries and models for material response, turbulence, burn, and high explosive behavior to algorithm changes in the areas of hydro, transport, solvers, and multi-physics coupling.
SNL	In some case changes to the codes may be required to handle advanced constitutive models or sub-grid models. The PEM staff and management work with PIs from Engineering codes.
Physics and Engineering Models	
LLNL	This product provides sub-continuum scale simulations, which are used in the development of new theoretical models as well as in producing parameterizations of physical properties used to populate material data libraries.

	Physics and Engineering Models (Theoretical Models and Experimental Integration; Model Implementation; Fundamental Physics Codes and Application; Material Data Libraries)
LANL	Provides for development of fundamental, first-principles theory in area of nuclear and atomic physics, equations of state, high explosives, materials response and damage, turbulence and mix, thermonuclear burn, and engineering analysis. Also provides for higher-risk, exploratory research (Weapons-Supported Research) necessary to pursue high-payoff weapons physics innovations. These theoretical developments drive the improved models instantiated in the Model Implementation Products. Implements (in software libraries) new and improved models developed in the Theoretical Models and Experimental Integration Product in area of materials response and damage, equations of state, turbulence and mix, thermonuclear burn, and engineering analysis. Develops, maintains, evolves, and applies codes whose algorithms represent high-fidelity solutions to fundamental, first-principles formulations for nuclear and atomic physics, equations of state, materials response, high explosives, turbulence and mix, and thermonuclear burn. These codes are the vehicle by which new, postulated theories developed in the Theoretical Models and Experimental Integration Product are verified and validated.
SNL	Contributes to the model implementation product. Gives theoretical underpinnings for sub-grid and constitutive models. Works with Model Implementation PIs. Model implementation is dependent on successful theoretical activities under the above product. These products are tightly integrated.
Verification and Validation	
LANL	Develops fundamental V&V and QMU methodologies and undertakes software quality assurance activities that are used in the assessment of material data libraries and models delivered for use in codes in the IC Sub-Program. Scrutinizes the material data libraries and models delivered by PEM to performance codes by conducting sensitivity analyses, uncertainty quantification, single- and multi-effects physics validation, and verification studies. Scrutinizes material (nuclear and atomic) data libraries delivered by PEM to astrophysical applications (for radiation hydrodynamics) and output diagnostics (for transport). Establish and maintain experimental databases needed to validate new models and material data libraries developed by PEM.
SNL	Verification and validation of sub-grid and constitutive models is reliant on V&V methods and engineering assessments to provide validated models.

	Physics and Engineering Models (Theoretical Models and Experimental Integration; Model Implementation; Fundamental Physics Codes and Application; Material Data Libraries)
Computational Systems and Software Environment	
LLNL	A delay in delivery of capability systems impacts the total resources available to the entire tri-lab program, limiting resources available to the Physics and Engineering model development. Contributes the required computational resources for code development and production parameter studies using the products of the Physics and Engineering models. Delay or inadequate capacity system resources slows down the progress of this area. The BlueGene/L system will be directly used for materials aging studies. Contributes the software environment needed to operate the computational resources for the development, test, and production usage of the new models and codes – especially for the BlueGene/L environment. A delay in delivery of system software and tools support makes it more difficult to use the computational resources effectively. User productivity and time-to-solution is impacted. Contributes the files systems and storage systems needed to operate the computational resources for all code use. A disruption or delay in delivery of these systems may make the computational resources unusable. The function of the parallel files systems will be especially important for the effective use of BlueGene/L for material studies. The Pre- and Post-Processing product contributes to an understanding of the Physics and Engineering Models. For highly scaled physics and materials codes on BlueGene/L, the volume of data produced coupled with unique architecture of BlueGene/L requires next-generation data visualization and analysis tools and servers. Delay in tool and server deployment from this product will have a large impact on the productivity and understanding of the Physics and Engineering Models efforts.
LANL	Ensures the hardware and software maintenance, reliability, availability, and security of LANL capability platforms (currently the Q platform) with which to scrutinize the effects of PEM material data libraries and models on predictive simulation of UGTs and full system scenarios. Procures, integrates, and maintains the capacity computing resources required for development and testing of PEM material data libraries and models and their integration into codes in the IC Sub-Program. Perform R&D work with selected computer vendors in the design and demonstration of next-generation (>3-5 years away) computing platforms that are cognizant of the memory bandwidth requirements imposed by the material data libraries and models supplied by PEM. Provide a reliable and resilient system software environment for material library and model development in the PEM Sub-Program by focusing on Linux software stack extensions (Science Appliance), efficient and portable MPI, useful IDEs (Eclipse environment), coverage tools (Alexandria), process migration, scalable run-time, and network device failover. Provide, support, and evolve the hardware and software necessary to meet the run-time and archival output requirements for material data libraries and models implemented in the PEM Sub-Program.

	Physics and Engineering Models (Theoretical Models and Experimental Integration; Model Implementation; Fundamental Physics Codes and Application; Material Data Libraries)
SNL	Provides the computing systems that are focused on the Mid-range Capability Gap, such as, workloads in the range of approximately 500-4,000 processors. Supports both production computing workload and Application and Algorithm development resources. May be well suited for extended job duration workloads.
Facility Operations and User Support	
LLNL	This product is required for all production operation of the computational resources needed by this subprogram, including tri-lab system access. Contributes the user support needed to access and operate the computational resources for the development, test, and production usage of the codes and applications. A disruption or delay in delivery of user support impacts the resources available to the entire tri-lab program, making it more difficult to use the computational resources effectively. User productivity and time-to-solution is impacted.
LANL	Deliver systems and network operations and maintenance and facilities maintenance and upgrades for all capacity and capability computing platforms used by the PEM Sub-Program. Provide on-call experts for timely consultation with developers and integrators of models and material data libraries in the PEM Sub-Program experiencing software and hardware problems on all computing platforms.

Table VI-3. All Subprograms as Related to Verification and Validation

	Verification and Validation (V&V Methods, Primary V&V Assessments, Secondary V&V Assessments, Engineering V&V Assessments, Specialized V&V Assessments, Data Validation and Archiving, University Partnerships)
Integrated Codes	
LLNL	MMPC provides the code capabilities for V&V assessments.
LANL	Provides the codes used in primary and secondary V&V assessments, acts on corrective actions resulting from those assessments, and improves software quality as guided by activities and training in the V&V Sub-Program. Improves software quality as guided by activities and training in the V&V Sub-Program. Uses findings in primary and secondary

	Verification and Validation (V&V Methods, Primary V&V Assessments, Secondary V&V Assessments, Engineering V&V Assessments, Specialized V&V Assessments, Data Validation and Archiving, University Partnerships)
	and V&V assessments to provides more robust and accurate (shock physics, transport, linear and nonlinear solvers, and coupled multi-physics) algorithms. Improves software quality as guided by activities and training in the V&V Sub-Program. Improves software quality as guided by activities and training in the V&V Sub-Program and acts on corrective actions identified in V&V assessments.
SNL	The Engineering Codes CALORE, FUEGO, SALINAS and DAKOTA will be used in executing the FY06 tri-lab level 1 V&V milestone. Normal user support is expected to be required, but additional support will be supplied if required. The code Alegra-HEDP will support a L2 V&V milestone. V&V and QMU applications require that codes are ready for stockpile computing such as, there is adequate SQE, regression testing, code verification, and acceptance tests. Provides the optimization framework and algorithms that are used by the verification and validation products at SNL. Provides the framework that is used by SNL, LLNL and LANL verification and validation products. The V&V program and QMU studies will rely on capabilities afforded by Dakota to perform UQ studies, sensitivity studies, and optimization studies.
Physics and Engineering Models	
LLNL	Provides guidance on experiments necessary for verifying new physics and engineering models. Provides the most up to date material property libraries for use in the integrated codes for doing the various V&V system assessments. Provides the best available physics models within the integrated codes for doing the various V&V system assessments.
LANL	Communicates verification and validation requirements imposed by new and improved theoretical models and works with V&V assessment teams in developing metrics, test suites, etc. Ensures that the latest software libraries embodying new and improved models in area of materials response and damage, equations of state, turbulence and mix, thermonuclear burn, and engineering analysis are available to V&V assessment teams. Ensures that the latest software libraries and databases embodying nuclear and atomic physics data, equations of state, and high explosive and foam materials response are available to V&V assessment teams. Improves software quality in fundamental codes as guided by activities and training in the V&V Sub-Program. Communicates validation requirements imposed by the theoretical models embodied in these codes to V&V assessment teams.
SNL	Models from PEM will be required for L1 milestone and support L2 milestones. Models from PEM are required for other V&V assessments. PEM models must be verified and validated in a manner consistent with the requirements of the V&V program and applications that require QMU assessments. V&V program requires a consistency and pedigree of material data and its usage.

	Verification and Validation (V&V Methods, Primary V&V Assessments, Secondary V&V Assessments, Engineering V&V Assessments, Specialized V&V Assessments, Data Validation and Archiving, University Partnerships)
Verification and Validation	
LLNL	Develops fundamental V&V and QMU methodologies and test suites to be used in periodic formal and quantitative code assessments by the primary, secondary, and engineering assessment teams. The test suites are archived, assessments are documented, and methodologies are delivered as standard tools.
LANL	Conducts code V&V assessments that utilize the methodologies and tools devised by the V&V Methods Product area. Work with other assessment teams in evolving the assessment rigor, formality, and corrective action feedback. Support V&V assessments by delivering the software and hardware infrastructure necessary for maintaining archival databases of data generated in small-scale and integral experiments as well as UGT events.
SNL	Methodologies for verification, validation, UQ and Sensitivity analyses are used extensively through V&V applications and all L1 and L2 milestones to which the V&V program contributes. Directly supports L1 milestones and supporting L2 milestones; Directly supports Alegra-HEDP Z-Pinch milestone.
Computational Systems and Software Environment	
LLNL	Contributes the required computational resources to enable the test, and usage of the 3D and full systems physics for the large codes. A delay in delivery of capability systems impacts the resources available to the entire tri-lab program, making it more difficult to perform the V&V testing of the Integrated code capabilities. Contributes the required computational resources for production parameter studies needed for V&V. Delay or inadequate capacity system resources slows down the progress of this area. Research and experience in advanced systems will contribute to preparation for future petascale calculations needed for future stockpile calculations. Contributes the software environment needed to operate the computational resources for the production V&V testing. If the environment isn't robust, it is more difficult to use the computational resources effectively and user productivity / time-to-solution is impacted. Contributes the files systems and storage systems needed to operate the computational resources for all production use. V&V activities also rely on access to older archived results. The Pre- and Post-Processing product helps support new computational paradigms and increased program emphasis of V&V activities. The large number of runs (100s to 1000s) and vast amount of (possibly geographically distributed) data requires new ways to manage and analyze large data. Delay in this product's deployment will have a large impact on the ability of V&V to analyze and post-process results in a timely way.
LANL	Ensures the hardware and software maintenance, reliability, availability, and security of LANL capability platforms (currently the Q platform) with which to conduct V&V assessments of predictive simulation of UGTs and full system scenarios. Procures, integrates, and maintains the capacity computing resources required for development of V&V

	Verification and Validation (V&V Methods, Primary V&V Assessments, Secondary V&V Assessments, Engineering V&V Assessments, Specialized V&V Assessments, Data Validation and Archiving, University Partnerships)
	Methods products and conducting the primary, secondary, and engineering V&V code assessments. Performs R&D work with selected computer vendors in the design and demonstration of next-generation (>3-5 years away) computing platforms that are cognizant of the computational loads imposed by rigorous V&V assessments, and UQ/sensitivity studies. Provides a reliable and resilient system software environment for code assessments in the V&V Sub-Program by focusing on Linux software stack extensions (Science Appliance), efficient and portable MPI, useful IDEs (Eclipse environment), coverage tools (Alexandria), process migration, scalable run-time, and network device failover. Provide, support, and evolve the hardware and software necessary to meet the run-time and archival output requirements for V&V assessments in the V&V Sub-Program. Provide for current and next generation production visualization needs of V&V assessments in the V&V Sub-Program. Associated activities include visualization hardware and user support of existing systems, next generation visualization R&D, expert visualization, legacy visualization tool support, and quantitative data analysis
SNL	Provides the computing systems that are focused on the Mid-range Capability Gap, such as, workloads in the range of approximately 500-4,000 processors. Supports both production computing workload and V&V and QMU Algorithm development resources. May be especially useful for parameter studies and QMU assessments. Provides the system software for both Capability and Capacity Systems the will be used by V&V and QMU workload.
Facility Operations and User Support	
LLNL	This product is required for all production operation of the computational resources needed by this subprogram, including tri-lab system access. Contributes the user support needed to access and operate the computational resources for data validation and archiving, and University partnerships. A disruption or delay in delivery of user support impacts the resources available to the entire tri-lab program, making it more difficult to use the computational resources effectively. User productivity and time-to-solution is impacted.
LANL	Deliver systems and network operations and maintenance and facilities maintenance and upgrades for all capacity and capability computing platforms used by the V&V Sub-Program. Provide on-call experts for timely consultation with V&V assessment teams in the V&V Sub-Program experiencing software and hardware problems on all computing platforms.
SNL	The V&V program has strong collaborations with the University of Utah in fire modeling and V&V of fire modeling codes; The V&V program has a collaboration with Stanford on turbulent fluid dynamics.

Table VI-4. All Subprograms as Related to Computational Systems and Software Environment

	Computational Systems and Software Environment (Capability Systems; Capacity Systems; Advanced Systems, System Software and Tools; I/O, Storage Systems; and Networking; Pre- and Post-Processing Environments)
Integrated Codes	
LLNL	Supplies requirements and feedback to CSSE to improve systems and environments deployed for ASC.
LANL	Supplies requirements and feedback to the CSSE Sub-Program on capability, capacity, and advanced systems hardware, software, and environments through code team development, alpha use, and testing activities. Work with the CSSE code optimization and performance modeling efforts in identifying and improving code execution performance.
SNL	There are requirements for the Engineering Codes to be running on ASC capability and capacity platforms. Provides the fundamental research in algorithms, advanced architectures, performance modeling, I/O and pre and post processing.
Physics and Engineering Models	
LLNL	Works closely with the staging teams for new capability and capacity systems; frequently the science codes are the early adopters of new systems and are used during the testing period to provide a thorough shake-out of new machines. Contributes to certifying that new systems are ready for general availability.
LANL	Supply requirements and feedback to the CSSE Sub-Program on capability and capacity systems hardware, software, and environments used to support theoretical model development, in implementing models into codes in the IC Sub-Program, in developing and applying fundamental physics codes, and in developing software libraries and databases that instantiate nuclear and atomic physics data, equations of state, and high explosive and foam materials response Work with the CSSE code optimization effort in identifying and improving execution performance.
Verification and Validation	
LLNL	This product contributes requirements and feedback to the CSSE subprogram.
LANL	Supply requirements and feedback to the CSSE Sub-Program on capability and capacity systems hardware, software, and environments used to develop tools in the V&V methods, code assessment, and data archiving activities.
Computational Systems and Software Environment	
LLNL	A delay in the deployment of the Purple system and BlueGene/L will result in a direct delay of other milestones in this subprogram. The capacity systems supplied by this product will be the development target of other products in this

	Computational Systems and Software Environment (Capability Systems; Capacity Systems; Advanced Systems, System Software and Tools; I/O, Storage Systems; and Networking; Pre- and Post-Processing Environments)
	subprogram. If the software environment is not deployed in a timely fashion, or is not robust – other milestones and efforts in this subprogram are directly impacted and delayed; likewise if the file systems are not operational and robust – other milestones and efforts in this subprogram are directly impacted and delayed. The Pre- and Post-Processing product delivers both hardware and software for the Computational Systems and Software Environment. Delays in researching, developing, integrating and deploying new data analysis and visualization tools will impact the ability of this subprogram to meet its overall goals and milestones.
LANL	Leverage, where possible, any hardware and software maintenance, reliability, availability, and security activity in support of LANL capability platforms (currently the Q platform) to similar capacity platform activities. Share computing facility requirements with other (capacity, advanced) systems. Comply with requirements and resources needed for software development activities in the CSSE Sub-Program. Transfer any mature technologies developed as a result of R&D work with selected computer vendors in the design and demonstration of next-generation (>3-5 years away) computing platforms to appropriate production efforts in the CSSE Sub-Program. Provide a reliable and resilient capability and capacity system software environment by focusing on Linux software stack extensions (Science Appliance), efficient and portable MPI, useful IDEs (Eclipse environment), code coverage tools (Alexandria), process migration, scalable run-time, and network device failover. Communicate problems, requirements, and corrective actions to other Product areas in CSSE. Provide, support, and evolve the hardware and software on capability and capacity systems necessary for application run-time and archival output needs. Provide feedback and requirements for capability and capacity system software and hardware necessary for current and next generation production visualization of application output data.
SNL	Provides development resources and some opportunity for large-scale Capacity dedicated system time testing and evaluation. Will support integration and deployment of products from other CSSE product areas. Provides the runtime, system software and system integration and management tools for Capability, Capacity and Advanced Systems the will be procured by CSUE product areas. This Product also provides the application performance and RAS Metrics that can be useful to guide decisions to upgrade or change system software. System integration and management tools are also used by many Pre and Post processing systems.
Facility Operations and User Support	
LLNL	This product is required for the operational aspects needed to support the work of all of the efforts in this subprogram. User Support services provides the direct source of feedback from customers about problems related to this CSUE subprogram. It also provides the documentation and training need by the subprogram products. A disruption or delay in delivery of user support impacts the resources available to the entire tri-lab program, making it more difficult to use

	Computational Systems and Software Environment (Capability Systems; Capacity Systems; Advanced Systems, System Software and Tools; I/O, Storage Systems; and Networking; Pre- and Post-Processing Environments)
	the computational resources effectively. User productivity and time-to-solution is impacted. This product includes procurement support for acquisitions of this subprogram.
LANL	Deliver systems and network operations and maintenance and facilities maintenance and upgrades for all capacity and capability computing platforms. Provide on-call experts for timely consultation with developers of system software in the CSSE Sub-Program experiencing software and hardware problems on all computing platforms.

Table VI-5. All Subprograms as Related to Facility Operations and User Support

	Facility Operations and User Support (Facilities, Operations, and Communications; User Support Services; Collaborations)
Integrated Codes	
LLNL	Supplies requirements and feedback to FOUS to improve facilities, operations, and support services.
LANL	Supply requirements and feedback to the FOUS Sub-Program on the facilities, operations, and support of capability and capacity systems through code team development, alpha use, and testing activities.
SNL	Provides an infrastructure for external collaborations, including facilities, administration and networking.
Physics and Engineering Models	
LLNL	Contributes requirements and feedback to the general operations and support of the computer facilities.
LANL	Supply requirements and feedback to the FOUS Sub-Program on the facilities, operations, and support of capacity systems used to support theoretical model development, in implementing models into codes in the IC Sub-Program, in developing and applying fundamental physics codes, and in developing software libraries and databases that instantiate nuclear and atomic physics data, equations of state, and high explosive and foam materials response.

	Facility Operations and User Support (Facilities, Operations, and Communications; User Support Services; Collaborations)
Verification and Validation	
LLNL	Contributes requirements and feedback to the general operations and support of the computer facilities.
LANL	Supply requirements and feedback to the FOUS Sub-Program on the facilities, operations, and support of capability and capacity systems used in V&V code assessment and storage hardware used in data archiving activities.
Computational Systems and Software Environment	
LLNL	A delay in the deployment of the Purple and BlueGene/L systems will impact delivery of other resources and milestones supplied by this subprogram. The capacity systems supplied by this product will be the development target of other efforts in this subprogram. Problems with their operational status will be the direct responsibility of this subprogram. If the software environment, and archive and file systems, are not operational robust – a substantial load is put on the operational staff and user services staff to track problems and maintain operational status. (Pre- and Post-Processing) Delivers both hardware and software for the Computational Systems and Software Environment. Delays in the procurement, installation, testing and deployment of data visualization and analysis hardware and tools will impact the ability of this subprogram to meet its overall goals and milestones.
LANL	Share computing facility operations and support requirements with other systems. Supply requirements and feedback to the FOUS Sub-Program on the facilities, operations, and support of capability and capacity systems used in system software development activities, for application run-time and archival output needs, and in current and next generation production visualization of application output data.
SNL	Provides the computing systems that are focused on the Mid-range Capability Gap. Close coordination and integration with 1.5.5 will be required to ensure Capacity System infrastructure requirements are met, such as, space, power, cooling, and network interfaces to storage, visualization and archiving resources. New capacity systems will also require staffing from 1.5.5 for system administration and user support.
Facility Operations and User Support	
LLNL	Interruptions in the facilities supported by this product causes a major load on the User Support services to interact with customers. User support services provides the direct customer problem tracking related to the Reliability, Availability, and Servicability (RAS) of the operational systems and tri-lab communications networks. Includes procurement support for acquisitions of this subprogram.
LANL	Use experiences gained in facilities operations, maintenance, and upgrades to anticipate user problems areas, thereby

	Facility Operations and User Support (Facilities, Operations, and Communications; User Support Services; Collaborations)
	coordinating fast and effective user support services. Track issues brought up by users and devise corrective actions for those issues directly related to facility operations and maintenance.

Table VI-6. All Subprograms as Related to External Programs

	External Programs
Integrated Codes	
LLNL	Simulation codes for Nuclear Explosive Package (NEP) engineering support DSW and LEP work at both LLNL (for example, W80-3) and LANL (for example, W76-1).
LANL	Provide DSW and the Science Campaigns with the simulation tools required for weapons certification, assessment, surety, SFI resolution, and design feasibility. These same tools are also feasible for design and assessment simulations of DOD conventional weapons. Provide DSW with the historical UGT calibration simulation tools required for benchmarking and quantifying simulation uncertainties (relative to the MMPC codes) in weapons certification, assessment, surety, SFI resolution, and design feasibility. Targets the reduction of numerical solution uncertainties known to exist in DSW certification by engaging for higher-risk, exploratory research (Weapons-Supported Research) necessary to pursue high-payoff numerical algorithm innovations in the area of shock physics, transport, linear and nonlinear solvers, and coupled multi-physics. Deliver simulation analysis and design support for W88 pit manufacturing, DOE Complex (e.g., LANL Sigma Foundry) casting design operations, Y-12 casting and welding operations, DOE Complex criticality safety scenarios, and DSW diagnostics output assessments and predictions.
Physics and Engineering Models	
LANL	Deliver theories useful in understanding basic physical phenomena of interest to experimental programs in DSW, the Science Campaigns, the DOD, and modeling and simulation programs in the DOE Office of Science. Software libraries embodying models for phenomena like materials response and damage and high explosive behavior can be

	External Programs
	useful for experimental programs in DSW, the Science Campaigns, for nuclear reactor programs in the NNSA, and for conventional weapons modeling and simulation program in the DOD. Atomistic, molecular dynamic, and chemistry codes generated in this product area represent tools for studying fundamental tools for studying and understanding phenomena such as material properties and behavior. These tools are need in many other programs such as those in the DOE Office of Science.
Verification and Validation	
LANL	Generic code V&V assessment tools (error estimates, QMU, convergence analysis), processes, and methodologies can be applied to similar assessments of simulation tools in other programs such as those being developed in the DOD and DOE Office of Science. These assessments lead to corrective actions that ultimately improve the code predictability, hence improve the simulation fidelity used for DSW certification. Generic code V&V assessment processes and methodologies can be applied to similar assessments of simulation tools in other programs such as those being developed in the DOD and DOE Office of Science. Archival databases of UGT events and other experiments is useful for DSW activities.
Computational Systems and Software Environment	
LANL	Other programs in need of and using HPC can benefit from ASC experiences and expertise gained in fielding capacity systems. Specifically, selected system software (e.g., Linux software stack) and vendor hardware used and developed for ASC platforms helps to advance future systems procured by other programs. Accelerates and potentially redirects vendor HPC strategies and plans to be more cognizant of HPC needs in scientific computing. This benefits other programs in need of and using HPC. System software and tools developed by ASC can ultimately find their way into commercial systems or standard operating systems (e.g., Linux). I/O and storage R&D driven by ASC capability and capacity needs helps to accelerate the availability and reliability of commercial vendors in this area (e.g., Panasas, Lustre, etc.). Visualization advances and needs helps to accelerate the availability, reliability, and usefulness of commercial vendor products (e.g., Computational Engineering International's EnSight) in this area.
Facility Operations and User Support	
LANL	Knowledge and experience gained from operations, maintenance, and upgrades of high-performance computing (HPC) facilities is useful for other programs engaged in HPC activities, such as Program Offices in the DOD and DOE Office of Science.

VII. 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 VII-1 summarizes ASC's top ten risks, which are managed and tracked.

Table VII-1. ASC's Top Ten Risks[7]

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.
2	Designers, analysts, DSW, or other Campaign programs lack confidence in ASCI 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.

[7] The ASC Top Ten Risks table was originally published in the *ASC Program Plan FY05*.

No	Risk Description	Risk Assessment			Mitigation Approach
		Consequence	Likelihood	Risk Exposure	
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 (SLEP, 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.
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.

No	Risk Description	Risk Assessment			Mitigation Approach
		Consequence	Likelihood	Risk Exposure	
9	Inadequate Problem Solving Environment 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.
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, ASCI Centers, and academia, and focus on test problem comparisons as part of software development process.

VIII. Performance Measures

Table VIII-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). 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 uncertainties 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.

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**	
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 A. Glossary

ASC	Advanced Simulation and Computing
CCF	Central Computing Facility
CSSE	Computational Systems and Software Environment (WBS 1.5.4)
DCE	Distributed Computing Environment
DMSC	Direct Simulation Monte Carlo
DNT	Defense and Nuclear Technologies Directorate at LLNL
DSW	Directed Stockpile Work
DTA	Design Through Analysis
ESN	Enterprise Secure Net
FOUS	Facility Operations and User Support
GPFS	Global Parallel File System
HPC	High Performance Computing
HPSS	High Performance Storage System
I/O	Input/Output
IC	Integrated Codes
ICC	Institutional Computing Cluster
ICSI	Integrated Cyber Security Initiative
KCP	Kansas City Plant
LANL	Los Alamos National Laboratory
LDAP	Lightweight Directory Access Protocol
LDCC	Laboratory Data Communications Center
LEP	Life Extension Program
LLNL	Lawrence Livermore National Laboratory
MEMS	Microelectromechanical Systems
MPI	Message Passing Interface
NAS	Network-Attached Storage
NFS	Network File System
NIF	National Ignition Facility
NNSA	National Nuclear Security Administration
NPR	Nuclear Posture Review
NSA	National Security Agency

nWBS	National Work Breakdown Structure
NWCC	Nuclear Weapons Compute Clusters
PaScalBB	Parallel Scalable Back Bone Concept
PEM	Physics and Engineering Models
PSI	Parallel Storage Interface
QMU	Quantify Critical Margins and Uncertainties
RAS	Reliability, Availability, and Serviceability
RDMA	Remote Direct Memory Access
SCC	Nicolas C. Metropolis Center for Modeling and Simulation
SCN	Secure Classified Network
SFI	Significant Finding Investigation
SLEP	Stockpile Life Extension Program
SNL	Sandia National Laboratories
SRN	Secure Restricted Network
SSP	Stockpile Stewardship Program
STS	Stockpile-to-Target Sequence
TSF	Terascale Simulation Facility
V&V	Verification and Validation
VST	Verification Software Toolkit
WAN	Wide Area Networking
WBS	Work Breakdown Structure

Appendix B. Points of Contact

WBS	Title	Contact
1.5.4	Computational Systems and Software Environment	Terri Quinn, LLNL, 925-423-2385, quinn1@llnl.gov Rich Graham, LANL, 505-665-5685, rlgraham@lanl.gov James L. Handrock, SNL, 925-294-3444, jlhandr@sandia.gov Sudip Dosanjh, SNL, 505-845-7018, ssdosan@sandia.gov
1.5.4.1	Capability Systems	Mark Seager, LLNL, 925-423-3141, seager1@llnl.gov Manual Vigil, LANL, 505-665-1960, mbv@lanl.gov Jim Tomkins, SNL, 505-845-7249, jltomki@sandia.gov
1.5.4.2	Capacity Systems	Mark Seager, LLNL, 925-423-3141, seager1@llnl.gov Manual Vigil, LANL, 505-665-1960, mbv@lanl.gov Carl S. Leishman, SNL, 505-844-3784, csleish@sandia.gov
1.5.4.3	Advanced Systems	Mark Seager, LLNL, 925-423-3141, seager1@llnl.gov Rich Graham, LANL, 505-665-5685, rlgraham@lanl.gov Sudip Dosanjh, SNL, 505-845-7018, ssdosan@sandia.gov
1.5.4.4	System Software and Tools	Terri Quinn, LLNL, 925-422-2385, quinn1@llnl.gov Rich Graham, LANL, 505-665-5685, rlgraham@lanl.gov Jim Ang, SNL, 505-844-0068, jaang@sandia.gov
1.5.4.5	I/O, Storage Systems, and Networking	Doug East, LLNL, 925-424-4148, east1@llnl.gov Rich Graham, LANL, 505-665-5685, rlgraham@lanl.gov James L. Handrock, SNL, 925-294-3444, jlhandr@sandia.gov
1.5.4.6	Pre- and Post-Processing Environments	Steve Louis, LLNL, 925-422-1550, stlouis@llnl.gov Rich Graham, LANL, 505-665-5685, rlgraham@lanl.gov Dino Pavlakos, SNL, 505-844-9089, cjpavla@sandia.gov
1.5.5	Facility Operations and User Support	Terri Quinn, LLNL, 925-423-2385, quinn1@llnl.gov Cheryl Wampler, LANL, 505-667-5243, clw@lanl.gov John Zepper, SNL, 505-845-8421, jdzeppe@sandia.gov
1.5.5.1	Facilities, Operations, and Communications	Doug East, LLNL, 925-424-4148, east1@llnl.gov Steve Shaw, LANL, 505-606-0203, shaw@lanl.gov John Noe, SNL, 505-844-5592, jpnoe@sandia.gov
1.5.5.2	User Support Services	Brian Carnes, LLNL, 925-423-9181, carnes1@llnl.gov Steve Shaw, LANL, 505-606-0203, shaw@lanl.gov John Noe, SNL, 505-844-5592, jpnoe@sandia.gov

WBS	Title	Contact
1.5.5.3	Collaborations	Terri Quinn, LLNL, 925-423-2385, quinn1@llnl.gov Cheryl Wampler, LANL, 505-667-5243, clw@lanl.gov Robert Thomas, SNL, 505-844-7450, rkthomas@sandia.gov
1.5.1.4.12	Caltech, Center for Simulating Dynamic Response of Materials	Dan Meiron, 626-395-3424, dim@its.caltech.edu Michael Aivazis, 626-395-3424, aivazis@caltech.edu Paul Dimotakis, 626-395-6811 Bill Goddard, 626-395-2731, wag@wag.caltech.edu Michael Ortiz, 626-395-4530, ortiz@aeor.caltech.edu Dale Pullin, 626-395-6081, dale@galcit.caltech.edu
1.5.1.4.12	Stanford, Center for Integrated Turbulence Simulation	Parviz Moin, 650-723-9713, moin@stanford.edu Juan Alonso, 650-723-9954, jjalonso@stanford.edu Heinz Pitsch, 650-736-1995, h.pitsch@stanford.edu William Dally, 650-725-8945, billd@csl.stanford.edu Pat Hanrahan, 650-723-8530, hanrahan@cs.stanford.edu
1.5.1.4.12	University of Chicago, Center for Astrophysical Flash Phenomena	Donald Q. Lamb, 773-702-7194, d-lamb@uchicago.edu Robert Rosner, 773-702-0560, r-rosner@uchicago.edu Todd Dupont, 773-702-3485, Dupont@cs.uchicago.edu Rusty Lusk, 630-252-7852, lusk@mcs.anl.gov Tomasz Plewa, 773-834-3227, tomek@flash.uchicago.edu Andrew Siegel, 773-834-8501, siegela@flash.uchicago.edu Jim Truran, 773-702-9584, truran@nova.uchicago.edu
1.5.1.4.12	University of Illinois, Center for Simulation of Advanced Rockets	Michael T. Heath, 217-333-6268, m-heath@uiuc.edu William A. Dick, 217, 244-7235, wdick@uiuc.edu Robert A. Fiedler, 217-333-3247, rfiedler@uiuc.edu
1.5.1.4.12	University of Utah, Center for Simulation of Accidental Fires and Explosions	David W. Pershing, 801-581-5057, David.Pershing@utah.edu Chuck Wight, 801-581-8796, Chuck.Wight@utah.edu Tom Henderson, 801-581-3601, tch@cs.utah.edu Philip Smith, 801-585-3129, smith@crsim.utah.edu Greg Voth, 801-581-7272, voth@chem.utah.edu Patrick McMurtry, 801-581-3889, mcmurtry@eng.utah.edu Eric Eddings, 801-585-3931, eddings@che.utah.edu Steve Parker, 801-585-1504, sparker@cs.utah.edu

Appendix C.
1.5.1.4.12 Alliance Support (LLNL, LANL, SNL)

The Alliance Support project—part of nWBS product 1.5.1.4 Focused Research, Innovation, and Collaboration—involves various activities in support and management of the ASC university alliance program. Primarily it supports the LLNL alliance strategy team (AST) member from LLNL and some members from LLNL of the tri-lab support teams (TSTs) for various alliance centers. The AST manages and coordinates the program in terms of reviews, reporting, communication, new solicitations, and program quality in general between labs and NNSA Headquarters and among the centers. The TSTs primarily provide support for the centers in terms of interactions with the laboratories on an individual researcher basis and visits between the centers and the labs and hold yearly spring TST reviews of the centers.

The project capabilities are primarily management and communication and some technical interaction.

The planned FY06 activities include preparing a solicitation for a follow-on alliance program to begin in FY08, provide a spring TST review of each center and hold a conference whose technical program highlights results of the current program, as well as various other interactions between centers, labs and headquarters, as appropriate.

Preliminary planned activities in FY07 include conducting a peer-reviewed solicitation for the expected follow-on alliance program, and interactions as above as appropriate.

California Institute of Technology, Center for Simulating Dynamic Response of Materials

The overarching goal of the Caltech ASC Alliance Center is the development of a virtual shock physics facility to simulate dynamic response in materials. An allied goal is to advance the state of the art in modeling using a multiscale paradigm. The research developments of the center are ultimately translated into algorithms that perform scalably on the ASC computing platforms. Finally, a significant additional thrust has been the integration of four validation experiments as part of our program. The center's modeling and algorithm development efforts are targeted at the integrated simulation of high velocity impact experiments wherein a detonation elicits shock response in a solid target. The fluid mechanics associated with the detonation simulation is performed using advanced Eulerian advection methods while the solid mechanics of the target are performed using a Lagrangian approach and tetrahedral finite elements. The two approaches are coupled using a novel fluid solid coupling approach based on level sets. The software environment that supports these simulations is known as the Virtual Test Facility (VTF).

Capabilities include the following:

- Integrated simulation capability: At present the VTF software has the following capabilities: parallel 3D AMR based Eulerian fluid mechanics solver via the AMROC framework, parallel 3D solid mechanics, parallel 3D solid shells, scalable communication and Eulerian-Lagrangian coupling algorithms, multiscale materials models for both solid and fluid. Integrated simulations can be optionally deployed via the Python based Pyre framework.

- Validation: A key part of the center's research program is the use of four key experiments to validate the VTF software. These experiments are: converging shocks and compressible turbulence experiment – used to validate the shock propagation and turbulence models developed by the center; dynamic deformation –validates the center's multiscale modeling an simulation of high strain rate deformation; dynamic fracture – validates the center's modeling of brittle dynamic fracture; and detonation-fracture – the center's integrated simulation capability as well as its modeling of ductile rupture in solids and detonation in combusting gases.
- Research in multiscale modeling: The center sponsors a research program to develop multiscale models for dynamic deformation of metals and high explosives as well as development of models for compressible turbulence in fluids.
- Research in computational science: The center carries out research to develop scalable algorithms to support the integrated simulation. Important contributions here include the fast level set algorithm, a scalable Eulerian-Lagrangian coupling algorithm and the Pyre framework as well as new WENO based advection algorithms for compressible turbulence simulations.

In FY06 we plan to integrate the LLNL Paradyn solver as a part of the VTF framework. This work is being undertaken with the collaboration of the Defense Technologies Engineering Division (DTED) and in particular with the Methods Development Group at LLNL. The integration of the Paradyn solver with the VTF will be performed only on LLNL computers and will not be distributed as part of the center's basic VTF software package.

Expected Deliverables FY06:

- Integrated simulation capability – Continue to improve the data structures used for adaptive mesh refinement in AMROC so as to improve scalability and load balancing. Provide for input of CAD descriptions so as to increase the usability of the solvers. We also plan the first release of the VTF software in Q1 FY06
- Converging shock experiment: Completion of large-aperture optics and beginning of Phase-1 shock-focusing experiments. Continue to provide validation data for simulations. Continue VTF simulations of Phase 0 and Phase 1 converging shock experiment including boundary layer effects
- Dynamic deformation experiment: Investigate the deformation of polycrystalline tantalum using the shear compression specimen and by evaluating the texture evolution in specimens subjected to high-strain-rate deformation. Develop digital image correlation (DIC) and high-speed full field thermal imaging techniques to measure the local deformation and temperature fields in the SCS specimen for validation of mesoscale models of plasticity in the VTF. Continue dynamic deformation validation runs using the VTF for polycrystalline aluminum and tantalum. Especial emphasis will be devoted to the development of quantitative validation measures.
- Dynamic fracture experiment: Conduct experiments to provide mixed mode and pure mode-II cohesive zone laws of adhesive bonds using asymmetric four-point bending fracture tests. Conduct separate set of experiments for obtaining dynamic cohesive zone laws under mode-I and mixed mode loading conditions to verify the sufficiency of quasi-static cohesive zone laws in the VTF simulations.
- Detonation-fracture experiment: Develop visualization techniques to image simultaneously propagating detonations and fracture. Compare fracture data with fully integrated VTF simulations.

- Multiscale modeling for solid dynamics: Develop model for microstructure in Fe due BCC to HCP phase transformation. Integrate the level set model of void coalescence into the VTF framework to conduct large-scale (many voids) coupled multiscale simulations of spallation of ductile crystal under shock loading. Conduct simulations to quantitatively assess the impact of microstructure on response of polycrystalline metals. Develop nanovoid based model for ductile fracture
- Computational science: Continue to improve pyre. Extend the support for distributed services. Continue to incorporate AMROC based simulations in the framework by providing support and application scripts for the Center's integrated applications.

Preliminary Planned Activities in FY07 include: validated simulations for converging shock experiment in phases 0, 1, 2 including compressible turbulence; validated simulations for dynamic deformation experiment; validated simulation for dynamic fracture; validated simulation for detonation fracture experiment including detonation driven ductile rupture; and second release of VTF software with validated models.

Stanford, ASC Alliance Center for Integrated Turbulence Simulations, CITS

CITS's mission is the development of a high-fidelity computational framework for the simulation of turbulent thermo-fluid systems involving a variety of physical phenomena and geometrically complex configurations. The simulations environment is based on multiple, integrated codes that address specific physical phenomena, such as detailed turbulence dynamics, multiphase interface tracking, combustion, etc. Strong emphasis is given to the development of efficient and scalable numerical algorithms for the ASC parallel computational platforms.

A complementary goal is the development of streaming supercomputer hardware and supporting software and algorithms; streaming represents the next generation of high performance scientific computing as demonstrated by the recent industrial interest.

Capabilities include the following:

- Integrated Simulations. CITS overarching problem is the simulation of the complete aero-thermodynamic flow path through a jet engine. CITS simulation environment is based on Python and built around the Center's flagship codes, CDP (Large Eddy Simulation approach) and TFLO (based on Reynolds-averaged Navier-Stokes equations). It also includes a set of general-purpose interpolation and communication libraries (CHIMPS, Coupler for High-performance Integrated Multi-Physics Simulations).
- Software Engineering. Scalability has been extensively pursued at the Center. Tests have been performed on several platforms; dedicated ALC runs (1,800 central processing units) have demonstrated nearly perfect scalability for TFLO. CDP demonstrated good scalability to 1350 processors. Code I/O has also received considerable attention; both CDP and TFLO use native MPI I/O procedures and have demonstrated I/O rates of 150Mb/sec or greater on a variety of problem sizes. On the streaming side, a new hierarchical programming language that makes it significantly easier to develop applications for exposed-communication architectures has been developed. Also a detailed architectural design of a stream processor was completed
- Physics Modeling. Accurate turbulence modeling has been the key feature of CITS. In addition models for characterizing combustion, heat release and the pollutant production in the engine combustion chamber have been developed and validated; work on soot modeling is now underway. Multiphase flow capabilities have also been substantially enhanced by introducing a new paradigm, the Resolved Level Set

Grid (RLSG) method, which directly uses the CHIMPS integration software to couple the liquid/gas interface tracking algorithm (based on a Cartesian mesh solver) and CDP.

- Verification and Validation. CITS has increased the visibility and internal dissemination of Verification and Validation activities to build a more widespread knowledge. Work on global grid refinement for unstructured grids has been completed and has enabled the largest (to the group's knowledge) polyhedral mesh simulation with 2 billion fully unstructured control volumes. CITS is also organizing a 2-day workshop on error estimation and uncertainty quantification to jumpstart activities in this arena.

In FY06, the work on the integration framework will continue with the objective of ensuring scalability and accuracy in the transfer of data between the various component codes. On the solver side, the algorithmic development will be related to the improvement of the linear system solver currently utilized. Another key aspect of the work in CDP will be related to the development, implementation, and testing of improved soot models.

Validation of the Center's new multiphase interface tracking approach will be completed.

The work on unstructured grid refinement algorithm will be continued by allowing local as well as global adaptation. Error estimation for time-periodic flows will be initiated using a dual formulation based on the time-spectral approach, creating a unique possibility in terms of efficiency for analyzing flow in turbo-machinery components.

On the streaming supercomputer project the plan is to refine the compiler for the hierarchical programming language, develop applications in this language, and port the programming system to the IBM Cell processor.

Several collaborations with the National Labs based on the use of CITS codes, algorithms or physical models have been initiated. The activities range from the modeling of landslide-generated tsunami waves to fire modeling. Important collaborations have been initiated, in particular with the LLNL/CASC Group for flow modeling activities and algorithmic developments.

In FY06, we expect completion of the first full-wheel simulation of the high-pressure component of a Pratt & Whitney jet engine- This landmark calculation will generate a substantial amount of data and will answer two fundamental questions related to engine components interaction and engine stability. It will also push the envelope in terms of computational resources used for a single calculation.

Research on accurate algorithms for compressible flow simulation will be completed and initial testing of the new approach will be carried out (this activity is carried out in collaboration with the University of Minnesota). CITS is also collaborating with Michigan State and Notre-Dame universities in an experimental program for validation of high fidelity numerical algorithms for compressible flow.

The first version of the Center simulation environment will also be made open-source.

Preliminary planned activities in FY07 include:

- Integrated simulation of the full jet engine, including the low- and high-pressure components and the fan.
- Validation of compressible flow algorithm using the Michigan and Notre-Dame data.
- Development of error estimation capabilities for periodic flows.

- Further development and distribution of the CITS legacy codes in the open domain.

University of Chicago, ASC Center for Astrophysical Thermonuclear Flashes

The goal of the Center is to solve long-standing problems of thermonuclear flashes on the surfaces of compact stars, such as neutron stars (X-ray bursts) and white dwarfs (novae); and particularly, 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 (the "FLASH code"), which is able to carry out numerical simulations of the various aspects of the "FLASH problem." In what follows, we highlight the capabilities of the code and the important astrophysical studies that have been accomplished using the code. We then specify some of the FY06 milestones for the Center's groups.

The FLASH code is a community code that is capable of simulating a wide variety of problems is astrophysics, laboratory fluid dynamics, and plasma physics. Its capabilities include non-relativistic and relativistic hydro, non-relativistic and relativistic MHD, a variety of equations of state, a variety of nuclear networks, multipole and multigrid self-gravity with both isolated and periodic boundary conditions, massless tracer particles, massive particles for treating dark matter, and diffusive radiation transfer. The code has been down-loaded by more than 500 scientists around the world. The FLASH code has enabled the Center to propose and simulate a self-consistent picture of C/O mixing in the surface layers of white dwarf stars prior to novae outbursts; and to simulate the entire white dwarf star during the deflagration phase of Type Ia supernovae, leading to the discovery of an entirely new and promising mechanism for such supernovae.

In FY06, the primary scientific activity of the Center in the coming year will be large-scale, integrated, multi-physics simulations of Type Ia supernovae, focusing on the deflagration phase. The primary computational physics and validation activities in the coming year will be the continued development of physics modules in support of these large-scale simulations of Type Ia supernovae and the initiation of new collaborations with the DOE labs in validation. The primary code activities in the coming year will be the continued development of FLASH 3, the migration of the FLASH code to new ASC platforms as they become available, and support of the large-scale astrophysics simulations of Type Ia supernovae. The primary visualization activities will be the continued development of FLASHVIEW and the visualization of the large-scale simulations of Type Ia supernovae carried out by the astrophysics group and of validation experiments carried out by the computational physics and validation group. The primary activities of the computer science group will be demonstration of the FLASH code on the next generation of scalable computers. The primary basic physics activities will be the continued study of the Rayleigh-Taylor instability, turbulence, and reactive flows.

Specific astrophysics milestones for FY06 include: extensive 3D simulations of the deflagration phase of Type Ia supernovae, enabling us to explore the sensitivity of the outcome to the location and the number of ignition points; development of an improved subgrid model for Type Ia supernova flames; and extensive 2-d simulations of the detonation phase, enabling us to determine the energy and the nucleosynthetic yield of the explosion. Specific computational physics and validation milestones for FY06 include: completion of a low-Mach number solver and application of the solver to the smoldering phase of novae; continued development of a level-set front tracker and

preliminary application of the front tracker to Type Ia supernova flames; continued simulations and study of the shock-cylinder experiment at LANL and initiation of a collaboration with Bruce Remington (LLNL) on laser-driven experiments. Specific code milestones for FY06 include: migration of the remaining physics modules to FLASH 3 and refinement of FLASH 3; migration of the FLASH code to new ASC platforms as they become available; and continued support of the simulations being carried out by astrophysics group. Specific visualization, computer science, and basic physics milestones for FY06 include: visualization of large-scale simulations carried out by the FLASH Center; further development of FLASHVIEW, the FLASH desktop visualization tool; demonstration of FLASH on the next generation of scalable computers, including the ASC BlueGene/L and Red Storm machines; and mathematical and numerical studies of flames and reactive flows.

The primary scientific activity of the Center in FY07 will be large-scale, integrated, multi-physics simulations of Type Ia supernovae, focusing on the smoldering phase prior to ignition and on the detonation phase. Other activities will include completion of the low-Mach number and level-set front tracker modules, continuation of validation studies, making FLASH 3 robust enough to replace FLASH 2, continued development of FLASHVIEW, and continued studies of reactive flows.

University of Illinois, Center for Simulation of Advanced Rockets

The goal of the University of Illinois Center for Simulation of Advanced Rockets (CSAR) 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. Each of these aspects is characterized by very high energy density, extremely diverse length and time scales, complex interfaces, and reactive, turbulent, and multiphase flows.

CSAR is focusing on the reusable solid rocket motor (RSRM) of the NASA Space Transportation System, better known as the Space Shuttle, as its long-term simulation vehicle. The RSRM is a well-established commercial rocket, is globally recognized, and design data and propellant configurations are available. The Center has a Space Act Agreement with NASA in place to share data and simulation results under an Export Control/ITAR relationship. Several smaller scale rockets are also simulated to provide validation data for CSAR codes. Simulations that include full geometric and materials complexity require a sequence of incremental developments—in engineering science, computer science, and systems integration—over an extended period.

Our approach to system integration has been to develop a single executable code containing modules for the various components and an interface code for tying them together. We are following an object-oriented design methodology that hides the data structures and other internal details of the individual component codes. This simplifies development and maintenance of the interface code and the component codes, and also makes it easier to swap different versions of the same component—a critical capability for determining the most efficient algorithms and implementations.

Broadly known as Rocstar, the CSAR simulation code is a fully coupled, multiscale, multiphysics suite of integrated modules for 3D simulation of solid propellant rocket performance on massively parallel computers. The suite is designed to be sufficiently general to solve any fluid/structure interaction problem. Components include fluid dynamics (Rocflo, Rocflu), entrained particle tracking and interaction (Rocpart,

Rocsmoke), solid mechanics (Rocsolid, Rocfrac), fracture (Rocfrac), particle packing (Rocpack), combustion (Rocburn, Rocfire), and software interface codes for coupling and mesh association (Roccom, Rocman, Rocface, Rocinteract, and others). Refinement of models reflects the synthesis of fundamental, subscale studies critical for detailed simulations of accident scenarios and for reliable simulation of multiscale phenomena such as combustion and turbulence.

The code has been applied to several research problems in addition to solid propellant rockets. These include validation studies employing super-seismic shocks, human (or animal) arteries, and acoustic interaction between helicopter rotor blades and the helicopter body. Rocpack has recently been licensed to the U.S. Army Engineering Research and Development Center for a preliminary study investigating packing of land mines in rocks and soil.

CSAR-NNSA/DP Interactions: Center personnel have traveled extensively and have been involved in a large number of technical and informational meetings. These included meetings intended to explore rocket science and technology, identify technical collaborators, describe the ASC/ASAP program, and establish relationships among Center investigators, DOE lab scientists, and industry leaders. One of the leading topics of discussion between lab staff and CSAR investigators has been and will continue to be in pursuing the potential use within the labs of specific technologies developed at CSAR. Immediate technology candidates include our technology for data transfer at component interfaces and our framework for integration of separately developed codes with automated load balancing.

Student-NNSA/DP Interactions: To date, 29 former CSAR students and four staff members have joined the DOE/NNSA labs as permanent employees. CSAR has been remarkably successful in encouraging student-lab interactions. Opportunities for UIUC graduate and undergraduate student interaction with the NNSA/DP laboratories include summer student internships, joint research, and CSAR undergrads in labs collaborating in research with NNSA/DP scientists.

Expected Deliverables in FY06:

- RSRM simulations — Semi-annual simulations of RSRM 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.
- Titan IV case rupture accident — In this simulation, the pressure builds up until the case fails. In test firing an early design (1991), a rocket motor exploded violently destroying the test stand, but there was no propellant detonation. This simulation will include the use of the new advanced material model for the propellant that includes the effects of voids and dewetting.
- 3D vortex shedding captured in RSRM simulations downstream of intersegment inhibitors
- Gravitational body forces added to Rocflo and Rocfrac modules
- Algorithm for propellant regression along case verified
- Automatic insertion of cohesive elements in Rocfrac verified
- Implementation of remeshing for tetrahedral meshes verified
- Material model and new finite element developed for case insulation

Preliminary planned activities in FY07 include:

- 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.
- Other major rocket simulations include aluminized propellant combustion and burnout in the U.S. Air Force ballistic test system (BATES) motor; an end-to-end validation study using a commercial attitude control motor (Aerojet); smoke, temperature and vorticity validation; and an enhanced simulation of the Titan IV case rupture accident.

University of Utah, Center for Simulation of Accidental Fires and Explosions

The principal objectives of C-SAFE are to advance the state of the art in high-performance computer simulation science by creating world-class software and by educating students, postdocs and professional staff in the science and art of high-performance simulation. C-SAFE software is particularly suited for creating, verifying, validating and visualizing simulations of complex physical and chemical behavior over wide ranges of time and space. The C-SAFE target scenario is to simulate the explosive response of a cylindrical steel container of PBX9501 embedded in a 10-m diameter jet fuel fire. A key goal is to create multi-physics simulation software for which the behavior at the resolved (grid) scale accurately reflects underlying physics associated with smaller unresolved scales, down to the scales of individual atoms and molecules.

The C-SAFE target simulation scenario places stringent demands on the software in order to produce validated results. The fire simulation uses Large Eddy Simulation (LES) on a structured grid to capture the effects of radiant and convective heating on the length and time scales relevant to large pool fires such as may be present after an airplane crash or other transportation accident. The Center has developed the methodology for identifying chemical surrogates for jet fuel and other complex hydrocarbon mixtures, as well as detailed kinetic mechanisms for combustion in air. Because energy transport in fuel fires is dominated by radiation from soot particles, C-SAFE has created a world-class center for understanding the chemistry of soot formation and has pioneered techniques for incorporating that knowledge into large-scale simulations.

Although the fire simulation occurs on time scales of seconds to minutes, the resulting explosion occurs over the course of a few milliseconds. The code therefore incorporates methods of detecting the rare trigger events and executing appropriate changes in time stepping, while incorporating only those physics models that are relevant to the process and time scale of interest. Creating validated simulations of explosions has required the development of new mechanics codes (such as, an extension of the Material Point Method) for simulating closely coupled fluid-structure interactions on multiple time scales in ways that allow seamless transitions between compression, metal plasticity, fracture and explosive release of gases at arbitrary locations throughout the simulation domain.

The chemical and mechanical properties of plastic-bonded explosives have been investigated from first principles using molecular dynamics simulations, the results of which are used to formulate validated homogeneous computational models and constitutive laws for use at the resolved grid scale of the simulations.

All of these capabilities are combined in a single scalable software infrastructure (Uintah Core Code Development), which allows large-scale interactive visualization, incorporation of adaptive mesh refinement (AMR) algorithms and infrastructure, as well

as continuous code verification through daily testing. The code has been ported to five major supercomputer architectures and exhibits excellent scaling characteristics to at least 2000 processors.

The principal scientific application of the code is analysis of heating rates and fire geometries on the violence of the resulting explosion (such as, limiting behaviors of fast and slow cookoff, as well as intermediate behaviors and transitions). Because the computational modules are designed to reflect underlying fundamental physics rather than empirical observations, the code also has proved capable of simulating many different types of complex processes such as cell membrane mechanics and interaction of projectiles with human tissue. Therefore, the intrinsic capabilities that were built into the software for one purpose can be leveraged for many different types of scientific investigations driven by high-performance computer simulations.

Expected deliverables in FY06:

- Verified and validated high-performance simulation code capable of predicting violence of explosion resulting from heating of PBX in a jet fuel fire
- Incorporation of adaptive mesh refinement and multigrid resolution into a true multimaterial CFD code closely coupled with solid materials, including parallel implementation of explicit fracture mechanics
- A suite of validated reaction tables and soot models appropriate to JP-8 fuel fires that can be incorporated into most CFD codes
- Temperature-dependent parameters for ViscoSCRAM model of PBX mechanical properties originally created at LANL
- Computational support for large-scale remote visualization in Uintah
- Completely integrated multi-physics multi-time scale simulation of fire, heat up and explosion of a steel container of PBX9501 (simulation target scenario)

Preliminary planned activities in FY07 include fully implicit version of the extended Material Point Method code for closely coupled fluid-structure interaction; validation of AMR infrastructure in the large-scale fire simulation code; temperature-dependent parameters for ViscoSCRAM model of PBX mechanical properties originally created at LANL; inclusion of thermal decomposition, damage, ignition and pressure-induced instability into the combustion simulation model for PBX9501; implement validated computational models for soot deposition on surfaces, densification and thermal conduction; and improved dynamic load balancing, scaling and performance

Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 9455-0808