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Advanced Simulation and Computing Implementation Plan, FY15, Rev. 1

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National Nuclear Security Administration

Advanced Simulation and Computing
IMPLEMENTATION PLAN

Version 1.0

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Version History

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0.5	*Michel McCoy, Bill Archer, M. Keith Matzen*	*09/15/14*	*Robert Meisner*	*09/16/14*	*Initial release*
1.0	*Michel McCoy, Bill Archer, M. Keith Matzen*	*01/27/15*	*Robert Meisner*	*01/27/15*	*Update after signed budget; changed IP to new NNSA template*

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Contents

I. Overview

The Stockpile Stewardship Program (SSP) is a single, highly integrated technical program for maintaining the surety and reliability of the U.S. nuclear stockpile. The SSP uses nuclear 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 requires the continued use of experimental facilities and programs, and the computational enhancements to support these programs.

The Advanced Simulation and Computing Program (ASC) is a cornerstone of the SSP, providing simulation capabilities and computational resources that support annual stockpile assessment and certification, study advanced nuclear weapons design and manufacturing processes, analyze accident scenarios and weapons aging, and provide the tools to enable stockpile Life Extension Programs (LEPs) and the resolution of Significant Finding Investigations (SFIs). This requires a balance of resource, including technical staff, hardware, simulation software, and computer science solutions.

As the program approaches the end of its second decade, ASC is intently focused on increasing predictive capabilities in a three-dimensional (3D) simulation environment while maintaining support to the SSP. The program continues to improve its unique tools for solving progressively more difficult stockpile problems (sufficient resolution, dimensionality, and scientific details), quantify critical margins and uncertainties, and resolve increasingly difficult analyses needed for the SSP. Where possible, the program also enables the use of high-performance simulation and computing tools to address broader national security needs, such as foreign nuclear weapon assessments and counter-nuclear terrorism.

In Prague (2009), and more recently Berlin (2013), President Obama articulated his vision of a world without nuclear weapons. These reductions will be made, however, while ensuring that the U.S. maintains a strong and credible strategic deterrent, which is safe, secure, and effective, for as long as such weapons exist.

The 2010 *Nuclear Posture Review Report* codified the role of the National Nuclear Security Administration (NNSA) in maintaining the deterrent. In areas essential for stockpile life extensions and stewardship, key investments have been made to:

- Strengthen the science, technology, and engineering base needed for conducting weapon system LEPs
- Mature advanced technologies to increase weapons surety
- Qualify weapon components and certify weapons without nuclear testing
- Provide annual stockpile assessments through weapons surveillance

This strategy includes developing and sustaining high-quality scientific staff, as well as supporting computational and experimental capabilities. These three components constitute the foundation of the nuclear weapons program.[1]

The continued success of the SSP and LEPs is predicated upon the ability to credibly certify the stockpile, without a return to underground nuclear tests (UGTs). Shortly after the nuclear test moratorium entered into force in 1992, the Accelerated Strategic Computing Initiative (ASCI) was established to provide the underpinning computational capability to support stockpile certification. While computing and simulation have always been essential to the success of the nuclear weapons program, the intent of ASCI was to re-envision how NNSA used these tools in support of the stockpile. The ASCI Program was essential to the success of the SSP, providing critical nuclear weapons simulation and modeling capabilities. Now designated as the ASC Program, the mission remains the same: provide the simulation and computational capabilities that underpin the ability to maintain a safe, secure, effective nuclear weapon stockpile, without a return to UGTs. Where possible, the program also enables the use of these tools and operational infrastructure to address broader national security needs, such as foreign nuclear weapon assessments and counter nuclear terrorism.

The capabilities that the ASC Program provide play a vital role in the Nuclear Security Enterprise, and are necessary for fulfilling the stockpile stewardship and life extension requirements outlined for NNSA in the Nuclear Posture Review (NPR). The Program develops modern simulation tools that provide insights into stockpile aging issues, provide the computational and simulation tools that enable designers and analysts to certify the current stockpile and life-extended nuclear weapons, and inform the decision making process when any modifications in nuclear warheads or the associated manufacturing processes are deemed necessary. Furthermore, ASC is enhancing the predictive simulation capabilities that are essential to evaluate weapons effects, design experiments, and ensure test readiness.

The ASC Program's advanced, leading-edge technologies in high performance computing (HPC) and predictive simulation are essential for meeting the short- and long-term needs of the stockpile. The ASC Program continues to improve its unique tools to solve stockpile problems—with a focus on sufficient resolution, dimensionality, and scientific detail—to enable Quantification of Margins and Uncertainties (QMU) and to resolve the increasingly difficult analyses needed for stockpile stewardship. The needs of the DSW and major modernization programs also drive the requirements for simulation and computational resources. These requirements include planned LEPs, stockpile support activities, and mitigation efforts against the potential for technical surprise. All of the weapons within the current stockpile are in some stage of the life-extension process. The simulation and computational capabilities are crucial for successful execution of thee lifetime extensions and for ensuring NNSA can certify these life-extended weapons without conducting an underground nuclear test.

[1] *2010 Nuclear Posture Review Report*, April 2010, p. 42.

Specific work activities and scope contained in this Implementation Plan (IP) represent the full-year annual operating plan for FY16. The Initial Implementation Plan effective October 1, 2014 should be consistent with: 1) the Department's Base Table when operating under a Continuing Resolution (CR); and 2) the final signed appropriation or full-year CR once enacted.

II. Corporate Program Goals

Preliminary targets are subject to change based on a final, enacted budget.

Program or Project Name	Performance Measure/ Indicator Title and Description	FY2015 Target	Endpoint Target
Advanced Simulation and Computing Program	Reduced Reliance on Calibration	46%	100% (FY24)

The contractor's *Performance Evaluation Plan* contains multisite targets that can be identified by the associate deputy administrator as base or stretch goals.

There are no multisite targets for ASC in FY15.

Along with the Contributing Factors and Site Specific Outcomes outlined in the *Performance Evaluation Plan*, the contractor's performance will be evaluated against the NNSA's *Strategic Plan*, NNSA performance priorities and deliverables, program execution plans, work authorizations, and other key inputs (for example, multiyear strategic objectives). In evaluating overall performance on the FY15 milestones, the contractor shall receive adjectival ratings "Excellent," "Very Good," "Good," "Satisfactory," or "Unsatisfactory" based on Federal Acquisition Regulation Subpart 16.401(e)(3).

At a minimum, all management and operating sites are expected to perform at the satisfactory level documented in the Strategic *Performance Evaluation Plan* for each site. If not stated specifically in the Strategic *Performance Evaluation Plan*, satisfactory performance includes achieving all milestones and/or keeping NNSA informed of obstacles to achieving milestones that may arise due to the scientific-discovery nature of the ASC work; meeting all reporting requirements; engaging in productive and constructive collaboration with other ASC partner sites especially to achieve joint milestones and to achieve joint, collaborative, scientific goals; productive and constructive peer review of ASC partners; constructive participation in ASC meetings and reviews; professional interactions especially between management and NNSA; and cost-effective management of ASC funds and facilities.

III. Major Activities

In FY14, ASC continued delivering science-based simulation tools for annual assessments and next-generation LEPs, focusing on improved physics, fidelity, and calculations in support of DSW and the National Code Strategy. In FY15 and beyond, ASC will be focusing on supporting the LEPs. To achieve this objective, ASC will continue strengthening the science basis and driving down uncertainties for weapons simulations to a degree where NNSA can credibly claim predictive capability; instituting a robust, formalized peer review system; increasing the number of production computing cycles to support increased use of simulation in stockpile activities and reliance on UQ in weapons decisions; and pursuing next-generation computing to meet time-urgent, future predictive science capability needs as documented in the *ASC Computing Strategy* and the *Predictive Capability Framework*.

The ASC Integrated Codes (IC) subprogram continued to add capabilities to their physics and engineering codes. A new 3D adaptive mesh refinement (AMR) capability was successfully applied to model the behavior of additively manufactured parts under extreme conditions. The AMR capabilities were critical in resolving the microstructure of the parts under consideration. Also during FY14, a multimaterial hydrodynamics capability provided for the use of a variety of mixed-cell pressure and temperature equilibrium models. This new capability allowed for better simulation of low-temperature experiments with nonequilibrium mixed-cell models, while also allowing the simulation of high-temperature and well-mixed flows using equilibrium assumptions. ASC engineering simulations continued to support the B-61 LEP and W-88 Alt programs. Within IC, ASC's collaborations with academia via the Predictive Science Academic Alliance Program (PSAAP II) continued with six newly selected Centers.

The ASC Physics and Engineering Modeling (PEM) subprogram continued to provide scientific models and databases used to describe a variety of physical processes relevant to Stockpile Stewardship. Some recent developments from the PEM subprogram in FY14 include 1) reactive molecular dynamics simulations on an unprecedented scale (length ~1 micron, time ~1 ns), confirming the hypothesis that voids play a critical role in determining the initiation threshold in energetic materials and pave the way to inform grain-scale hydrocode simulations in the future; and 2) predictions of four distinct theories for the equation of state (EOS) of lithium deuteride, providing the capability to create more accurate databases to match these simulations and existing experimental data obtained by the science campaigns in both high-energy-density and focused experiments.

Within the Computational Systems and Software Environment (CSSE) subprogram, the vendor for the first ASC advanced technology system (ATS), which is named Trinity and will be deployed at Los Alamos National Laboratory (LANL) in the first quarter of FY16 and capable of 33.6 petaFLOP/s, has been selected. In early FY15, ASC intends to make an award for the Sierra ATS at Lawrence Livermore National Laboratory (LLNL). The acquisition and operation of the commodity technology systems (CTS), in the Facilities

Operations and User Support (FOUS) program element, has been pushed back a year at all three of the NNSA laboratories, with a FY15 start. The FastForward and DesignForward engagements with industry, in the Advanced Technology Development and Mitigation (ATDM) subprogram, have begun to accelerate industry's R&D technology roadmap for the program's future exascale-class computational needs.

IV. Funding Guidance

To support the scope of work contained in this IP, funding will be distributed through the existing Approved Funding Program (AFP) process. The AFP is adjusted on an as needed basis for the execution of congressionally approved programs, projects, or activities (PPAs). Specific work activities are authorized via this document, with incremental funding changes made through the AFP, and authorized via work authorizations and obligated via formal contract modification.

Program/Operational Control Level	President's FY2015 Budget Request	FY2015 CR Operating Target	FY2015 Enacted/Full-Year CR	Difference between Request versus Enacted
ASC	$610.1M	$569.3M	$598.0M	-$12.1M

V. Description of Planned Activities

The purpose of this IP is to outline key work requirements to be performed and to control individual work activities within the scope of work. Contractors may not deviate from this plan without a revised work authorization (WA) or subsequent IP.

Specific quantifiable subprogram deliverables are negotiated and/or updated during an annual process to document and track subprogram Level 2 Milestones. Successful progress toward completing these milestones is tracked on a quarterly basis. Progress towards completion of subprogram deliverables contribute toward an aggregate assessment of the Campaign's progress toward a quantifiable total number of deliverables for the current fiscal year.
Annual performance expectations for each M&O contractor outlined in this document will be considered in determining the contractor's performance rating and fee earned through the NNSA Corporate Performance Evaluation Process (CPEP).

The table below lists the current ASC Level 2 Milestones for FY15. A more comprehensive list (including milestone description and grading/exit criteria) is included in the individual subprogram detail in the appendices.

Table V-2. ASC Level 2 Milestone for FY15[2]

Sub-Program	ID#	Milestone Title	Complete Date	Site
IC	5206	Deliver Enhancements of Mesh Relaxation and Remap	3/31/15	LLNL
IC	5207	Evaluate and Improve Interactions of Turbulent Mix and Arbitrary Lagrangian-Eulerian Advection	6/30/15	LLNL
~~IC~~	~~5208~~	~~Evaluate the Use of Arbitrary Lagrangian-Eulerian/Adaptive Mesh Refinement in Full-System Modeling, Part 1~~	~~9/30/15~~	~~LLNL~~
IC	5166	Production Release of the Eolus Project Diagnostics Codes	9/30/15 ~~6/30/15~~	LANL

[2] Factors such as FY15 Congressional Appropriations, NNSA/DP directives, and National Security considerations may necessitate a change in the current milestone set.

Sub-Program	ID#	Milestone Title	Complete Date	Site
IC	5167	Eulerian Applications Project Support for the FY16 Predictive Capability Framework Peg Post	9/30/15	LANL
IC	5319	Thermal/Mechanical Coupling in SIERRA for Pressurization and Breach	9/30/15	SNL
IC, V&V	5320	Verification and Validation Propensity Improvements via Solution Verification Automation	9/30/15 ~~6/30/15~~	SNL
IC, PEM	5321	A Model for Simulating Photoconductivity Effects in Small-Scale Integrated Circuits in Support of Stockpile Modernization	9/30/15	SNL
IC, ATDM, CSSE	5215	Demonstrate Advances in Proxy Applications through Performance Gains and/or Performance Portable Abstractions	9/30/15	LLNL LANL SNL
PEM	5209	Material Model Development for Reuse Applications	9/30/15	LLNL
PEM	5168	Replacement of the Legacy Opacity Code LEDCOP with the ATOMIC Opacity Code for Production of New Opacities	9/30/15	LANL
PEM	5169	Parameterization and Implementation of the Pseudo-Reaction-Zone High Explosive Model	9/30/15	LANL
PEM	5322	Direct Simulation Monte Carlo Simulation of a Massively Parallel, Chemically Reacting, 3D Re-Entry Flow	9/30/15	SNL
V&V	5210	Applications of Uncertainty Quantification Techniques to Predictions of Pit Reuse Success	3/31/15	LLNL
V&V	5211	Assess Filtering Methodologies for Uncertainty Quantification	6/30/15	LLNL
V&V	5170	Secondary Validation Suite Support for Energy Balance II	6/30/15 ~~3/31/15~~	LANL

Sub-Program	ID#	Milestone Title	Complete Date	Site
V&V	5323	Assess Ion Extraction and Beam Transport Models, Including Parameter Sensitivity and Uncertainty Quantification, for Neutron Tube Applications	9/30/15	SNL
V&V	5324	Blind Validation for a Directed Stockpile Work III–V Small-Scale Integrated Circuit	9/30/15	SNL
ATDM*	5212	Implement a Proxy Application in Support of Researching Parallel Input/Output and Burst Buffer Strategies	6/30/15	LLNL
ATDM, CSSE	5171	Demonstrate an Initial Burst Buffer Application Programming Interface	9/30/15	LANL
ATDM*	5325	Programming Models Analysis for Next-Generation Platforms	9/30/15	SNL
CSSE	5213	Commodity Technology System-1 Contract Awarded	9/30/15	LLNL
CSSE	5216	Planning for Pre-Exascale Platform Environment	9/30/15	LLNL LANL SNL
FOUS	5214	Livermore Computing High Performance Computing Enduring Facility Master Planning—Modernization and Repurposing	3/31/15	LLNL
FOUS	5172	Physical Infrastructure Integration for Trinity	9/30/15	LANL

* The long description for this Level 2 milestone is available upon request from the ASC Program Office.

VI. Reporting Requirements

The following systems and processes for program management and control of the ASC Program are in place:

- **Quarterly Program Reviews**. Management & Operating (M&O) contractors report Level 2 milestone status to Headquarters using the Milestone Reporting Tool. In preparation for each quarterly review, each site and Federal Program Manager will assess the status of each milestone by providing a score (Green, Yellow, Red, Blue, or Black). In addition, supporting details for the assessment of each milestone will be reported and any programmatic risk will be identified.
- **Monthly Financial Reporting**. Monthly cost/financial expenditure data will be reported by the Office of Planning, Programming, Budgeting and Evaluation, NA-MB, and available to the NNSA Program Managers.
- **Other NNSA Program Reviews**. Special technical and program reviews requested by NNSA Program Managers and other senior NNSA officials for oversight and program management responsibilities will be supported by the sites.
- **Bi-Weekly Subprogram Teleconference**. Federal Program Managers conduct bi-weekly teleconferences to discuss upcoming meetings and to provide an opportunity to exchange information of programmatic and technical interest and need.
- **Program Change Control**. Change control for program activities conducted within this IP will be managed and tracked on the Revision Summary at the front of this document.
- **Budget Control Levels**. The budget control level allows the federal Program Manager to shift funding within the ASC Campaign subprograms. All requests to shift resources between subprograms must be approved in advance by the appropriate NNSA Program Manager.
- **Contractor Performance Evaluation Plan (CPEP)**. Each NNSA M&O contractor is evaluated utilizing the individual contract's Performance Evaluation Plan. Program Managers are required to establish the expectations for the M&O contractor(s) via this IP and associated Work Authorizations. The annual evaluation of each M&O contractor is performed per the CPEP Process Policy Guide. The Federal Program Managers provided quarterly evaluations, which are included in the annual Performance Evaluation Report produced by the NNSA Field Office.

VII. Key Execution Year Reference Documents

The following documents are incorporated by reference:

- *ASC Computing Strategy* (May 2013)
- *ASC Right Size* (October 2010)
- *ASC Business Model* (July 2005)
- MOU between DOE Office of Science and DOE NNSA Office of Defense Programs for the coordination of exascale activities (April 2011)
- *ASC Program Management Plan* (July 2010)
- Approved Funding Program Input sheet (AFP) and regular monthly financial plan adjustments, including Work Breakdown Structure (WBS), Budget and Reporting (B&R) code, and other necessary information for each site in the monthly Approved Funding Program updates

VIII. Major Risks and Handling Strategies

A number of factors must operate in concert to ensure the work proceeds as planned. Deviation from any one of these factors may cause delays in milestone schedules, reductions in scope, or increased technical risks and uncertainties. Technical risks specific to an individual milestone are covered in the individual subprogram appendices to this document.

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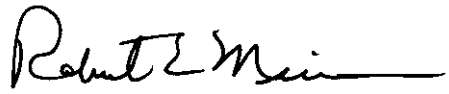
X. Approvals

The undersigned acknowledge that they have reviewed the ASC Implementation Plan and agree with the information presented within this document. Changes to this Implementation Plan will be coordinated with, and approved by, the undersigned, or their designated representatives.

Approved by:

Robert Meisner,
NNSA ASC Program Director  01/27/15
Signature Date

Concurrence:

Michel McCoy, LLNL ASC Executive	*Concurrence received*	9/15/14
Bill Archer, LANL ASC Executive	*Concurrence received*	9/15/14
M. Keith Matzen, SNL ASC Executive	*Concurrence received*	9/13/14

Appendix A: Key Terms

The following definitions and explanations are for terms and acronyms relevant to the content presented within this document and its appendices.

3D	Three Dimensional
ACES	New Mexico Alliance for Computing at Extreme Scale
ACSLS	Oracle's Automated Cartridge System Library Software
AFP	Approved Funding Program
AMR	Adaptive Mesh Refinement
AMT	Asynchronous Many Task
API	Application Programmer or Programming Interface
ASC	Advanced Simulation and Computing (formerly ASCI)
ASCI	Accelerated Strategic Computing Initiative
ASCR	Office of Science's Advanced Scientific Computing Research
ATDM	Advanced Technology Development and Mitigation
ATS	Advanced Technology System
B&R	Budget and Reporting
BB-API	Burst Buffer Application Programming Interface
BSF	Boiler Simulator Facility
CBTF	Component-Based Tool Framework
CCC	Capability Computing Campaign
CCE	Common Computing Environment
CD	Critical Decision
CORAL	Collaboration of Oak Ridge, Argonne, and Livermore
CPU	Central Processing Unit
CQMOM	Conditional Quadrature Method of Moments
CRADA	Cooperative Research and Development Agreement
CSSE	Computational Systems and Software Environment
CTS	Commodity Technology System

D&E	Development and Engineering
DAG	Directed Acyclic Graph
DBD	Dielectric-Barrier Discharge
DOE	Department of Energy
DRAM	Dynamic Random Access Memory
DSL	Domain-Specific Language
DSW	Directed Stockpile Work
EDR	Enhanced Data Rate
EOS	Equation of State
ESP	IBM's Early Ship Program
EVTS	Enhanced Verification Test Suite for Physics Simulation
FDR	Federated Data Rate
FOUS	Facility Operations and User Support
GPGPU	General-Purpose Graphics Processing Units
GPU	Graphics Processing Unit
HMC	Hybrid Memory Cube
HPC	High-Performance Computing
HPCG	High Performance Conjugate Gradient
HPSS	High-Performance Storage System
HQ	ASC Headquarters
HSI/HTAR	Hierarchical Storage Interface/ High-Performance Storage System Tape Archiver
I/O	Input/Output
IB	Infiniband
IC	Integrated Codes
IDM	Identity Management System
IHPC	Inter-Site High Performance Computing
ISC	International Supercomputing Conference
ITIL	Information Technology Infrastructure Library
KCP	Kansas City Plant
LANL	Los Alamos National Laboratory
LC	Livermore Computing

LCLR	Local Checkpoint, Local Restart
LDMS	Lightweight Distributed Metric Service
LDRD	Laboratory Directed Research and Development
LEC	Lagrangian-Eulerian Compatibility
LEP	Life Extension Program
LES	Large Eddy Simulation
LFLR	Local Failure Local Recovery
LLNL	Lawrence Livermore National Laboratory
LWK	Lightweight Kernel
MIC	Many Integrated Core
Mini-App	Mini Application
MMS	Method of Manufactured Solutions
MPI	Message Passing Interface
NAS	Network-Attached Storage
NERSC	National Energy Research Scientific Computing Center
NFS	Network File System
NGBB	Next-Generation Backbone
NNSA	National Nuclear Security Administration
NPR	Nuclear Posture Review
NRE	Non-Recurring Engineering
NSCC	National Security Computing Center
NUMA	Non-Uniform Memory Access
nWBS	National Work Breakdown Structure
OCF	Open Computing Facility
OFC	Oxy-Fuel Combustor
OS	Operating System
PCF	Predictive Capability Framework
PDE	Partial Differential Equation
PECASE	Presidential Early Career Award for Scientists and Engineers
PEM	Physics and Engineering Models
PESP	Predictive Engineering Science Panel

PF	petaFLOP/s
PI	Principal Investigator
PKI	Public Key Infrastructure
PLFS	Parallel Log File System
PSAAP	Predictive Science Academic Alliance Program
PSP	Predictive Science Panel
QASPR	Qualification Alternatives to the Sandia Pulsed Reactor
QMU	Quantification of Margins and Uncertainties
R&D	Research and Development
RAIT	Redundant Array of Independent Tapes
RFI	Request for Information
RFP	Request for Proposal
RHEL	Red Hat Enterprise Linux
RMCRT	Reverse Monte Carlo Ray Tracing
RPM	Red Hat Package Manager
SAML	Security Assertion Markup Language
SC	Supercomputing (Conference)
SCC	Strategic Computing Complex at Los Alamos
SCF	Secure Computing Facility
SFI	Significant Finding Investigation
SIMD	Single Instruction, Multiple Data
SLURM	Simple Linux Utility for Resource Management
SNL	Sandia National Laboratories
SNSI	Secret National Security Information
SRN	Sandia Restricted Network
SSP	Stockpile Stewardship Program
SST	Structural Simulation Toolkit
TLCC	Tri-Lab Linux Capacity Cluster
TOSS	Tripod Operating System Software
UGT	Underground Test
UQ	Uncertainty Quantification

V&V	Verification and Validation Program
WAN	Wide Area Network
WBS	Work Breakdown Structure
WESC	Weapons Effects Steering Committee
WEST	Workshop on Exascale Software Technologies
WC	Workload Characterization

Appendix B: Integrated Codes Subprogram (WBS 1.5.1)

Note: The content for the IC subprogram is available upon request from the ASC Program Office.

Appendix C: Physics and Engineering Models Subprogram (WBS 1.5.2)

Note: The content for the PEM subprogram is available upon request from the ASC Program Office.

Appendix D: Verification and Validation Subprogram (WBS 1.5.3)

Note: The content for the V&V subprogram is available upon request from the ASC Program Office.

Appendix E: Advanced Technology Development and Mitigation Subprogram (WBS 1.5.6)

Note: Additional content for the ATDM subprogram is available upon request from the ASC Program Office.

The Advanced Technology Development and Mitigation (ATDM) sub-program includes laboratory code and computer engineering and science projects that pursue long-term simulation and computing goals relevant to the broad national security missions of the National Nuclear Security Administration (NNSA).

Accomplishments

ASC accomplishments from quarter 4, fiscal year 2013, and through quarter 3, fiscal year 2014, are reflected below for the ATDM subprograms.

- Released FastForward2 request for proposal (RFP) and evaluated proposals (LANL)
- Organized the new program element and assigned a program manager/point of contact (LANL)
- Began a task force to determine the physics and workflow requirements for a new weapons performance code that includes the ability to simulate parts of the hostile environment problem and the resulting performance impacts (LANL)
- Assigned a lead for the new code development project (LANL)
- Began tri-lab interactions on the relevant aspects of co-design and other computer science efforts, including the abstraction layers and programming models (LANL)
- Organized new program element and assigned a program point of contact (SNL)
- Oversaw the execution of SNL's portion of the tri-lab Level 2 milestone *Evaluate Application Performance on Advanced Architectures* (SNL)
- Explored design tradeoffs for scheduling within a resilient, asynchronous, distributed-memory task-directed acyclic graph (DAG) runtime using Structural Simulation Toolkit (SST)/macro simulations (SNL)
- Developed an SST/macro implementation of the distributed task-DAG runtime and used it to study the performance and fault-resilience limits of the task-DAG approach for a port of mini-FE on an advanced technology architecture (SNL)
- Based on the results of SST/macro experiments, began implementing components of a resilient, asynchronous, distributed-memory task-DAG runtime to be used for SNL's FY15 Level 2 milestone (SNL)

Level 2 Milestone Descriptions

Milestone (ID#5171): Demonstrate an Initial Burst Buffer Application Programming Interface		
Level: 2	**Fiscal Year**: FY15	**DOE Area/Campaign**: ASC
Completion Date: 9/30/15		
ASC nWBS Subprogram: ATDM, CSSE		
Participating Sites: LANL		
Participating Programs/Campaigns: ASC		
Description: This milestone is a LANL deliverable supporting the development of hierarchical file systems to enable checkpoint restart at scale. This milestone focuses on demonstrating the initial prototype for the burst-buffer API on a test bed or other representative system. The prototype burst-buffer API was delivered in FY14. Evaluating the performance of the API through micro-benchmark drivers and applications such as Partisn and XRAGE will be the focus of this FY15 milestone. This should be demonstrated at the largest scale limited by the burst-buffer test beds available. The API should be evaluated during the integration, and pros/cons of the API will be reported as lessons learned. In addition, performance issues with the proposed burst-buffer hardware architectures will be documented and communicated back to the vendors to drive improved designs for our applications.		
Completion Criteria: This milestone will be completed when: • Demonstrate functioning API with micro-benchmarks, mini-apps, and or one application at largest scale available with burst-buffer test bed hardware. • A report and/or slides have been completed detailing lessons learned, both successes and failures, in regards to performance and initial API.		
Customer: ASC IC		
Milestone Certification Method: A program review is conducted and its results are documented. 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: CSSE advanced architecture test beds		

Milestone (ID#5215): Demonstrate Advances in Proxy Applications through Performance Gains and/or Performance Portable Abstractions		
Level: 2	**Fiscal Year**: FY15	**DOE Area/Campaign**: ASC
Completion Date: 9/30/15		
ASC nWBS Subprogram: IC, ATDM, CSSE		
Participating Sites: LLNL, LANL, SNL		
Participating Programs/Campaigns: ASC		
Description: This milestone is a tri-lab deliverable supporting the ongoing co-design efforts in the program (IC and CSSE) as well as the new ATDM activities. In FY14, a milestone evaluating the performance and underlying bottlenecks of key proxy applications (proxy apps) on advanced architecture test beds or ATS was completed. In addition, each lab has been developing and exploring promising new parallel programming models that will provide abstractions for performance portability, especially at the node level. This milestone focuses on building upon those findings through a combination of internal performance improvements, deeper evaluation of abstractions, and external co-design influence. Each lab will choose one or more ~~at least two~~ proxy applications and refactor them through the use of new programming models and tools, algorithms, or domain-specific languages (DSLs), resulting in either demonstrable speedup, improved portability through abstractions, or as a stretch goal, both. If only one proxy application is chosen, two or more refactored versions will be provided. Improvements will be demonstrated across at least two advanced architectures (test bed or ATS). Performance improvements will be relative to proxy apps and related metrics gathered in the FY14 milestone. Programming abstraction demonstrations will use at least one proxy app developed at another laboratory (in collaboration and agreement with that lab) to demonstrate broad applicability across variable programming styles. Successful and unsuccessful attempts will be reported as lessons learned. The tri-lab co-design project will work closely with the *Forward vendors to make available the studied proxy apps and related data (for example, traces or simulator results) for vendor research.		
Completion Criteria: This milestone will be completed when: • At least two proxy apps (or at least two implementations of one proxy app) from each lab have demonstrated performance improvements or improved portability across two advanced architectures. • A report has been completed by the three labs detailing lessons learned—both successes and failures—in regards to performance and/or portability improvements. • The milestone team has communicated appropriate information, including source code, metrics, trace data, and simulator analysis for use in vendor-focused research.		
Customer: ASC application code teams		

Milestone (ID#5215): Demonstrate Advances in Proxy Applications through Performance Gains and/or Performance Portable Abstractions
Milestone Certification Method: A program review is conducted and its results are documented. 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: ASC advanced hardware; CSSE and IC Staff (ATDM)

Projects for the Next-Generation Architecture and Software Development Product (WBS 1.5.6.2)

This product is focused on long-term computing technology research to influence the shift in computing technology to extreme, heterogeneous architectures and to mitigate its impact and advance its capabilities for Advanced Simulation and Computing (ASC) simulation codes.

Next-Generation Computing and Enablement and Co-Design (LLNL)

Accomplishments in FY14:

- Released FastForward2 RFP and evaluated FastForward2 proposals
- Researched tools and techniques for next-generation computing and contributed to co-design efforts
- Executed LLNL portion of the tri-lab Level 2 milestone to evaluate application performance on advanced architectures

Planned Activities in FY15:

- Conduct co-design activities with co-design centers and vendors, and evaluate next-generation technologies
- Research and develop tools and techniques to effectively utilize emerging next-generation architectures, including tools for measuring impact on power, energy, and performance of applications; next-generation resource management framework; performance modeling; and techniques for input/output (I/O) stack optimizations for future parallel file systems
- Evolve the development environment to include next-generation debugging and to support programming models used in IC
- Participate in the technical management of DesignForward projects

- Execute LLNL portion of the tri-lab Level 2 milestone to demonstrate advances in proxy applications through programming abstractions or performance gains
- Procure and deploy prototypes and leverage test beds to allow exploration of how emerging technologies support ASC applications

FastForward—Industrial Partnerships for Extreme-Scale Technology Research and Development (LLNL)

Accomplishments in FY14:

- Provided technical coordination and contractual management for FastForward contracts
- Issued FastForward2 RFP and oversaw proposal evaluation

Planned Activities in FY15:

- Provide technical coordination and contractual management for FastForward2 contracts

Co-Design and Programming Model Research (LANL)

Accomplishments in FY14:

- Explored next-generation programming techniques in the context of ASC codes/mini-apps
- Defined and extended proxy apps in support of FastForward1 and Trinity with respect to both the Eulerian and Lagrangian application projects
- Extended parallel file-system simulation capabilities for future file systems

Planned Activities in FY15:

- Extend and enhance next-generation programming techniques in the context of an ASC integrated code
- Extend and support program compiler and analysis tool-chain on next-generation architectures for characterization and analysis of ASC applications
- Characterize and validate proxy applications in support of the tri-lab CSSE/IC Level 2 milestone, DesignForward, and FastForward2 efforts, and in support of preparing Eulerian and Lagrangian application project codes for Trinity
- Extend parallel file-system simulation capabilities for hierarchical file-systems (Burst Buffer) and make it a usable tool for design and validation

Programming Models and Abstractions (SNL)

Accomplishments in FY14:

- Oversaw the execution of SNL's portion of the tri-lab Level 2 milestone *Evaluate Application Performance on Advanced Architectures*
- Provided draft technical requirements for ATS-3 request for information (RFI) and draft RFP
- Explored design tradeoffs for scheduling within a resilient, asynchronous, distributed-memory task-DAG runtime using SST/macro simulations
- Developed an SST/macro implementation of the distributed task-DAG runtime and used it to study the performance and fault-resilience limits of the task-DAG approach for a port of mini-FE on an advanced technology architecture
- Based on the results of SST/macro experiments, began implementing components of a resilient, asynchronous, distributed-memory task-DAG runtime to be used for SNL's FY15 Level 2 milestone

Planned Activities in FY15:

- Execute SNL's portion of the tri-lab Level 2 milestone *Demonstrate Advances in Proxy Applications Through Performance Gains and/or Performance Portable Abstractions*
- Execute Level 2 milestone "*Programming Models Analysis for Next-Generation Platforms*" by prototyping asynchronous task-based programming models on Mantevo mini-apps
- Deliver a five-year plan for deployment of Kokkos to ATDM codes in collaboration with the task parallel and data management CS efforts
- Evaluate portability and performance of Kokkos-based proxy applications on the latest relevant next generation testbeds and deliver a formal SAND report of results that summarizes and provides lessons learned from prototype mini-apps to ATDM code teams
- Design and document the application-programming interface for the key-value storage service
- Implement and demonstrate a simple prototype key-value storage service that uses available application memory to share data between tasks within an application
- Design and document abstractions/interfaces required for sharing mesh and particle data
- Design and document abstractions/interfaces required to support task-based programming models and application resilience (for example, local checkpoint/recovery)

- ~~Evaluate the performance and usability of Kokkos in proxy applications representative of implicit finite element production codes~~
- ~~Develop an implementation of an asynchronous many task (AMT) runtime on an advanced technology system~~
- ~~Develop optimized dynamic scheduling and work-stealing methods for AMT runtime~~
- ~~Integrate in-memory data storage capabilities (Kelpie) into AMT runtime~~
- ~~Investigate approaches to reduce data-movement for integrated application workflows~~

DesignForward—Industrial Partnerships for Extreme-Scale Technology Research and Development (LBNL)

Accomplishments in FY14:

- Re-issued the RFP for the System Integration focus areas and managed the award selection process
- Provided technical coordination and contractual management for DesignForward Interconnect contracts

Planned Activities in FY15:

- Provide technical coordination and contractual management for DesignForward contracts in the Interconnect and System Integration contracts

Appendix F: Computational Systems and Software Environment Subprogram (1.5.4)

The mission of this national sub-program is to build integrated, balanced, and scalable computational capabilities to meet the predictive simulation requirements of the NNSA. This sub-program strives to provide users of ASC computing resources a stable and seamless computing environment for all ASC-deployed platforms. Along with these powerful systems that ASC will maintain and continue to field, the supporting software infrastructure that Computational Systems and Software Environment (CSSE) is responsible for deploying on these platforms includes many critical components, from system software and tools, to I/O, storage and networking, to post-processing visualization and data analysis tools. Achieving this deployment objective requires sustained investment in applied research and development (R&D) activities to create technologies that address ASC's unique mission-driven needs for scalability, parallelism, performance, and reliability.

Accomplishments

ASC accomplishments from quarter 4, fiscal year 2013, and through quarter 3, fiscal year 2014, are reflected below for the CSSE subprograms.

- Released CORAL (Collaboration of Oak Ridge, Argonne, and Livermore) RFP evaluated responses, awarded CORAL Non-Recurring Engineering (NRE) contract, and planned for CORAL development environment (LLNL)
- Led the tri-lab process for CTS-1; completed market survey and developed CTS-1 RFP (LLNL)
- Ran two Capability Computing Campaign (CCC) processes on Sequoia platform (LLNL)
- Released Tripod Operating System Software (TOSS) 2.2 (based on Red Hat Enterprise Linux (RHEL) 6.5, the latest release from Red Hat) and initiated development of TOSS 3 (LLNL)
- Extended PISTON, a portable hardware-accelerated visualization library, to BlueGene, graphics processing unit (GPU), and Intel Many Integrated Core (MIC), including distributed memory and unstructured mesh support (LANL)
- Finalized design and developed initial burst buffer application programming interface (BB-API) (LANL)
- Completed PowerWall theater technology upgrade and supported and maintained production visualization systems and tools in weapons programs (LANL)

- Awarded Trinity RFP following establishment of joint technical requirements and the execution of design and independent project reviews (LANL)
- Completed extensive investigation of dynamic random access memory (DRAM) faults spanning LANL, the National Energy Research Scientific Computing Center (NERSC), and Oak Ridge National Laboratory on Cray systems (LANL)
- Established, for the NNSA/ASC program and the Department of Energy (DOE)/Office of Science's Advanced Scientific Computing Research (ASCR), a contract with Micron for research and development (R&D) into Hybrid Memory Cube (HMC) functions in memory, HMC multicube modules, and analysis of search proxy applications (SNL)
- Completed development of Local Checkpoint, Local Restart (LCLR) software, along with runtime API specification, for replacing a failed node during job execution (SNL)
- Introduced new Intel SandyBridge/XeonPhi advanced architecture test bed for porting export controlled code; added two systems with IBM Power 8 and ARM processor nodes, respectively; upgraded NVIDIA boards on another system (SNL)
- After extensive testing, released SST V4.0.0 with new models, including ones for hierarchical memories, flexible network routing, and scheduling for power (SNL)
- Unveiled the High Performance Conjugate Gradient (HPCG) benchmark list at the International Supercomputing Conference 2014 (ISC14), furthering the goal of standardizing on a benchmark more relevant to ASC applications than HPLinpack (SNL)

Level 2 Milestone Descriptions

Milestone (ID#5213): Commodity Technology System-1 Contract Awarded		
Level: 2	**Fiscal Year**: FY15	**DOE Area/Campaign**: ASC
Completion Date: 9/30/15		
ASC nWBS Subprogram: CSSE		
Participating Sites: LLNL		
Participating Programs/Campaigns: ASC		
Description: Based on tri-lab CTS-1 process and review, LLNL successfully awards the procurement for the next-generation tri-lab Linux CTS-1.		
Completion Criteria: Signed contract		
Customer: ASC		
Milestone Certification Method: Signed contract 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: ASC CSSE and FOUS personnel, LLNL procurement staff		

Milestone (ID#5216): Planning for Pre-Exascale Platform Environment		
Level: 2	**Fiscal Year**: FY15	**DOE Area/Campaign**: ASC
Completion Date: 9/30/15		
ASC nWBS Subprogram: CSSE		
Participating Sites: LLNL, LANL, SNL		
Participating Programs/Campaigns: ASC		
Description: This milestone addresses planning for hardware architectures and associated system environments anticipated in the 2016–2021 timeframe for advanced technology platforms. The study will be strongly aligned with the concurrent development of the usage models for the ATS-1 (Trinity) and ATS-2 (Sierra) platforms. Given the ATS-1/2 baseline(s), user and application environment requirements for future ATS will be considered. A review of the applicable R&D landscape will be performed, followed by a gap analysis, and finally a next-steps proposal. Known areas for attention include: strategies for application porting, readiness and scaling, based on expected programming models and tools for application development/execution; strategies for maximizing I/O efficiency as part of an overall computational analysis workflow; strategies for delivering system performance, reliability and associated resource management that enables real use of such systems at their intended capability; strategies for maximizing whatever energy-efficient utilization can be achieved for what are expected to be expensive systems to operate. The ability to deliver next-generation platform environments that provide an effective, efficient computing ecosystem in support of the ASC mission is the driver for this work.		
Completion Criteria: A report covering the strategy to provide the platform environment components needed for successful ASC use of advanced technology platforms.		
Customer: DSW customers and ASC IC and ATDM sub-programs		
Milestone Certification Method: Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion. A program review is conducted and its results are documented.		
Supporting Resources: Tri-lab CSSE staff with input from IC and FOUS staff.		

Projects for the Commodity Technology Systems Product (WBS 1.5.4.8)

This level 4 product provides 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, procurement and integration coordination, and installation. This product also provides market research for future Commodity Technology Systems (CTS).

Production Planning and Integration (LLNL)

Accomplishments in FY14:

- Led the tri-lab process for the next CTS-1
- Conducted a market survey and developed the CTS-1 RFP

Planned Activities in FY15:

- Successfully award the contract for CTS-1, based on tri-lab CTS-1 process and review
- Plan for deployment of LLNL CTS-1 systems

Computing Platform Integration and Deployment (LANL)

Accomplishments in FY14:

- Participated in the CTS-1 market survey
- Provided production support of TLCC2 systems in both the classified and unclassified computing environments

Planned Activities in FY15:

- Continue to operate Luna and the other capacity systems in both the classified and unclassified computing environments
- Provide production support for CTS systems
- Participate in the tri-lab selection for the NNSA ASC CTS-1 procurement

ASC Commodity Systems (SNL)

Accomplishments in FY14:

- Monitored industry hardware and software roadmaps to understand opportunities for cost-effective integration of new commodity technology into future CTS, and implications or requirements for future common computing environment (CCE) software development

Planned Activities in FY15:

- Participate in CTS-1 selection and contract reviews

Projects for the Advanced Technology Systems Product (WBS 1.5.4.3)

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 test bed 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.

Sequoia Tri-Lab Advanced Technology Platform (LLNL)

Accomplishments in FY14:

- Ran two CCC processes
- Continued to investigate optimal performance tuning for specific codes
- Made changes necessary to support running up to 20,000 simultaneous jobs in support of uncertainty quantification (UQ) suites

Planned Activities in FY15:

- Run two CCC processes
- Continue to investigate optimal performance tuning for specific codes

Sierra Tri-Lab Advanced Technology System (LLNL)

Accomplishments in FY14:

- Released CORAL RFP; evaluated CORAL RFP responses and awarded CORAL non-recurring engineering contract
- Negotiated Sierra build contract and submitted for approval
- Completed Sierra Critical Decision (CD)-1/3a
- Provided initial technical coordination and contractual management for CORAL non-recurring engineering and Sierra contracts

Planned Activities in FY15:

- Provide technical coordination and contractual management for CORAL non-recurring engineering and Sierra contracts

- Begin application preparations for Sierra system through Center of Excellence

Hyperion Test Bed (LLNL)

Accomplishments in FY14:

- Supported the scalability testing of the Lustre file system, high performance storage hardware, system software, and application middleware
- Explored new software models to evaluate the use of high performance storage-class memory and the design impacts of storage-class memory on future system software and hardware architectures
- Supported the scalability testing of performance and debugging tools, system software, and application middleware

Planned Activities in FY15:

- Procure and deploy a technology refresh of the Hyperion phase 2 servers, including high performance cluster interconnect, and potentially storage class memory
- Explore new system software models to evaluate the use of high performance storage class memory and the design impacts of storage class memory on future system software and hardware architectures
- Continue to support scalability testing on system software, middleware, storage, and file systems

~~Advanced Architecture Test Bed Research and Development (SNL)~~

~~**Accomplishments in FY14:**~~

- ~~Installed and integrated a pre-general-availability Power 8 node as part of IBM's Early Ship Program (ESP) to support investigating new programming models, evaluation of compilers, and to perform application performance analysis~~
- ~~Installed and integrated multiple APM Xgene ARM 64 bit processors using HP moonshot cartridge technology (McDivitt cartridges) well before general availability (these processors have supported early compiler, performance analysis, and light weight kernel operating system activities)~~
- ~~Installed and integrated an HMC test bed in collaboration with Micron Technologies for the purposes of researching advanced memory technologies~~
- ~~Installed and integrated latest generation Intel Phi nodes on the SNL restricted network (SRN) in support of production code performance analysis~~
- ~~Installed and integrated Intel Silvermont processor to support early investigations of Knights Landing node and core level application and network considerations~~

~~**Planned Activities in FY15:**~~

- ~~Provide platforms to support investigating new programming models and evaluating compilers and application performance (including existing system technology refresh and network relocation based on program needs)~~
- ~~Provide platforms and/or devices for advanced power and energy research and in situ application power and energy analysis~~
- ~~Provide platforms for advanced node and platform-level architecture analysis and investigations supporting next-generation platforms~~

~~Application Performance Analysis (SNL)~~

~~Accomplishments in FY14:~~

- ~~Configured Mantevo mini-apps; ran on advanced architectures test beds to evaluate performance and programming challenges of next-generation architectures~~
- ~~Worked with the selected Trinity vendor and the tri-labs in the implementation of mini-apps and capability applications for procurement acceptance~~
- ~~Developed and deployed (as part of the Mantevo.org suite) an AMR mini-app (miniAMR)~~

~~Planned Activities in FY15:~~

- ~~Work with co-design centers and activities that apply to mini and proxy applications~~
- ~~Apply mini applications in support of the Trinity procurement~~
- ~~Support Level 2 milestone *Using Performance Modeling and Simulation Tools and Techniques to Gauge Key Application Performance Characteristics of the Trinity Platform*~~

Alliance for Computing at Extreme Scale Trinity Advanced Technology System (LANL, SNL)

Accomplishments in FY14:

- Completed an independent cost review
- Completed a technical evaluation and source selection of the responses to the Trinity RFP; evaluated Trinity/NERSC-8 RFP responses and made selection
- Completed the acquisition planning process for contract award
- Completed the CD 2/3b process for procurement approval
- Supported Trinity acquisition activities
- Finalized Trinity procurement
- Awarded Trinity contract

- Updated the existing CCC process to accommodate the ATS platforms

Planned Activities in FY15:

- Provide technical coordination and management for the Trinity contract
- Deliver and install Trinity
- Continue Trinity development and engineering (D&E) collaborations between selected vendor and ACES

Alliance for Computing at Extreme Scale Cielo Capability Computing Platform (LANL, SNL)

Accomplishments in FY14:

- Completed the CCC5 and CCC6 capability campaigns
- Upgraded the Cielo operating environment
- Completed the CD 4 process

Planned Activities in FY15

- Complete the Cielo campaigns for FY15 (CCC7 and CCC8)
- Continue to run Cielo in production capability mode
- Provide operations in support of CCCs

Projects for the Next-Generation Computing Technologies Product (WBS 1.5.4.9)

The Next-Generation Computing Technologies product includes costs for the planning, coordinating, and executing of the next-generation R&D computing technology activities. These activities will prepare the ASC applications and computing environment for the next computing paradigm shift to extreme parallelism, via heterogeneous and/or multi-core nodes.

Next-Generation Computing Environment (LLNL)

Accomplishments in FY14:

- Developed initial LLNL plan for software for the Sierra ATS, including programming model, code correctness, power, resilience, and performance tools
- Explored next-generation topics, including characterization of power consumption of key application codes, evaluation of development environment software on advanced

architecture test systems, performance characterization, and next-generation resource management

- Participated in planning activities for next-generation computing, including joint meetings with ASCR, meetings and workshops with IC, and interactions with academic collaborators
- Conducted co-design activities with ASC and ASCR co-design centers and vendors, and researched and evaluated next-generation technologies

Planned Activities in FY15:

- Develop next-generation CTS and run-time level support, including center-wide resource management, accelerator support, and performance monitoring
- Provide technical coordination for 2017 ASC ATS contracts
- Identify technology gaps in available systems, and procure and deploy prototypes and test beds to allow exploration of how those technologies support ASC applications
- Refine and begin execution of LLNL plan for the software environment for the Sierra ATS

Future Architecture Planning and System Requirements (LANL)

Accomplishments in FY14:

- Provided program and project management for computing platforms, including requirements gathering and analysis
- Identified network and archive requirements for the Trinity and CTS-1 systems
- Participated in site-wide planning for power upgrades for future systems

Planned Activities in FY15:

- Provide program and project management for computing platforms, including requirements gathering and analysis
- Plan infrastructure to support pre-exascale and exascale systems
- Participate in site-wide planning for power and cooling upgrades for future systems

Future-Generation Computing Technologies (LANL)

This project was renamed for FY15 from the FY14 Next-Generation Computing Technologies project.

Accomplishments in FY14:

~~This is a new project for FY15.~~

- Analyzed and implemented data-parallel methods via extensions to Nvidia's Thrust library using volume tracking as a representative algorithm
- Explored and tested data-intensive computing paradigms for in-transit analysis and checkpoint-restart workloads for future development in ASC codes

Planned Activities in FY15:

- Investigate leveraging cloud and big data technology for ASC data analytics
- Research NVRAM for memory and storage hierarchy
- Investigate alternative burst buffer designs for in-situ
- Develop data structures and algorithms for physics code and backend optimizations for data and task parallel
- Implement and extend data-parallel methods via extensions to Nvidia's Thrust library using hydrodynamic algorithms using AMR meshes as a representative algorithm
- Develop in-transit analysis workloads and a data-aware computing interface to allow ASC codes to leverage data-intensive compute models

Architecture Office (SNL)

Accomplishments in FY14:

This is a new project for FY15.

Planned Activities in FY15:

- Support SNL engagement with industry *Forward R&D projects
- Collaborate technically and coordinate with the joint ASC/ASCR R&D project with Micron Technology
- Initiate discussions with industry to determine both technology roadmaps and opportunities for influencing future hardware architectures for ATS-3 and beyond

Heterogeneous Computing (SNL)

Accomplishments in FY14:

- Redesigned Kokkos' thread team strategy for fine-grained parallelism and enhanced from a globally fixed thread team size to kernel-by-kernel selection of thread team size with no degradation in performance
- Implemented the initial minFENL mini-app and exercised an initial version of a manycore enabled sparse linear algebra library built on Kokkos

- Performed user review of Kokkos focused on driving usability improvements, documentation, and tutorials to support broad adoption by the application developer community
- Researched performance interactions between message passing interface (MPI) and KokkosArray levels of parallelism, including data movement and effective overlapping of communication and accelerator-resident computation

Planned Activities in FY15:

- Collaborate with library and application teams to prototype strategies to migrate their capabilities to heterogeneous computing architectures
- Research hierarchical, heterogeneous domain decomposition to address Non-Uniform Memory Access (NUMA) performance concerns and work decomposition in an MPI + central processing unit (CPU) + accelerator strategy

Advanced Architecture Test Bed Research and Development (SNL)

This project's funding remained in WBS 1.5.4.9 and was therefore moved here for Rev. 1 of this document.

Accomplishments in FY14:

- Installed and integrated a pre-general-availability Power 8 node as part of IBM's Early Ship Program (ESP) to support investigating new programming models, evaluation of compilers, and to perform application performance analysis
- Installed and integrated multiple APM Xgene ARM 64 bit processors using HP moonshot cartridge technology (McDivitt cartridges) well before general availability (these processors have supported early compiler, performance analysis, and light weight kernel operating system activities)
- Installed and integrated an HMC test bed in collaboration with Micron Technologies for the purposes of researching advanced memory technologies
- Installed and integrated latest generation Intel Phi nodes on the SNL restricted network (SRN) in support of production code performance analysis
- Installed and integrated Intel Silvermont processor to support early investigations of Knights Landing node and core level application and network considerations

Planned Activities in FY15:

- Provide platforms to support investigating new programming models and evaluating compilers and application performance (including existing system technology refresh and network relocation based on program needs)
- Provide platforms and/or devices for advanced power and energy research and in situ application power and energy analysis

- Provide platforms for advanced node and platform-level architecture analysis and investigations supporting next-generation platforms

Application Performance Analysis (SNL)

This project's funding remained in WBS 1.5.4.9 and was therefore moved here for Rev. 1 of this document.

Accomplishments in FY14:

- Configured Mantevo mini-apps; ran on advanced architectures test beds to evaluate performance and programming challenges of next-generation architectures
- Worked with the selected Trinity vendor and the tri-labs in the implementation of mini-apps and capability applications for procurement acceptance
- Developed and deployed (as part of the Mantevo.org suite) an AMR mini-app (miniAMR)

Planned Activities in FY15:

- Work with co-design centers and activities that apply to mini and proxy applications
- Apply mini applications in support of the Trinity procurement
- Prepare for FY15 IC/ATDM/CSSE ~~Support~~ Level 2 milestone *Demonstrate Advances in Proxy Applications through Performance Gains and/or Performance Portable Abstractions* ~~*Using Performance Modeling and Simulation Tools and Techniques to Gauge Key Application Performance Characteristics of the Trinity Platform*~~

Projects for the System Software and Tools Product (WBS 1.5.4.4)

This level 4 product provides the system software infrastructure, including the supporting OS 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.

System Software Environment for Scalable Systems (LLNL)

Accomplishments in FY14:

- Released updates to TOSS (version 2.1.1–3, 2.1.1–4, and 2.2.2) that included Lustre version 2.4, security updates, and bug fixes
- Released TOSS 2.2 (based on RHEL 6.5, the latest release from Red Hat)
- Tested and deployed a new version of the workload manager, Moab version 7.2, which enabled more direct communication between Moab and Slurm, the computing resource manager, to increase the throughput of jobs
- Developed and deployed an Infiniband (IB) OpenSM Monitoring Service, which provided an application interface to IB diagnostics, monitoring, management, and control functions
- Initiated development of TOSS 3 (based on RHEL 7)

Planned Activities in FY15:

- Provide ongoing TOSS software development and support
- Develop/deploy TOSS 2.X (based on RHEL 6.X)
- Develop/deploy TOSS 3.X (based on RHEL 7.X)
- Develop enhancements to the IB OpenSM Monitoring Service, which provides an application interface to IB diagnostics, monitoring, management, and control functions
- Investigate alternative architectures for commodity Linux clusters (for example, ARM)

Applications Development Environment and Performance Team (LLNL)

Accomplishments in FY14:

- Supported and improved the BlueGene/Q development environment for Sequoia/Vulcan
- Continued to support and further enhance the TLCC2 environment
- Assessed needs for upcoming CTS-1 environment by investigating new hardware, operating system (OS)/TOSS, program development, and programming model requirements
- Supported tri-lab code teams with performance tuning and debugging support in CCC activities on Sequoia
- Continued the development of new performance analysis, modeling, and code correctness capabilities with a particular focus on scalability

Planned Activities in FY15:

- Begin scoping of 2017 system requirements for development environment
- Research and further develop resilience strategies based on SCR Lib for 2015 and future systems
- Provide support for identified emerging programming models
- Plan for development environment for CTS-1
- Support tri-lab code teams in CCC activities on Sequoia

High Performance Computing Systems Research (LANL)

Accomplishments in FY14:

- Analyzed and developed advanced HPC system software, including transparent check-pointing, synchronization, power-capping, distributed job management, and interconnect topology performance models
- Analyzed DOE production system statistics and developed models related to reliability of memory subsystems (includes LANL, ORNL, LBNL systems)
- ~~Analyzed and implemented data-parallel methods via extensions to Nvidia's Thrust library using volume tracking as a representative algorithm~~
- ~~Explored and tested data-intensive computing paradigms for in-transit analysis and checkpoint-restart workloads for future development in ASC codes~~

Planned Activities in FY15:

- Analyze and develop advanced HPC system software, including persistence of deep memory hierarchies, modeling interconnects, and mixed scheduling with traditional MPI and many-task (fine grained-ensemble) workloads
- Analyze and extend models of DOE production system statistics related to reliability, including system characterization, code characterization, and SRAM aging
- ~~Implement and extend data-parallel methods via extensions to Nvidia's Thrust library using hydrodynamic algorithms using AMR meshes as a representative algorithm~~
- ~~Develop in-transit analysis workloads and a data-aware computing interface to allow ASC codes to leverage data-intensive compute models~~

Advanced System Test Beds (LANL)

Accomplishments in FY14:

- Managed and enhanced advanced system test beds for system software, programming models, tools, and applications, spanning both CSSE and advanced IC project use
- Upgraded laboratory infrastructure, including cooling and network

- Upgraded network

Planned Activities in FY15:

- Manage advanced technology computer test beds for CSSE and IC project use
- Refresh technology in Darwin test bed system with state-of-the-art technology and vendor loans of future products, focusing on representing most likely hardware for ATS-1, ATS-2, and ATS-3

System Software Stack Advancement (SNL)

Accomplishments in FY14:

- Defined power/energy API at all levels identified in scope of *Power API Use Case* document
- Vetted foundational aspects of Power API against prototype implementation and documented results
- Enabled two-way communication between Lightweight Kernel (LWK) and dynamic adaptive runtime system
- Completed external review of Power API specification; incorporated feedback and changes into specification
- Conducted initial discussions, including milestones and deliverables, with Trinity vendor targeted to implementing Power API specification

Planned Activities in FY15:

- Perform benchmark analysis of node virtualization layer running on a production ASC platform
- Integrate power/energy measurement and API on Trinity's early-spec platform
- Evaluate effectiveness of LWK and dynamic adaptive runtime system combination for ASC workloads
- Prototype portions of the published Power API specification using PowerInsight as the measurement and control mechanism
- Evaluate the integration of a dynamic runtime system with interconnect capabilities

High Performance Computing Hardware Architecture Simulation (SNL)

Accomplishments in FY14:

- Analyzed the predictive capabilities of mini AMR against the CTH code
- Verified newly introduced SST/Micro threading code via experimentation with Mantevo applications using OpenMP

- Used scheduler and power models to assess the performance impact on energy of proposed cluster-level task allocation strategies integrated with a power estimation methodology
- Continued ongoing usability and integration efforts, as evidenced by the release of SST/Micro V4.0.0

Planned Activities in FY15:

- Report on architectural analysis of Trinity components (pre-test)
- Provide a pre-configured, "abstract machine model" and associated proxy architecture parameters that proxy application developers can use for co-design analysis
- Merge SST (macro/micro) with a unified, parallel discrete event simulator core and a common component interface to allow integration of macro or micro components into the HPC architectural simulation framework

Interprocess Communication System Software Stack (SNL)

Accomplishments in FY14:

- Completed a study of inter-job network interference for large-scale systems, including the development of an MPI benchmark that measures network traffic interference between jobs
- Implemented and evaluated the effectiveness of using single-instruction, multiple-data (SIMD) vectorization and other node-level hardware capabilities to accelerate MPI tag matching
- Released an enhanced version of the Portals 4.0 reference implementation

Planned Activities in FY15:

- Continue to develop and enhance Portals to meet the ongoing interconnect requirements of applications and services
- Study the impact of low-power processors on interconnect performance
- Explore power/energy tradeoffs in the communication software stack

Resilience (SNL)

Accomplishments in FY14:

- Demonstrated favorable trends with parallel scale-up for finite-difference stencils robust to silent data corruption, including an example shock-physics solver that tolerates up to 100,000x higher bit-flip rates with a robust stencil versus a standard stencil

- Demonstrated local failure local recovery (LFLR) resilient computing model for partial differential equations (PDE) mini-app in simulated and real (2048 core Chama cluster) scalable environments with MPI process loss
- Defined prototype LFLR persistent storage API and semantics

Planned Activities in FY15:

- Demonstrate research code framework incorporating one or more representative candidates for robust PDE solvers and hardware silent-error models expected to be applicable at extreme scale
- Develop proof-of-concept example for using symbolically represented constraints to automatically generate a solver algorithm with resilience to a hardware silent-error model
- Deploy local failure/local recovery technologies for checkpoint/restart in a mini-driver application to investigate and qualify its impact on application architecture/design
- Assess the LFLR model with more complex simulation code running on the production systems along with more realistic hard failures, including a loss of multiple processes and alternate recovery (for example, roll-forward) schemes
- Develop and demonstrate an application performance model based on operating system interference to evaluate the performance of resilience mitigation mechanisms
- Using the performance model, characterize the CPU detour footprint of LFLR and communication characteristics most impacted by this mitigation method

Projects for the Input/Output, Storage Systems, and Networking Product (WBS 1.5.4.5)

This level 4 product provides I/O (data transfer) storage infrastructure in balance with all platforms and consistent with integrated system architecture plans. The procurement of all supporting subsystems, 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, 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 high-performance storage system (HPSS) or future hierarchical storage management system disks, tape, robotics, servers, and media. This product also includes relevant prototype deployment and test bed activities. Projects and technologies in the advanced networking and interconnect areas 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.

Archive Storage (LLNL)

Accomplishments in FY14:

- Continued ongoing High-Performance Storage System (HPSS) software development and support, with focus on development and testing of HPSS 7.P, which features partitioned metadata and is currently targeted for General Availability in CY15 as HPSS 7.5
- Deployed HPSS 7.4.2 with conversion to native 64-bit architecture, support for IPv6, dynamic update of devices/drives, Redundant Array of Independent Tapes (RAIT), and enhanced repack of legacy small files into aggregates
- Evaluated, procured, and deployed upgrades to enterprise tape drive environment for increased archive capacity and bandwidth, and positioning for large-scale repack
- Converted from Solaris to TOSS on X86-based platforms and Oracle's Automated Cartridge System Library Software (ACSLS) to v8.3 for Oracle libraries
- Consolidated archive hardware into smaller footprint by retiring over 20 racks of aging gear, creating operational efficiencies and significantly reducing support costs
- Provided ongoing support of currently deployed archival storage systems, including selection, deployment, support, and maintenance of all archival storage hardware and media, customer and interface support, ongoing tech refresh, and data stewardship

Planned Activities in FY15:

- Continue ongoing HPSS software development and support, with focus on inspection, integration testing, and release of HPSS 7.5, which features partitioned metadata
- Begin planning for production deployment of HPSS 7.5, including evaluation and potential procurement and deployment of new HPSS Core Server platforms and metadata disk subsystems to exploit scalability of partitioned metadata
- Develop and deploy hard quota and user notification features in archival quota system
- Begin repack of nine-year-old T10K Gen1 media (1-TB native) to T10K Gen2 media (8-TB native) to minimize data loss due to aging media and to reclaim slot capacity in libraries
- Deploy HPSS disk subsystems to increase disk cache capacity and disk file residency
- Deploy network upgrades from 10Gbe to 40Gbe for increased archive performance
- Provide ongoing support of currently deployed archival storage systems, including selection, deployment, support, and maintenance of all archival storage hardware and media, customer and interface support, ongoing tech refresh, and data stewardship

Parallel and Network File Systems (LLNL)

Accomplishments in FY14:

- Focused user support activities on lscratch1 in support of production CCCs on Sequoia
- Supported the development, testing, and deployment of Lustre version 2.4 in classified and unclassified environments
- Completed Lustre software stabilization allowing the migration of all production file systems to common ZFS-based Lustre
- Actively participated in the continuing community software development efforts of Lustre 2.4 and beyond
- Maintained and supported Lustre and network-attached storage (NAS) file systems, including middleware and higher level I/O libraries for users

Planned Activities in FY15:

- Enhance ZFS-based Lustre metadata performance in support of user and purge performance
- Support the development, testing, and deployment of new Lustre versions in classified and unclassified environments
- Complete analysis of reliability and availability realized through the selective mounting of file systems on SCF platforms
- Deploy file system resources in support of CTS-1 deliveries
- Complete deployment of new NAS home directory hardware in open computing facility (OCF) and secure computing facility (SCF) centers
- Investigate pNFS production viability leveraging the Hyperion test environment

Networking and Test Beds (LLNL)

Accomplishments in FY14:

- Evaluated Open Compute Platform for use as compute, data, and Lustre resource
- Evaluated ARM64 as compute platform, and collaborate with RedHat to address deficiencies in software
- Performed RedHat Enterprise 7 alpha and beta testing
- Evaluated Nvidia Kepler discrete GPUs and drivers
- Continued evaluating and testing Infiniband Federated data rate (FDR), deployed in test bed cluster
- Evaluated virtual machines for data movement

Planned Activities in FY15:

- Deploy small ARM64 cluster for software development and debugging working with RedHat; continue to address software shortcomings
- Support Intel Haswell in TOSS 2 and 3; test and evaluate
- Integrate RHEL7 into TOSS 3 and test
- Evaluate Ares, Stormlake, and Mellanox enhanced data rate (EDR)
- Evaluate and support TOSS 3 in CTS-1 systems

File Systems, Archival Storage, and Networking (LANL)

Accomplishments in FY14:

- Performed an assessment of network file system (NFS) and commercial archival solutions and verified parallel file system software releases (Lustre)
- Provided application readiness and system management personnel support on capacity platforms and continued building an MPI support capability and initiated an OpenMP support capability
- Continued Parallel Log File System (PLFS) development under the EMC Corporation Cooperative Research and Development Agreement (CRADA), including burst buffer integration and support for production and testing with production ASC codes
- Designed a prototype burst-buffer enablement library to insulate application developers from the complexities of next-generation file-systems

Planned Activities in FY15:

- Provide on-going support and testing for production file-systems and HPSS
- Deploy initially an open source or commercial archival solution in LANL production environment
- Provide application readiness support on commodity platforms, including MPI and threading models such as OpenMP
- Prototype and test a burst-buffer enablement library to insulate application developers from the complexities of next-generation file-systems, and schedulers

Production Input/Output Services (SNL)

Accomplishments in FY14:

- Deployed HPSS 7.4 releases integrating RAIT and performance enhancements
- Negotiated ownership and support of the Hierarchical Storage Interface/HPSS Tape Archiver (HSI/HTAR) tools from Gleicher Enterprises for use by ASC

- Completed transfer of all T10KA data media to T10KC high capacity tapes
- Enhanced data transfer capability on inter-site HPC (IHPC) to LLNL rzuseq for SNL code developers

Planned Activities in FY15:

- Finalize HPSS version 7.5 deployment schedule to implement distributed core servers
- Design and prototype v8.1 with partitioned database across multiple systems, with a target of 30,000 file creates per second
- Proceed with development and testing of v8.1

Scalable Data Management (SNL)

Accomplishments in FY14:

- Developed and demonstrated a globally accessible data service for in-memory data storage
- Analyzed topological placement issues related to coupled codes and in-transit data services
- Explored resilience/durability of in-transit workflows, which coincides with the completion of an early career laboratory-directed research and development (LDRD) on distributed transactions

Planned Activities in FY15:

- Develop an I/O mini-app capable of representing SIERRA I/O patterns and demonstrating new capabilities developed by the scalable data management team
- Explore use of alternative storage architectures for SIERRA application workflows, in support of FY16 milestone to demonstrate analysis, visualization, and I/O capabilities for SIERRA

Scalable File Systems (SNL)

Accomplishments in FY14:

- Refactored Sirocco's local storage management service for improved performance; in particular, the log-based on-disk storage service can now achieve near theoretical peak bandwidth to underlying physical store
- Added protocol to accomplish batched I/O and transactional I/O for Sirocco, needed for bulk operation processing

Planned Activities in FY15:

- Implement extended feature support for Sirocco using the peer-to-peer protocols

- Complete performance and correctness testing in preparation for deployment on Trinity

Projects for the Post-Processing Environments Product (WBS 1.5.4.6)

This level 4 product provides integrated post-processing environments to support end-user 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 metadata and scientific data management, as well as general-purpose and application-specific visualization, analysis, and comparison. Research includes innovative data access methods and visualization of massive, complex data—the use of open-source foundations will continue to be an important strategy for development of shareable advanced techniques. The product must develop solutions to address interactivity, scaling, tri-lab access for petascale platforms, and data analysis techniques needed to support effective verification and validation (V&V) and comparative analysis. Solutions for emerging platform architectures may in turn require customization and/or re-architecting of software to leverage hardware features. A continuing emphasis will be placed on tools for improving end-user productivity. The product also provides and supports infrastructure including office and collaborative space visualization displays, mechanisms for image data delivery, and graphics rendering hardware.

Scientific Visualization (LLNL)

Accomplishments in FY14:

- Provided consulting and maintenance for the data analysis and visualization hardware platforms and software environment
- Provided initial start up and ongoing data analysis and visualization support for users of the Max data analysis cluster deployed to support Sequoia users
- Provided operational support for projection systems and other equipment associated with ASC visualization theaters
- Supported large-scale visualization and data analysis efforts, including the creation of movies and visuals
- Developed an initial flow visualization capability using steam-line tracing algorithms to be deployed in Lorenz using WebGL
- Experimented with flow exploration and seeding strategies to determine data access patterns for streamline tracing

- Prepared for next-generation data analysis through research in multiresolution techniques, data compression, and topological methods

Planned Activities in FY15:

- Evaluate, select, and deploy visualization hardware to support ASC data analysis needs
- Continue to maintain the data analysis and visualization hardware platforms and software environment and provide operational support for all visualization facilities, including supporting projection equipment and facilitating the use of the data analysis clusters and associated storage
- Support large-scale data analysis and visualization activities, including supporting ASC scientists with creation of visuals and movies for presenting and analyzing scientific data
- Exploit research results in data analysis and visualization for ASC simulations, including data compression, topological methods, and optimization of streamline tracing algorithm

Scientific Workflow and Data Management (LLNL)

Accomplishments in FY14:

- Released new versions of Hopper and Chopper with a focus on helping users deal with exceptionally large collections of data, including a file transfer wizard that optimizes the transfer path in terms of both speed and efficiency of resources
- Investigated the inclusion of RobinHood-based Lustre metadata in Hopper and Chopper, with the expectation of significantly improving directory list and disk usage operations in Lustre file systems
- Developed and released new versions of Lorenz that support the growing number of users who are turning to Web-based tools for interacting with the computing center
- Extended the MyLC dashboard to securely support operations as alternate users

Planned Activities in FY15:

- Release new versions of Hopper and Chopper with a focus on incorporating MPI and non-MPI based parallelism for copy and directory operations
- Incorporate RobinHood-based Lustre metadata in Hopper and Chopper, significantly improving disk usage and related scanning operations for users
- Extend the MyLC dashboard to include more complete information about changes occurring within the center, and provide users with a variety of ways to subscribe to this information
- Investigate workflow-related frameworks and techniques and prototype elements of an identity management replacement tool

Visualization and Data Analysis (LANL)

Accomplishments in FY14:

- Completed PowerWall theater technology and supported and maintained production visualization systems and tools in weapons programs
- Provided technical review on visualization and data-intensive computing for Trinity and ASC CSSE exascale planning
- Extended PISTON, a portable hardware-accelerated visualization library, to BlueGene, GPU, and MIC, including distributed memory and unstructured mesh support
- Applied in situ data analysis framework to ASC codes and evaluated optimization strategies for data flow in visualization, analysis, and parallel storage systems

Planned Activities in FY15:

- Continue to support and maintain production visualization systems and production visualization tools, including directly with designers, and to support the production integration of visualization hardware for Trinity and CTS
- Move R&D tech transfer to production in-situ, improving feature set and statistics for in situ data analysis framework to additional ASC codes
- Continue development of PISTON portable hardware-accelerated visualization library
- Continue expert technical analysis of visualization and big data for ASC

Scalable Data Analysis (SNL)

Accomplishments in FY14:

- Delivered initial ensemble analysis on the classified network for use in sensitivity analysis for electrical circuit simulations
- Developed and integrated select many-core algorithms into SNL production toolset
- Developed an in-situ capability using Catalyst for applications using the SIERRA toolkit
- Released *ParaView* 4.1, in conjunction with Kitware, Inc., with a number of SNL-provided improvements, including support for a zero-copy infrastructure for the Catalyst in situ library and a redesigned color-map editor

Planned Activities in FY15:

- "Harden" the Catalyst in situ capability through deep evaluation of overheads, including memory and performance

- Begin integration of analysis and visualization capabilities with the Sandia Analysis Workbench (in support of FY16 and FY17 Level 2 milestones related to application workflow demonstrations)
- Prototype integration of multi/many core code into production tools
- Continue *ParaView* and Catalyst releases, with production support
- Deliver scalable analysis and visualization capabilities for Cielo and Sequoia customers

Appendix G: Facility Operations and User Support Subprogram (WBS 1.5.5)

This sub-program provides both necessary physical facility and operational support for reliable, cross-lab production computing and storage environments as well as a suite of user services for effective use of ASC tri-lab computing resources. The scope of the facility operations 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. FOUS also covers physical space, power and other utility infrastructure, and local area network (LAN)/wide area network (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. Industrial and academic collaborations are an important part of this sub-program.

Accomplishments

ASC accomplishments from quarter 4, fiscal year 2013, and through quarter 3, fiscal year 2014, are reflected below for the FOUS subprograms.

- Deployed Sequoia visualization cluster Max (LLNL)
- Deployed expanded Lustre file system hardware (marzen, porter, stout) in advance of ZFS-based software transition (LLNL)
- Integrated Splunk into daily monitoring (LLNL)
- Deployed new and updated existing system status, events, hotline scheduler and hotpad tools for improved user communication and hotline operations (LLNL)
- Completed value engineering design of the new unclassified HPC facility to house unclassified systems, including the next-generation CTS-1 clusters (LLNL)
- Completed 80% of the Strategic Computing Complex (SCC) cooling project that brings water-cooling into the SCC for future equipment requiring water-cooling (LANL)
- Completed SCC power distribution unit consolidation in preparation for new higher density platforms (LANL)
- Saved 36 million gallons of city/well water by using water from LANL's Sanitary Effluent Reclamation Facility (SERF) (LANL)
- Initiated work on SCC facility network for automation and notification for handling electrical and mechanical signals for operating SCC computer room (LANL)

- Delivered user support for Sandia National Laboratories (SNL) users of Sequoia, including Tier 1 issue response, and application porting and tuning support; developed with the SIERRA team a workaround for a loader limitation (SNL)
- Continued to improve collaborative tools and self-help resources, particularly in support of the New Mexico Alliance for Computing at Extreme Scale (ACES), including deployment of joint live chat capability between SNL and LANL support teams, redesign and initial development of HPC OneStop portal and ACES Web pages, and identification of Knowledge Base candidates for expanded self-help (SNL)
- Deployed production version of Lightweight Distributed Metric Service (LDMS) on SNL internal and collaborative partners large-scale production HPC platforms, and prepared a Red Hat Package Manager (RPM) for including LDMS into TOSS distributions (SNL)
- Upgraded SNL's two 10-GE links to LANL to a single 100-G link (SNL)
- Continued to integrate next SARAPE development phases; integrated improved authentication capabilities (SNL)

Level 2 Milestone Descriptions

Milestone (ID#5214): Livermore Computing High Performance Computing Enduring Facility Master Planning—Modernization and Repurposing		
Level: 2	**Fiscal Year**: FY15	**DOE Area/Campaign**: ASC
Completion Date: 3/31/15		
ASC nWBS Subprogram: FOUS		
Participating Sites: LLNL		
Participating Programs/Campaigns: ASC		
Description: All computational equipment will be relocated from B115 to other enduring HPC facilities, eliminating ongoing building maintenance costs to the program. Ownership of B115 and B117 will be returned to the institution to repurpose for other non-load-intensive data center uses. The unclassified server room floor in B453 will be modernized, with all infrastructure relocated temporarily and then returned, reracked, and re-cabled at completion. B453's chilled water plant will be modernized to increase capacity in preparation for the 2017 system.		
Completion Criteria: A report documenting completion of the work will be developed.		
Customer: ASC		
Milestone Certification Method: Professional documentation, such as a report or a set of viewgraphs with a written summary, is prepared as a record of milestone completion. The "handoff" of the developed capability (product) to a nuclear weapons stockpile customer is documented.		
Supporting Resources: LLNL FOUS staff, electrical and mechanical outside subcontractors.		

Milestone (ID#5172): Physical Infrastructure Integration for Trinity		
Level: 2	**Fiscal Year**: FY15	**DOE Area/Campaign**: ASC
Completion Date: 9/30/15		
ASC nWBS Subprogram: FOUS		
Participating Sites: LANL		
Participating Programs/Campaigns: ASC		
Description: Design, build, and integrate under-floor electrical and water-cooling distribution system for Trinity/ATS-1 platform.		
Completion Criteria: Under floor electrical and water-cooling distribution system ready for Trinity hook-up.		
Customer: NNSA/ASC HQ, tri-lab weapons applications community		
Milestone Certification Method: A program review is conducted and its results are documented. 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: LANL facilities team, LANL support organizations		

Projects for the Collaborations Product (WBS 1.5.5.3)

This level 4 product provides programmatic support for collaboration with external agencies on specific HPC projects. This product also includes collaborations with internal or external groups that enable the program to improve its planning and execution of its mission.

Program Support (LLNL)

Accomplishments in FY14:

- Continued FY14 procurement, contract management, and extreme-scale computing planning
- Supported annual HPC Best Practices meeting with Office of Science for FY14, titled *HPC Operations Review Meeting*
- Supported bi-annual Predictive Science Panel (PSP) meetings
- Supported Presidential Early Career Award for Scientists and Engineers (PECASE) awardee

- Managed new PSAAP II program for the six new Academic Alliance Centers

Planned Activities in FY15:

- Continue FY15 procurement, contract management, and program planning needs
- Support annual HPC Operations Review meeting with Office of Science
- Support bi-annual PSP meetings
- Provide contract management and procurement support of tri-lab procurements and system deliveries

Program Support (LANL)

Accomplishments in FY14:

- Supported PSAAP efforts at LANL
- Published ASC eNews newsletter
- Participated in Principal Investigator (PI) and PSP meetings
- Provided LANL support for ASC Headquarters (HQ)

Planned Activities in FY15:

- Support PSAAP II collaborations
- Host PSP meeting
- Publish ASC eNews online newsletter
- Participate in PSP and PI meeting
- Provide LANL support for HQ

Program Support (SNL)

Accomplishments in FY14:

- Organized and hosted fifth Predictive Engineering Science Panel (PESP) meeting and side meetings of PESP sub-panels
- Organized and hosted ASC PI meeting at Kansas City
- Organized attendance, booth, and meeting logistics for Supercomputing 2014 (SC14) Conference
- Supported programmatic needs of the PSAAP II program and the DOE Exascale Initiative
- Managed the SAIC/Leidos contract to provide various administration support for HQ

Planned Activities in FY15:

- Organize and host sixth PESP meeting
- Support external review panel meetings for Qualification Alternatives to the Sandia Pulsed Reactor (QASPR), the Engineering Sciences External Advisory Board, and the Computer and Information Sciences External Advisory Board
- Support programmatic needs of the PSAAP II program
- Complete lead lab responsibilities for SC14 Conference
- Support programmatic needs of NNSA tri-lab ASC program and ASC executive committee

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

Accomplishments in FY14:

- Procured, integrated, and tested several components of the manufacturing visualization capability, including ART DTrack2 optical tracking system, head-mounted display, Virtalis Visionary Render software, Liberty portable magnetic tracking system with 4D wand tracking, and PTC Creo importer; completed software quality and security procedures required for implementation in manufacturing environment
- Demonstrated that a native Creo dataset can be quickly imported into Visionary Render and viewed in immersive 3D stereo with desktop monitors or projected with a stereo projector (the operator was able to view the image with 3D stereo glasses and manipulate items with the 3D wand and track head movement)
- Utilized Penguin cluster to develop and benchmark MPI-based codes for computed tomography and super-resolution imaging in support of stockpile stewardship

Planned Activities in FY15:

- Update the ART optical tracking system with a 3D fly stick to manipulate images; develop a virtual training demonstration with immersive 3D stereo and head and fly-stick tracking
- Demonstrate collaborative viewing of a stereo immersive scene in Visionary Render
- Upgrade the immersive environment with high-resolution stereo projection
- Develop specifications to upgrade the classified simulation modeling terminal servers
- Develop a dynamic virtual factory simulation of the proposed Lithium Production Facility

Projects for the System and Environment Administration and Operations Product (WBS 1.5.5.4)

This product provides requirements planning, initial deployment, configuration management, and ongoing operational support for reliable production computing and storage environments. Activities include system and network administration and operations, user support, hardware maintenance, licenses, and common tri-lab computing environment integration and support.

System and Environment Administration and Operations (LLNL)

Accomplishments in FY14:

- Dismantled and disposed of uDawn, rzDawndev, and Dawn; retired Coastal
- Deployed Sequoia visualization cluster Max
- Deployed expanded Lustre file system hardware (Marzen, Porter, Stout) in advance of ZFS-based software transition
- Continued 24x7x365 monitoring and diagnostics of facility and systems
- Upgraded Weapons & Complex Integration's test and development cluster on the open computing facility (replaced rzalastor)
- Integrated Splunk into daily monitoring
- Procured replacement NFS home directory servers
- Upgraded/nfs/tmp servers with new storage back-end
- Deployed full identity management capability (classified accounts) on SCF by replacing Identity Access Management
- Upgraded to RSA 8 in the secure computing facility and Secret National Security Information (SNSI) environments
- Consolidated infrastructure systems to a virtual machine environment
- Completed Web firewall improvements to support the use of the Atlassian collaboration tools

Planned Activities in FY15:

- Continue to deploy Virtual Machine based infrastructure servers and migrate services to new platforms
- Retire Juno and Graph
- Migrate NFS home directories to new hardware
- Integrate identity lifecycle policies and capabilities with institutional data sources

- Investigate options for replacing the identity management system (IDM) workflow, approvals, and provisioning processes
- Establish distinct development, pre-production, and deployment environments for the security infrastructure
- Implement log-based security event analysis and detection

Hotlines and System Support (LLNL)

Accomplishments in FY14:

- Continued to provide ongoing support services for hotline operations, documentation, and training, including BlueGene/Q training on site at SNL and LANL
- Continued to migrate existing Livermore Computing (LC) Websites to the new LLNL standard Website format
- Consolidated and automated nightly email notifications to users, greatly reducing the volume of email sent while significantly improving the readability of the notifications
- Deployed new and updated existing system status, events, hotline scheduler, and hotpad tools for improved user communication and hotline operations
- Continued to assist users in the migration of applications to the BlueGene/Q architecture
- Began migrating, reorganizing, and consolidating existing online documentation onto the LC Confluence server
- Worked with the Computer Security Organization to streamline the provisioning of new user accounts for all tri-lab users

Planned Activities in FY15:

- Continue to provide ongoing support services for hotline operations, documentation, and training
- Continue to migrate, reorganize, and consolidate existing user documentation to the LC Confluence server
- Learn about accelerator technologies and their software libraries (GPUs, MIC) in preparation for providing support to the user community in their use
- Provide trusted agent support to for National Security Systems Public Key Infrastructure (PKI) on the Enterprise Secure Network
- Become familiar with the Service Now Incident Management software in preparation for migration to it from Front Range in FY16

Facilities, Network, and Power (LLNL)

Accomplishments in FY14:

- Completed value engineering design of the new unclassified HPC facility to house unclassified systems, including the next-generation CTS-1 clusters
- Began a project to bring in electrical equipment that allows for more widely varying voltages in preparation for the 2017 system
- Completed the cutover of the B453 chilled-water system small staging chiller with a larger in-line chiller to increase reliability and reduce nuisance staging of the chilled water system
- Continued to enhance diagnostic and monitoring of IB fabrics on Sequoia and other IB-attached Lustre file systems
- Continued to analyze and evaluate emerging network technologies

Planned Activities in FY15:

- Begin construction of the new unclassified HPC facility to house unclassified systems, including the next-generation CTS-1 clusters
- Begin to purchase long lead electrical equipment to house electrical equipment that allows for more widely varying voltages and block load in preparation for the 2017 system
- Complete commissioning of the B453 chilled-water system cutover project
- Relocate all computational equipment from B115 to other enduring HPC facilities, eliminating ongoing building maintenance costs to program; continue to enhance diagnostic and monitoring of IB fabrics on IB-attached Lustre file systems
- Continue to analyze and evaluate emerging network technologies

System Administration and Storage (LANL)

Accomplishments in FY14:

- Supported HPC systems by conducting ongoing daily system and storage administration with continuous monitoring of production systems and infrastructure servers
- Upgraded ASC systems to TOSS-2
- Ensured workload was carried out by proper configuration of queues and scheduling policies plus daily monitoring and problem resolution relating to workloads running on ASC/HPC computing resources
- Procured NFS servers to replace end-of-life equipment

- Started upgrading Ethernet, Infiniband, and Archive infrastructures in preparation for Trinity system

Planned Activities in FY15:

- Support HPC systems by conducting ongoing daily system and storage administration with continuous monitoring of production systems and infrastructure servers
- Provide support for Trinity (ATS-1) and CTS-1 site preparation project
- Provide support for CTS-1 integration and production readiness

Operations and Procurement Support (LANL)

Accomplishments in FY14:

- Provided 24x7x365 operations and monitoring of ASC/HPC computing resources
- Provided hardware maintenance for ASC/HPC computing equipment
- Coordinated efforts for destruction of Redtail, Yellowrail, and Hurricane platforms
- Provided technical and administrative support for procurement of HPC platforms, supporting hardware and software, and other products and services required by HPC
- Initiated work on SCC facility network for automation and notification for handling electrical and mechanical signals for operating SCC computer room

Planned Activities in FY15:

- Provide 24x7x365 operations and monitoring of ASC/HPC computing resources
- Develop reports for projecting out-year hardware maintenance costs for current and future ASC platforms
- Provide technical and administrative support for procurement of ASC/HPC platforms, supporting facility hardware, software, and other products and services required by ASC/HPC

Computing Platform Integration and Deployment (LANL)

Accomplishments in FY14:

- Provided requirements for SCC floor plan for Trinity and CTS-1
- Participated on the ASC CTS acquisition team for CTS-1 technology and acquisition requirements

Planned Activities in FY15:

- Deploy CTS-1 at Los Alamos

- Develop plan and schedule for system accreditation

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

Accomplishments in FY14:

- Provided on-going consulting and user support services, documentation, and training for LANL and tri-lab users of ASC platforms and architectures
- Partnered with ACES collaboration for initial work on Trinity usage model
- Transitioned smoothly from CCC-5 to CCC-6 on Cielo

Planned Activities in FY15:

- Prepare Trinity (ATS-1) system documentation and training materials
- Develop CTS-1 system documentation and training materials
- Provide ongoing consulting and user support services, documentation, and training for ASC platforms and architectures

Facilities, Networking, and Power (LANL)

Accomplishments in FY14:

- Provided ongoing operations and maintenance of electrical and mechanical systems for ASC computing facilities
- Upgraded SCC power substations in preparation for Trinity system
- Completed power distribution unit consolidation in preparation for new higher density platforms that will reside in the SCC
- Completed 80% of the SCC Computer Cooling Equipment Project
- Drafted version of Next Generation Backbone (NGBB) document
- Provided ongoing operations and maintenance of HPC networking components

Planned Activities in FY15:

- Provide support for Trinity (ATS-1) and CTS-1 platform integration into SCC computing facility
- Provide ongoing operations and maintenance of electrical and mechanical systems for ASC computing facilities
- Integration of NGBB technology in support of Trinity (ATS-1) and CTS-1 platforms

Production Computing Services (SNL)

Accomplishments in FY14:

- Continued operations support for Cielo, RFP activity on Trinity, and coordination with LLNL on Sequoia software stack needs for SNL mini-Sequoia system
- Continued operations of storage systems, archive systems, and production systems supporting ASC and nuclear weapons programs
- Deployed production version of LDMS on SNL internal and collaborative partners large-scale production HPC platforms
- Developed RPM for TOSS to include LDMS
- Provided additional resources for PSAAP program use in the Open HPC network

Planned Activities in FY15:

- Begin construction plans for new computing facility
- Begin procurement activity for next-generation capacity systems
- Perform ACES integration activities for Trinity; engage with the Lawrence Berkeley National Laboratory NERSC production operations team in implementing LDMS
- Continue operations of all production systems

User Support (SNL)

Accomplishments in FY14:

- Provided user support for SNL and tri-lab ASC computing
- Delivered user support for SNL users of Sequoia, including Tier 1 issue response, and application porting and tuning support
- Continued to improve collaborative tools and self-help resources, particularly in support of ACES, including deployment of joint live chat capability between SNL and LANL support teams, redesign and initial development of HPC OneStop portal and ACES Web pages, and identification of Knowledge Base candidates for expanded self-help
- Continued to partner with LANL to strengthen joint user support for ACES platforms; prepared to provide Trinity user support, including beginning development of Trinity usage model document
- Continued to leverage Information Technology Infrastructure Library (ITIL) as a framework for improving the HPC OneStop Service Desk processes and practices

Planned Activities in FY15:

- Provide user support for SNL and tri-lab ASC computing systems

- Develop expertise in support of next-generation architectures and software environments
- Ramp up to deliver user support for Trinity

Facilities, Networking, and Power (SNL)

Accomplishments in FY14:

- Upgraded SNL's two 10-GE links to LANL to a single 100-G link
- Deployed two 10-GE encryptors at each site to double the aggregate available bandwidth
- Managed operation of the DisCom wide area network (WAN)

Planned Activities in FY15:

- Analyze networking technologies for next-generation upgrade of DisCom WAN
- Design expansion of Building 725 computer floor space
- Transition 100GE connection to LANL into production state
- Publish definitive evaluation of power requirements comparing identical TLCC2 platforms (one air cooled, one liquid cooled)

Projects for the Common Computing Environment Product (WBS 1.5.5.6)

The goal of the CCE product is to enable a common environment across the tri-labs that was initially deployed on the TLCC systems. The scope of this product includes funded R&D projects to address gap areas identified by the tri-lab technical working groups.

The CCE working groups and projects focus on a common software stack, including but not be limited to, OS software; application development tools; resource management; HPC monitoring and metrics; and common tri-lab environment issues such as configuration management, licenses, WAN access, and multi-realm security.

System Software Deployment for Commodity Technology Systems

Accomplishments in FY14:

- Released updates to TOSS (version 2.1.1-3, 2.1.1-4, and 2.2-2) that included Lustre version 2.4, security updates, and bug fixes
- Released TOSS 2.2 (based on RHEL 6.5, the latest release from Red Hat)
- Initiated development of TOSS 3.X (based on RHEL 7.X)

- Continued Simple Linux Utility for Resource Management (SLURM) support efforts through tri-lab collaboration
- Initiated development of a tri-lab-coordinated software engineering and release process, accommodating 1) OS development, integration, test and distribution from a central and shared build farm; and 2) patch, module, and software package utilization of the central resource
- Initiated cross project working groups at a tri-lab face-to-face project meeting to tackle software environment deployment, Lustre integration, and IB toolset usage

Planned Activities in FY15:

- Provide ongoing TOSS software development and support
- Develop/deploy TOSS 2.X (based on RHEL 6.X)
- Develop/deploy TOSS 3.X (based on RHEL 7.X)
- Prepare for deployment of the next generation of ASC CTS systems (CTS-1), which may include software integration and testing for the tri-lab environment
- Continue SLURM support efforts through tri-lab collaboration
- Develop identified collaborative system software tasks, including investigation of new architectures (for example, general-purpose graphics processing units (GPGPUs) and ARM), integration of virtualization, logging/monitoring improvements, and testing infrastructure improvements

Programming Environment Development/Support for Tri-Lab Systems

Accomplishments in FY14:

- Evaluated tri-lab needs, with regard to performance analysis and debugging, with evolving MPI+X programming model(s), providing node-centric performance information, power utilization information, and information to help minimize data movement overheads, and developed libquo, a high-level programming interface for codes that may benefit from evolving process binding policies during their execution
- Provided MVAPICH enhancements for better security; evaluated MPI performance across architectures and process and memory binding policies
- Completed development with ORNL to add their enhanced collectives into Open MPI 1.7.4 release
- Delivered enhanced capabilities addressing user-identified needs for the TotalView debugger through the BIGCAT tri-lab collaboration and scalability efforts
- Added advanced capabilities in the Components Based Tools Framework (CBTF) to enhance available experiments and use in tri-lab developed tools (including support for threading, I/O, and memory usage analysis)

Planned Activities in FY15:

- Validate deliverables on tri-lab contracts for TotalView BIGCAT effort and open-source tools contracts
- Provide user interface enhancements to CBTF
- Provide enhancements and bug fixes to Open MPI/MVAPICH based on tri-lab need; assess MPI performance across many architectures; assess the impact of process and memory binding policies on application performance; and provide results to end users
- Continue development and support efforts for debuggers, performance analysis tools, and MPI as programming models and architectures evolve

High Performance Computing Environment Integration for Tri-Lab Systems

Accomplishments in FY14:

- Released SARAPE updates to securely and safely manage personal data within SARAPE required by new LLNL EZid system
- Incorporated new security assertion markup language (SAML) capability (beginning with the tri-labs), allowing SARAPE users to log in through their home site, which communicates authenticated data to certain SARAPE fields from corporate databases, thus simplifying the local approval processes while providing verified data to the target site
- Added PSAAP II universities and partners to the SARAPE process, including identifying and training Guest Processing Agents at each university site during Q1, and started managing PSAAP user accounts at the tri-labs during Q2
- Continued Workload Characterization (WC) Tool efforts to meet new and/or expanded ASC HQ reporting requirements; addressed issues in evolving tri-lab computing environments; deployed RAILS 3.x version of WC Tool

Planned Activities in FY15:

- Develop increasingly automated functions in SARAPE, including mySARAPE page to allow authenticated users fuller access to account requests and status at all sites
- Migrate CCE tri-lab activities tracking and documentation from gforge to Confluence Wiki or other appropriate repositories
- Continue WC Tool efforts to meet new and/or expanded ASC HQ reporting requirements; address issues in evolving tri-lab computing environments; investigate and develop streamlined ASC HQ reporting tools

Monitoring and Metrics Integration for Tri-Lab Systems

Accomplishments in FY14:

- Continued development of Splunk tools as needed across the sites (LANL, LLNL, SNL), including Splunk filters for syslog information that is site specific
- Deployed LDMS for use as common data collection, transport, and storage tool on tri-lab HPC systems, with RPM packaging deployed on Chama and bi-lab Dedicated Access Time session conducted to analyze application performance impacts of monitoring
- Began investigation of how expected architectural changes and increased scale will impact the ability to effectively monitor; analyzed information pertinent to application performance and system operation
- Began investigations into monitoring on the Intel Phi co-processor with respect to fidelity and both Phi and host impact

Planned Activities in FY15:

- Continue development of Splunk tools as needed across the sites (LANL, LLNL, SNL)
- Explore environmental, resource utilization, and health-testing-related HPC monitoring and analysis tools and infrastructure currently being developed/utilized across the tri-lab (for example, Cerebro, Gazebo, LDMS, Lorenz)
- Explore opportunities for collaborative development, integration, and deployment of monitoring and analysis tools and infrastructure across tri-lab ASC resources

Projects for the Special Purpose Facilities, Systems, Operations, and Support Product (WBS 1.5.5.7)

This product provides special purpose high performance computing resources to the DOE community and the necessary support and maintenance of these systems and facilities. This includes special security controls and special purpose facilities in addition to the standard high performance computing operations and support activities necessary to support these resources.

Exploitation (LLNL)

Accomplishments in FY14:

- Delivered several reports and provided briefings NNSA

Planned Activities in FY15:

- Deliver studies of interest and provide briefings to NNSA

High Performance Computing and Code Support (LLNL)

Accomplishments in FY14:

- Supported and provided system administration services for special-purpose networks and clusters
- Adapted physics to codes to support foreign analysis

Planned Activities in FY15:

- Provide additional hardware and system administration services for special-purpose networks and clusters
- Adapt physics to codes to support foreign analysis

Special Purpose Computing (LANL)

Accomplishments in FY14:

- Provided ongoing operations and maintenance for computing facilities
- Provided luster hardware and software support
- Performed Weapons Effects Steering Committee (WESC) project startup

Planned Activities in FY15:

- Provide ongoing operations and maintenance for computing facilities
- Provide luster hardware and software support
- Continue work on WESC project

Special Purpose Computing (SNL)

Accomplishments in FY14:

- Continued operations of storage systems, archive systems, and production systems supporting the LLNL, LANL, and SNL National Security Computing Center (NSCC) programs
- Acquired a flexible computing platform for the NSCC to provide capacity computing and, when needed, expanded capability computing (Dark Bridge upgrade)
- Supported porting activities, problem solving and security approvals for tri-lab codes
- Provided debugging and visualization tools as requested by remote customers
- Began addressing user support needs for the NSCC, with ad hoc user support and initial planning sessions for defining the support process

Planned Activities in FY15:

- Continue operations of computing platforms, storage subsystems, and data archive
- Expand capabilities for remote access, data transfer, and remote graphics services
- Implement COI data protection mechanisms
- Initiate procurement activity for NSCC computing resources
- Complete security plan and usage models
- Fully deploy a user support process for NSCC

Appendix H: Academic Alliance Centers

The cooperative agreements with the new PSAAP II Centers were completed in mid-FY14, and funding was released in March of 2014. Accomplishments listed below represent those from the time the funding was received until the end of FY14.

University of Utah

The Uncertainty Quantification-Predictive Multidisciplinary Simulation Center for High Efficiency Electric Power Generation with Carbon Capture

High-Level Accomplishment:

- Integrated VisIt (LLNL scalable visualization tool) into Uintah to allow for VisIt builds to seamlessly read Uintah data across all HPC machines

Accomplishments in FY14:

- Developed a version one interface between the Utah large eddy simulation (LES) coal combustion application, Arches, and the DSL, Nebo; refactored Arches to provide DSL functionality for clear and concise interface to Uintah task scheduling and data warehouse variable retrieval
- Completed formulation of the conditional quadrature method of moments (CQMOM) for computing multivariable Eulerian particle distributions for the pulverized coal combustion application
- Implemented a two-step devolatilization model in Arches, allowing for coal type dependency to be derived from the more complete but complex CPD devolatilization model; tested and validated it for the Utah SUFCO coal with experimental data taken from the University down-fired Oxy-Fuel Combustor (OFC)
- Demonstrated reverse Monte Carlo Ray Tracing (RMCRT) for a virtual radiative heat flux radiometer; used in a UQ analysis for validation with laboratory experiments
- Completed validation with Arches, employing a range of experimental data from the laboratory scale through to the Alstom Boiler Simulator Facility (BSF); built on this validation (the first LES prediction was made of a full-scale oxy-coal boiler)
- Held the Uintah Deep Dive 2014, which was an interactive discussion with national lab and Utah computer science experts to detail the Uintah Computational Framework and to learn more about analogous projects being pursued at the Labs

Planned Activities in FY15:

- Make available at the labs the Uintah runtime scalability improvements to reach the size of all HPC machines

- Perform in-situ visualization and analysis
- Extend DSL implementation to full Arches application
- Extend the Discrete Ordinates Method for radiative heat transfer to include anisotropic scattering; evaluate to determine the optimum ordinate directions for oxy-coal combustion application
- Incorporate models for coal particle fragmentation, particle deposition, and late stages of burnout into Arches; evaluate with formal validation and UQ
- Develop and teach foundational graduate course on validation with UQ with the University of Utah, University of California at Berkeley, and Brigham Young University

University of Illinois, Urbana-Champaign

Center for Exascale Simulation of Plasma-Coupled Combustion

High-Level Accomplishment:

- Designed specific physics model (two-temperature flow-like plasma, two-step chemistry) for ASC's year-1 predictive simulation, with flexibility to introduce more detailed physical models for subsequent predictions

Accomplishments in FY14:

- Designed codelet-0 and codelet-1 as representative of PlasComCM to facilitate development and testing of exascale tools
- Serial profiled and optimized codelet-0 and, based on that, PlasComCM, to understand opportunities for vectorization, a first step toward refactorization and implementation on heterogeneous systems
- Designed a dielectric-barrier discharge (DBD) plasma jet orifice actuator that shows an order-one effect in stand-alone experiment on both H2 and CH4 flames
- Completed over-decomposition analysis of codelet-1 using ROSE and AMPI
- Designed specific physics model (two-temperature flow-like plasma, two-step chemistry) for year-1 predictive simulation, with flexibility to introduce more detailed physical models for subsequent predictions
- Rewrote codelet-0 for in OpenCL and OpenMP/MPI to provide variants for analysis of performance on heterogeneous systems and facilitate subsequent development

Planned Activities in FY15:

- Complete design and acquire data (turbulence PIV, combustion/plasma species, temperatures) for year-1 target sustained combustion prediction
- Perform full predictive simulation and critical evaluation of prediction quality

- Complete development of codelet-2 as a model for bridging to GPUs as a surrogate for accelerators anticipated on exascale systems
- Perform detailed inference-based UQ of reduced models for spark-induced combustion ignition
- Complete planned experiments on electrode degradation and develop physics-based models
- Organize and run the first Workshop on Exascale Software Technologies (WEST) near an NNSA lab

Stanford University

Predictive Simulations of Particle-Laden Turbulence in a Radiation Environment

High-Level Accomplishment:

- Completed simulations of coupled turbulence/particle/radiation in periodic boxes and demonstrated self-sustaining mechanism of coupling between turbulence, particle transport, and radiation

Accomplishments in FY14:

- Analyzed turbulence/particle/radiation coupling and determined controlling parameters and definition of weak/strong coupling regimes as target for experimental campaign
- Completed simulations of coupled turbulence/particle/radiation in periodic boxes and demonstrated self-sustaining mechanism of coupling between turbulence, particle transport, and radiation
- Designed experimental apparatus, identified particle and lamp characteristics and radiation loading
- Developed Liszt 2.0 in Terra/Lua; formulated relational representation of meshes and implementation of particle primitives in Liszt 2.0
- Designed and implemented Soleil (turbulence/particle/radiation code in Liszt 2.0) and demonstrated single-CPU computations
- Initially implemented conjugate gradient and fast direct solvers in the Legion C++ API

Planned Activities in FY15:

- Demonstrate Liszt/Legion integration and develop Liszt mapper for Legion
- Demonstrate Soleil on CPU/GPU systems and large-scale clusters
- Simulate fully developed turbulent duct with particles and radiation forcing on large-scale clusters and demonstrate scalability

- Develop verification suites for single-particle transport under radiation
- Measure heat transfer loads for weakly coupled case and compare to simulations
- Analyze radiation modeling errors from snapshots of coupled simulations using Monte Carlo Ray Tracing

University of Florida

Center for Compressible Multiphase Turbulence

High-Level Accomplishment:

- Ported Rocflu (the Center's multiphysics code) on Mustang (LANL) and Vulcan (LLNL) for the demonstration problem (macroscale); fixed a number of compile issues; coupled Rocflu to Dakota for carrying out bundled runs; blending parallel post-processing subroutines (Paraview format) with Rocflu

Accomplishments in FY14:

- Ported Rocflu (the Center's multiphysics code) on Mustang (LANL) and Vulcan (LLNL) for the macroscale demonstration problem; fixed a number of compile issues; coupled Rocflu to Dakota for carrying out bundled runs; blended parallel post-processing subroutines (Paraview format) with Rocflu
- Developed 3D meshes at microscale to study shock-particle interaction for single-layered cubic array; performed suite of 3D inviscid simulations to determine Mach number/volume fraction dependencies on force history for shock-particle interaction
- Built CMT-Nek as a trunk off Nek-5000
- Developing macro/meso scale models for the university's framework for the uncertainty budget; assimilated Rocflu with Dakota for predicting macro/meso-scale responses by constructing surrogate models
- Identified target kernel as matrix multiplier in Nek5000, which forms the basis for the Center's new code, CMT-Nek; carried out a performance analysis on the matrix multiplier using CHiLL and identified the fastest variants
- Used MonEQ power API to measure power on IBM BG/Q during runtime
- Completed initial computation-time estimation experiments (Kriging) and published a manuscript detailing results; established foundation structures and methods for behavioral emulation and validated the methodology using proof-of-concept micro- and meso-scale experiments; published a conference manuscript detailing the results

Planned Activities in FY15:

- Speed up Rocflu and test its scalability to O(10,000) processors/cores at the macroscale; implement new physics-based models from the university's DNS microscale simulations; implement and test real EOS and study the effect of different

initial particle distribution; improve the unsteady force model to track Lagrangian particles

- Set up grid generation for 3D simulations for FCC and BCC geometries at microscale
- Implement two-way coupling for CMT-Nek of the Eulerian-Eulerian approach to dispersed phases; implement point-particle models to represent polydisperse phases
- Develop a framework to combine predicted responses of different models for uncertainty budget (that is, 1D, 2D, and 3D) using a multifidelity surrogate
- Explore alternative methods of application decomposition and interpolation schemes to optimize computation-time estimators; explore efficient synchronization and congestion modeling techniques and evaluate their speed, accuracy, and scalability tradeoffs for BE; and scale FPGA-based simulator prototype to multiple devices

Texas A&M University

Center for Exascale Radiation Transport

High-Level Accomplishment:

- Performed transport calculations using the PDT transport code with 128k cores with an efficiency of over 70 percent, and performed calculations using over 1 million parallel processes

Accomplishments in FY14:

- Performed transport calculations using PDT transport code with 128k cores with an efficiency of over 70 percent; performed calculations using over 1M parallel processes
- Extended parallel performance model for PDT, thereby improving ability to correct flaws and improve efficiency
- Began preliminary experiments to exercise the experimental system that will be used for calibrating the first impurity model (IM1)
- Identified quantities of interest for IM1
- Performed preliminary testing of an aSA multigrid algorithm for least-squares Sn formulation and obtained excellent results
- Developed an exponentially-convergent 1D Monte Carlo algorithm for thermal radiation transport in the high-energy density regime

Planned Activities in FY15:

- Perform transport calculations with PDT transport code using nested parallel data structures and algorithms on 384k cores
- Develop hierarchical system models and use these models to guide data distribution and computation in STAPL components used by PDT

- Extend parallel sweep performance model to include iteration estimates and memory use
- Complete the IM1, solid block, and single–gap ABC experiments together with the associated UQ analysis
- Demonstrate a neutron transport validation problem performed with the thermal radiation transport solver in PDT
- Implement an unstructured polyhedral mesh parallel sweeping capability in PDT transport code

University of Notre Dame

Center for Shock Wave Processing of Advanced Reactive Materials

High-Level Accomplishment:

- Demonstrated for predictive science the quasi-steady computational theory of homogenization using micro-solver, *PGFem3D*, and ported it to the LLNL Vulcan computer

Accomplishments in FY14:

- Demonstrated the quasi-steady computational theory of homogenization using micro-solver, *PGFem3D*, and ported it to the LLNL Vulcan computer
- Derived and implemented the Lagrangian-Eulerian Compatibility (LEC) condition
- Initiated the image-based modeling, at crystal, layer, and particle levels
- Performed extensive verification using Enhanced Verification Test Suite for Physics Simulation (EVTS) codes, and the Method of Manufactured Solutions (MMS)
- Initiated validation experiments (micro, micro-to-macro, and macro-scale tests)
- Performed analysis of existing Macro- and micro- (M&m) codes, prototyping in MPI
- Ported Eulerian Macro-code, *WAMR*, to HPX
- Created C-SWARM architecture plans, defined initial Domain Specific embedded Language (DSeL) specifications and software implementation roadmap
- Integrated verification and software engineering practices
- Integrated DSeL specifications with M&m code structures and HPX requirements
- Integrated image-based modeling between predictive science and experimental physics plans

Planned Activities in FY15:

- Develop mini-apps in HPX

- Develop suitable phenomenological constitutive equations, chemical kinetics, and phase transformation models
- Identify UQ characteristics and couple C-SWARM with DAKOTA
- Validate selected Macro- and micro-properties for Ni/Al
- Continue C-SWARM software architecture development, DSeL, and mini-apps installment
- Continue performance metrics assessment; prototype graph library with M&m codes
- Develop transient Micro-scale model and time integrators
- Implement mini-apps and review the C-SWARM specifications
- Validate selected properties using phenomenological models and integrate with software engineering practices
- Integrate DSeL software and system modeling with C-SWARM architecture plans, and integrate mini-apps with M&m codes