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ASCI Program 4Q FY99-Quarterly Progress Report Unclassified Projects

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U.S. Department of Energy

Lawrence
Livermore
National
Laboratory

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ASCI Program 4Q FY99 - Quarterly Progress Report Unclassified Projects

Lawrence Livermore National Laboratory

Problem Solving Environment (PSE)

LLNL Quarterly Progress Report for PSE - 4Q FY99

- **Principal Investigator - Terri Quinn (quinn1@llnl.gov, 925-423-2385)**

- **Project Description**

PSE is made up of four technical areas, ASCI Simulation Development Environment (ASDE), Data Exploration and Management (DEM), Data Transfer and Storage (DTS), and Distributed Systems (DS).

ASDE (Mary Zosel, PI)
The goal of ASDE is to create a truly scalable simulation development environment across ASCI platforms. Specific objectives are to improve the environment to accelerate application development, to improve reliability of codes, and to enable better scalable performance.

DEM (Sam Uselton, PI)
DEM's effort is to provide an interactive environment for efficiently and visualizing massive amounts of data. WE are working to help scientists spend more time concentrating on data understanding by providing tools that both enhance interactions and minimize unnecessary manipulations of data.

DTS (Steve Louis, PI)
The goal of DTS is to provide multiple gigabytes/sec parallel data transfer, multiple petabytes of archival mass storage, and new architectures for "end-to-end" I/O all helping to ensure the highest utilization of ASCI resources.

DS (Barry Howard, PI)
DS consists of secure networking, secure distributed computing, and resource management for ASCI platforms. These three research and development activities are fundamental to the creation of the basic infrastructure for the ASCI computing environment.

- **Accomplishment Highlights**

Baby-white System was integrated into our test bed. Baby-white is 16 NightHawk 1 nodes in four frames with peak capability of 114 GFLOPS. It is a prototype node for the ASCI white system. A write-up appeared in the ASCI Update newsletter dated 9/99.

PFTP deployment for HPSS was completed 9/29. PFTP deployment consists of delivery into production of the ability to use PFTP to stripe from the SKY machine directly to 4-wide HPSS tape in the SCF. We are seeing a 30MB/sec file transfer rate direct to tape with this new capability.

We made two improvements in our simulation development environment. We released a new version of TotalView in July, including new features for scientific notation default variable display, non-threaded performance monitoring on the IBM platforms, and enhanced structured array displays. Also we released the updated sPM604e performance monitor code which supports process and thread measurements on an SMP processor.

A standalone 2-d Lagrange code for single fluid gas dynamics was developed and integrated into the SAMRAI framework. This code has been tested against several test problems, namely, the Noh, the Sedov blast wave, and the interacting blast wave problems. We can now run multiple patch, single level calculations in parallel. A remap capability was also developed and incorporated into the SAMRAI framework, allowing us to run either in Lagrangian or Eulerian (i.e., Lagrange plus remap) mode.

In our Scientific Data Management project we released two tools as part of our meta-data strategy. We are using meta-data as a way to provide quick analysis of simulation data sets. We released the production version of Enotes. This is a meta-data editor and browser that has been deployed along with Eserver on a customer's network. ASCI scientists are using the tool for creating and viewing weapons information records. We have a tool to automatically generate meta-data for simulation runs called SimTracker. We released a production version of this too this quarter. SimTracker has been deployed with two LANL and two SNL code systems and it is in process of being deployed with another SNL and LANL code system. Interest continues to grow in SimTracker, as evidenced by the many requests we get for the software. Development is being done both at LLNL and SNL, with new user-requested features being added on a continuous basis.

An unstructured-grid component of our linear solvers was developed and was integrated into two codes. Currently both BoomerAMG (our parallel algebraic multigrid solver) and PILUT (our parallel incomplete factorization solver) are available. More work is needed to provide additional solvers, test and tune, etc. Initial indications of the usefulness of hypre in the two codes are extremely encouraging.

• Milestone Status

The past two PSE LLNL quarterly reports reported on milestones identified in our project plans. These contain IP milestones and lower-level milestones. DOE has asked to start reporting on IP milestones only. This report does that.

Milestone: Evaluate Current State of CBE Deployment and Create Plan to Remedy missing Features and tools
Status: Dropped
Expected Completion Data: N/A
Impact: There is a risk that some code team needs will not be met as soon as they like.
Remediation: This is being done on an ad-hoc basis.

Milestone: TotalView-Additional Feature Prototype Release Q4
Status: Completed in July

Milestone: Thread Safety Analysis
Status: Not complete - Unknown - we have dropped continued funding of the ANL work - so don't know when they will finish their ADI3 interface.
Expected Completion Data: unknown
Impact: Most users use MPI (MPICH) in a basically safe way, but the lack of the ADI3 interface is more serious, because it means that all LLNL users must stop using MPICH and move to MPI when GangLL is enabled on our systems. We will no longer have MPICH as a back up.
Remediation: PNNL is working on a LAPI version of MPICH that will allow it too work under GangLL. (Also months late - but we are not funding them, so have no leverage.) Current plan is to tell users they must move to IBM's MPI. Ideally, continued funding for ANL will be found to continue to encourage the ADI3 work that allows thread safety.

Milestone: ASCI Capps Codes: Complete Initial Set of Applications for the ASCI Capps Code Suite
Status: 90% complete Three apps are close to release. However in the current unsettled security climate, we will not attempt to go into the
Expected Completion Data: unknown – waiting on review

Impact: none
Remediation: none

Milestone: Finish an AMR Lagrange Application in Both 2d and 3d for Shock Hydrodynamics
Status: not complete – has a different funding source for FY00 The original milestone was also based on being able to use source code for certain kernels and/or as reference material. However, we have so far been unable to obtain the needed source code. The possibility of using the source on this project in the future remains uncertain.
Expected Completion Data: FY00
Impact: As this work is a speculative research project, there is no direct impact on SAMRAI or any other project.
Remediation: Due to unavailability of the needed source codes, we are developing all computational kernels "from scratch" using the open literature and unpublished tech reports.

Milestone: Develop new methods for adaptive mesh refinement - linear solver
Status: Delayed to Q3 FY00, now funded under ASCI Apps
Expected Completion Data: Q3 FY00
Impact: The impact is minimal because the code teams do not need this capability until next calendar year.
Remediation:

Milestone: Development of a Parallel Solver for Differential-Algebraic Equation (DAE) Systems
Status: Complete

Milestone: PVODE and KINSOL Extensions and Preconditioners Suitable for Classes of PDE-Based Problems
Status: Complete

Milestone: Scalability and Bandwidth Improvements to MPI-IO for HPSS
Status: 50% complete
Expected Completion Data: 2/11/00
Impact: Since we have not deployed HPSS release 4.1 that contains the MPI-IO interface, there is little impact due to this delay.
Remediation: none needed

Milestone: Research Report on IPv6 Optimizations for SMP Architectures
Status: 66% complete
Expected Completion Data: 4/6/00
Impact: Delays FY00 IPv6 VIA work start
Remediation: Dropped the performance evaluation for multi-threaded SMP stack.

Milestone: Extend DFS/HPSS to ASCI DFS users
Status: Delayed due to HPSS rel 4.1 deployment delays. HPSS rel 4.1 includes the DFS
Expected Completion Data: Q2 FY00
Impact: Little impact since DFS is not yet widely used.
Remediation: none needed

Milestone: Collaborate with Transarc to improve DFS over WAN
Status: dropped due to lack of manpower
Expected Completion Data: Q4FY00
Impact: We may not be getting the best performance of DFS over the wide area network. This effort was to use the expertise of Transarc to evaluate and tune DFS performance.
Remediation: none needed

Milestone: HPSS Release 4.2
Status: 40% complete
Expected Completion Data: 12/29/00
Impact: Release 4.1 and its sub-releases incorporated items that were destined for R4.2 which minimized the impact of this collaboration-wide product slip. Delay of R4.2 slips the availability of functionality to HPSS users and administrators such as improved security (ACLs) and increased scalability.
Remediation: Eliminate some Release 4.2 functionality to shorten schedule.

Milestone: Deploy HPSS Client Software
Status: dropped - not needed since pftp solution is satisfactory
Expected Completion Data: n/a
Impact: n/a
Remediation: n/a

Milestone: Requirements and Design for Release 5.0
Status: 0% complete
Expected Completion Data: 3/30/01
Impact: The product-wide release slip will delay the delivery of Release 5.0 functionality to users and administrators.
Remediation: Tighten HPSS release cycle times by limiting the amount of functionality attempted by a single release. Schedule more sub-releases as necessary.

Milestone: Complete Development of a Gatekeeper Policy Module
Status: 66% complete - this software is now being rolled into HPSS Release 4.2
Expected Completion Data: 12/29/00
Impact: The new Gatekeeper design made it a more integral part of the HPSS product. General availability of the scheduling capabilities for HPSS administrators will slip.
Remediation: Attempt to deploy Gatekeeper functionality early at LLNL. This will depend on significant local modification and a study of the feasibility of such an approach.

Milestone: Query Access to Simulation Data - Investigate alternate strategies for providing fast query access.
Status: 60% Contractor participating in this activity had resource problems.
Expected Completion Data: 3/23/00
Impact: Delayed evaluating commercial technology and assessment for its usefulness for ASCI scientific data. This is turn delay implementing a prototype system.
Remediation: none needed

Milestone: Complete and Deploy E-Search; Meta-data Search Tool
Status: not complete – We completed the integration of the Esearch front-end into Emajor. That was mostly a GUI task. We have not acquired from Sandia or deployed the Esearch back-end (the guts of the tool that does all the work.
Expected Completion Data: 12/30/99
Impact: This delay has not had an impact because of the DCE and security plan delays.
Remediation: none needed

Milestone: Report on the Feasibility of Usefulness of Commercial Data Mining Tools
Status: 50% complete - We had difficulty getting evaluation licenses for several of the products we are evaluating. The summer student assigned to work evaluating several products was unable to complete the task in the time allotted since we underestimated the amount of startup time the student needed.
Expected Completion Data: 11/30/99
Impact:

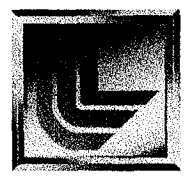
Remediation: We've prioritized and reduced the number of packages we are evaluating. We are evaluating packages that are parallel capable and can work on high-performance computing platforms and meet a minimum data size requirement.

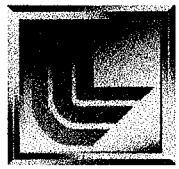
• Issues

DOE security issues continue to delay PSE deliverables in Distributed Systems due to personnel being called on to higher priority tasks and to other PSE projects like SDM which are being delayed because security plan approvals are slow in coming.

Tightening of security for lab interactions with foreign nationals is hindering our collaborations with universities and other research labs.

Distance and Distributed Computing (DISCOM^2)





LLNL Quarterly Progress Report for DisCom^2 - 4Q FY99

- **Principal Investigator – Dave Wiltzius**

- **Project Description**

The Distance and Distributed Computing and Communication (DisCom^2) Program is intended to deliver key computing and communications technologies that complement the ASCI vision. DisCom^2 will create the technologies to efficiently integrate distributed resources with high-end computing resources at a distance.

- **Accomplishment Highlights**

Parallel file transfers were demonstrated on the LLNL-SNL/CA testbed between LLNL computing resources. This was a demonstration of PFTP between IBM SP2 Baby and the unclassified SGI visualization server over 4 Fast Ethernet paths.

The lossless compression effort demonstrated a factor of 5-7 compression (current products offer about a factor of 2 lossless compression). However, due to prioritization of efforts for FY00, this compression effort was terminated as of the end of FY99.

Purchased and deployed a 8 nodes of a 4 processor Compaq SMP with a Quadrics switch. This SMP cluster will run Linux. Starting in FY00 development on this cluster will create an application environment that is very similar to the proprietary UNIX environment provided by Compaq for their SMP clusters.

- **Milestone Status**

SP2 Pilot Extension Subproject

Milestone, Improve Performance of Pilots (8/99) – Status: Delayed

Expected Completion Date: 11/99

The ASCI networks at LLNL won't be deployed until 6/00 so the impact of this milestone being delayed a few months is not expected to be significant. However, the most challenging part of this effort is the demonstration and tuning of PFTP between the IBM SP2 Baby and the SGI. We have achieved over 20Mbytes/sec over 4 Fast Ethernet (100 Mb/s each) paths. We have demonstrated 11Mbytes/sec for a single FTP session, but have found hardware and software issues in making this scale to about 44Mbytes/sec for a 4 stripe PFTP transfer.

The remediation for this delay is a more substantial effort in FY00 to address performance problems.

Distance Computing Network Subproject

Milestone, Compression for ASCI Applications – Status: Complete

Expected Completion Date: 9/99

Milestone, VIA for ASCI Blue-Pacific – Status: Canceled

Expected Completion Date: 7/99.

This effort was not initiated, since funds were diverted to better support network management efforts on behalf of DisCom. Since the VIA effort is more research than development, the impact would be a possibly delayed deployment of VIA on IBM systems in 3-5 years.

The remediation for the cancellation of this effort is to track the OS bypass efforts, and when/if VIA is destined for ASCI environments, collaborative efforts can be initiated to help with the development.

Partnership for Wide Area Connectivity

Milestone, Follow-on contract with Bellcore (now Telcordia) placed – Status: Delayed

Expected Completion Date: 7/99

This effort completed 8/99, a one month delay. There was no impact.

This contract allowed Telcordia to work with the tri-Lab RFI for the DisCom wide-area network. Telcordia was able to participate when SNL completed the first draft of the RFI.

Distributed Resource Management Subproject

Milestone, Research dynamic co-scheduling and other scheduling mechanisms – Status: Delayed

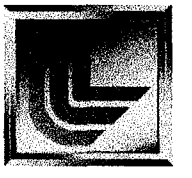
Expected Completion Date: 12/99

The dynamic co-scheduling effort was an advanced part of the DRM proposal. Several other elements of the DRM solution needs to be in place to realize the dynamic co-scheduling development effort. Delaying the dynamic co-scheduling effort a few months should have an insignificant effect.

The remediation for this delay is to track the progress of the DRM deployment carefully. Resources will be allocated if necessary to ensure that the dynamic co-scheduling is aligned with the DRM deployment.

- **Issues**

None.



Numerical Environment for Weapon Simulation (NEWS)

LLNL Quarterly Progress Report for NEWS - 4Q FY99

- **Principal Investigator - Steve Louis, LLNL**

- **Project Description**

Weapons analysts will be challenged to see and understand the data produced by new ASCI codes, as these data will vastly exceed today's in quantity and complexity, requiring innovative approaches to data storage, data visualization, and data analysis. The Numerical Environment for Weapons Simulation (NEWS) Program deploys the necessary terascale infrastructure technologies in data and visualization to support stockpile stewardship objectives, in concert with advanced ASCI computers and new physics simulations. NEWS provides the DP laboratories' implementation of the *Data and Visualization Corridor* (DVC) concept, linking results of weapons codes to stockpile stewardship understanding, judgment, and decisions. NEWS plans call for a series of increasingly powerful systems: V.0 Corridors in FY99-FY00, V.1 Corridors in FY01-FY02, and V.2 Corridors in FY03-FY04. These systems are integrated, multi-directional, high-bandwidth *information pipelines*, connecting users to physics simulations and to data, driven by ASCI requirements in the following technical areas: (1) visualization engines, (2) exploration modalities, (3) data manipulation engines, and (4) data delivery infrastructure.

- **Accomplishment Highlights**

Visualization Engines

Installation, integration and deployment of most visualization engine upgrades were completed and made available to ASCI users in 3Q FY99. The secure configuration (a.k.a. Tidalwave) underwent a final processor upgrade (16 CPUs converted from R10K 250MHz to R12K 300MHz) in 4Q FY99. The open configuration (a.k.a. Riptide) underwent a final disk upgrade (4.0 TB total of new Ciprico RAID with new smaller footprint 50 GB disks) in 4Q FY99. Two TB of extant Riptide disk will move to Tidalwave in 1Q FY00, providing 5.5 total TB of disk on Tidalwave and 4.0 total TB on Riptide.

Exploration Modalities

Secure LLNL DVC Assessment Theater located in Bldg. 132 upgrade to a fifteen-projector 5x3 system (~20Million pixels) was completed, tested and made fully operational in 4Q FY99. A Fakespace VersaBench immersive display system has been installed for development and user evaluation in the open DVC environment in Bldg. 451. Several single and quad 2x2 flat panel displays were received and installed in Bldg. 132 (Room 1418) and in Bldg. 451. All of these data exploration capabilities were successfully demonstrated during the September 15 Tri-Lab VIEWS Program Review.

Data Engines

Installation, integration and initial deployment of data engine upgrades were completed in 3QFY99. Beta test, security approval and subsequent production usage of data server components was completed in 4Q FY99. All hierarchical data management robotic hardware and software upgrades were completed in 3Q FY99. The 10.5 TB Fibre Channel disk cache installed at the end of 3Q FY99 was deployed for production use in 4Q FY99. New STK 9840 high-speed tape drives tested at the end of 3Q FY99 were also deployed for production use in 4Q FY99.

- **Milestone Status**

List status of any project milestones in the FY99 ASCI Implementation Plan (IP) for this project that were either: 1) due this quarter or, 2) which were due in previous quarters but which were delayed. If the status of a milestone is anything other than "completed", explain when you expect it to be completed, the impact on the project of its not being completed on time, and what the remediation plan is .

Visualization Engines

2Q FY99	Installation of visualization engine disk (Original disk installation project milestone was completed in 2Q FY99. An additional 4.0 TB disk procurement was completed in 4Q FY99 to alleviate space shortages, as described previously in the 3Q FY99 Progress Report)	COMPLETED

Exploration Modalities

2Q FY99	Expansion of desktop support to 16 highest-end users Expected completion date: 2Q FY00 Impact of delay on this project: Minimal. Limits use to initial eight DNT users. Remediation plan for this delay: Identify next set of high priority DNT users and determine proper desktop capabilities, based on current industry offerings. FY00 implementation plan calls for supporting a total of 30 DNT users.	DELAYED
3Q FY99	Installation of Fakespace VersaBench immersive display Completion date: 4Q FY99	COMPLETED
3Q FY99	Installation of tiled flat-panel displays in DNT office Completion date: 4Q FY99	COMPLETED

Data Engines

3Q FY99	Installation/expansion of data engine pre-/post processing Available to DNT users 4Q FY99.	COMPLETED
3Q FY99	Installation/expansion of hierarchical data management Available to DNT users 4Q FY99.	COMPLETED

Data Delivery

2Q FY99	Deployment of RGB video switch Expected completion date: 2Q FY00 Impact of delay on this project: Minimal. Prevents dynamic configuration changes. Remediation plan for this delay: Identify DNT needs for sharing available IRs, fiber and flat-panel capabilities, based on feedback from user community. Gather security plan approvals and information from LANL's previous deployment of similar switch.	DELAYED

- **Issues**

Integration of NEWS tasks into the VIEWS Program in FY00
NEWS tasks and milestones delayed to FY00 have been incorporated into the VIEWS program for FY00. Procurements, installation, integration and ongoing maintenance activities for visualization engines, exploration modalities, data management engines and data delivery infrastructure will now be managed and coordinated under VIEWS Operational Deployment activities. A new project manager for LLNL Operational Deployment was hired in September, reporting to the VIEWS PI and Deputy PI.

Increased Emphasis on Office and Immersive Visualization Capabilities for 4Q FY99
Arrival of the Fakespace VersaBench, and the individual and 2x2 flat-panel tiled displays in 4Q FY99 will allow introduction and early evaluation of immersive workbench capabilities as well as high-resolution multi-frame office display capabilities. Members of VIEWS Operational Deployment efforts will work closely with DNT users to understand the best ways to deploy new capabilities in Bldg. 132 and Bldg. 111 DNT scientist offices. A senior video technician was hired in September to assist with these and other tasks.

Linux Clusters for Data and/or Visualization Engines
A DEC Alpha Linux cluster environment usable as a scalable data management or visualization engine continues to be explored in coordination with ongoing LLNL DisCom efforts and related Tri-Lab VIEWS collaborations. The proposed VIEWS LLNL testbed plans to leverage this Linux cluster to prototype new capabilities. A preliminary four-node SGI PC cluster capable of running Linux has been shipped to Stanford University as part of an ongoing LLNL collaboration with Professor Pat Hanrahan.

VIEWS Facilities Planned for Bldg. 111
An additional data exploration facility is planned for LLNL Bldg. 111 having capability to house several individual scientist work spaces, multi-user collaborative and immersive work spaces, back-projected tiled screen capabilities, and secure machine room space. Discussion and prioritization of specific need are ongoing with members of the DNT community and with A-Program leaders. Projected availability of this space is 2Q FY00 with deployment of new capabilities targeted for completion 3Q-4Q FY00.

September 15 Tri-Lab VIEWS Review
A DOE team of 17 experts (including four LLNL employees) visited the three DOE DP labs on September 13 (LANL), 14 (SNL-NM) and 15 (SNL-CA and LLNL). A Site Visit Report has been drafted reflecting a rough consensus of the review team. The site visit team found that the laboratory managers and program staff understand well the program objectives, timeframe and technical requirements. They found that weapons designers and analysts appear to be well served by the infrastructure deployed, but that there are increasing requirements that need to be met in FY00 and beyond. Providing high-end visualization capabilities to DNT scientists and engineers will continue to be a priority. LLNL will use recommendations of this report to guide its improvement of capabilities for large-scale data exploration in FY00.

Specific facilities issues raised in the Site Visit Report (and planned VIEWS activities to address these) include:

- Additional direct data delivery connections to individual offices are recommended at LLNL
  (VIEWS will provide more fiber connections for up to 30 DNT offices in FY00)

- Access to shared facilities should be made easier (more "walk-in" facilities)
  (VIEWS will take steps to eliminate procedural hurdles for B132 and B111 use)

- The 2x2 flat-panel technology demonstrated at LLNL was impressive and useful
  (VIEWS will provide more 2x2 flat panels to B111 and B132 DNT offices in FY00)
  (VIEWS will continue vendor dialogue to increase resolution and reduce panel separation)

- Use of dynamic video switching and digital delivery should continue to be pursued
  (VIEWS will investigate deployment of a large 30x30 video switch capability in FY00)
  (VIEWS will investigate digital delivery including new digital interfaces and software)

Platforms

LLNL Quarterly Progress Report for Blue-Pacific and White - 4Q FY99

THIS SECTION CONTAINS IBM CONFIDENTIAL INFORMATION COVERED BY NON-DISCLOSURE AGREEMENTS.

- **Principal Investigator – Mark K. Seager**

- **Project Description**

Blue-Pacific and its sister system Blue-Mountain form the second major step along the ASCI Platforms curve. Developed by IBM and sited at Lawrence Livermore, ASCI Blue-Pacific SST hyper-cluster system delivers 3.9 TeraOP/s, 2.6 TB of memory and 62.5 TB global disk to the ASCI program classified ultra-scale code development and programmatic activities. The ASCI Blue-Pacific CTR system delivers over 914 GigaOP/s, 500 GB of memory and 20 TB of global disk to the ASCI program unclassified ultra-scale code development and programmatic activities.

White forms the third major step along the ASCI Platforms curve. Developed by IBM and to be sited at Lawrence Livermore, ASCI White MuSST SMP cluster system will enjoy in excess of 10.2 TeraOP/s, 4.0 TB of memory and 150 TB global disk to the ASCI program classified ultra-scale code development and programmatic activities. The ASCI White CODE system will deliver over 2.6 TeraOP/s, 1.952 TB of memory and 30 TB of global disk to the ASCI program unclassified ultra-scale code development and programmatic activities.

These two platforms lines are tightly coupled and are managed as a single entity.

- **Accomplishment Highlights**

The Blue-Pacific platform (SST and CTR) has been heavily used in production status during the 4QFY00. Programmatic usage is high in order to meet the CY00 code development milestone.

Development for the White NightHawk-2 nodes and Colony network as well as the Mohonk software base is proceeding according to plan.

- **Milestone Status**

38 Scalable Development Environment Sep-99 Not funded $1,500,000

This milestone is partially complete. We are waiting on SMP improvements in the C and F90 compilers and modifications to the IDENT daemon. This milestone should be complete in 1QFY00. There is no unclassified impact to the program due to the delay of these features.

38a PChkpt/Restrt Design Document Review Sep-99 Not funded $500,000

The parallel checkpoint/restart design document was received in 4QFY99. However, the review was not complete before the end of the quarter. We anticipate the review to complete in 1QFY00. There is no impact to the program due to the completion delay of this milestone.

39 16-way MUSPPA Design Review Sep-99 Not funded $600,000

The 16-way MuSPPA design document was received in 4QFY99. However, the review was not complete before the end of the quarter. We anticipate the review to complete in 1QFY00. There is no impact to the program due to the completion delay of this milestone.

40 Nighthawk Baby w/ Colony and Mohonk Beta Sep-99 Not funded $5,000,000

This milestone was partially completed in 4QFY99. We anticipate that this milestone will be complete in 1QFY00. There is no impact to the program due to the completion delay of this milestone.

41 TotalView Scalability Enhancements Beta-Test Sep-99 Not funded $300,000

This milestone will be completed in 1QFY00. There is no impact to the program due to the completion delay of this milestone.

42 On-Site Systems Programmer Sep-99 Balance $76,393 $152,784

This milestone was completed.

TS Technical Services, SP software problem analysis, two persons for three months Sep-99 $81,000

This milestone was completed.

- **Issues**

Reaching the 10.2 TeraOP/s demonstration milestone in March of 2000 is a very aggressive goal. However, there are currently no known impediments to reaching this goal.

LLNL Quarterly Progress Report for IBM

PathForward - 4Q FY99

THIS SECTION CONTAINS IBM CONFIDENTIAL INFORMATION COVERED BY NON-DISCLOSURE AGREEMENTS.

- **Principal Investigator – Mark K. Seager**

- **Project Description**

The PathForward Interconnect Project is intended to enable a quantum leap in interconnect technology. However, it is not our intention to dictate to industry how to build computer systems or design interconnect fabric. Instead, the interconnect performance requirements described below define the achievements necessary for ASCI to support the Stockpile Stewardship program. PathForward will be considered successful if the technologies that are developed under this program are installed as integral and scalable technology in future ASCI and other National Security community computer systems. The ASCI program believes that computer systems will consist of commercially viable components to the greatest degree possible. We are looking for industry to take bold, innovative steps in developing interconnect technology on the path to 30 teraOPS and beyond.

- **Accomplishment Highlights**

This project is proceeding according to plan on budget.

- **Milestone Status**

Milestone 6 - Copper transceiver chip design released to fabrication. It is anticipated that this milestone will be completed in 1QFY00. There is no programmatic impact from the delay of this milestone.

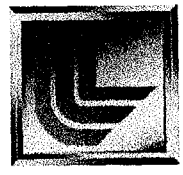
Milestone 8 - Review of switch chip design specification. This milestone is complete.

Milestone 11 - Parallel optical link design specification. This milestone is complete.

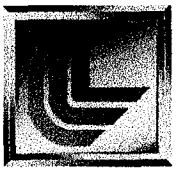
- **Issues**

There are no known issues for this project at this time.

Stockpile Computing (Operations)



LLNL Quarterly Progress Report for Stockpile Computing (SC) - 4Q FY99



- **Principal Investigator - Mike McCoy**

- **Project Description**

Stockpile (Production) Computing provides and maintains the computers, networks and services required for accomplishing computational science. In addition, this program element is responsible for integrating and maintaining the deliverables from NEWS, DisCom and the PSE into the production environment fostering its evolution into a production terascale simulation environment. Classified and unclassified computing services are provided 24 hours a day, seven days a week, 365 days a year for stockpile stewardship customers computing locally and remotely (coming from other laboratories, like Sandia and LANL, and from ASCI University Alliance Centers). The production computing environment includes large symmetric multiprocessor (SMP) clusters, massively parallel systems (in particular classified and unclassified ASCI terascale computers), supporting servers, terabyte storage archives, data assessment theaters for visualizing huge data sets, and finally networking infrastructure to tie all of these together.

The primary objective of Stockpile Computing is to provide and maintain a 24-hour per day stable production simulation capability required for maintaining the safety, reliability, and performance of the U.S. nuclear stockpile in the absence of test-based methods.

- **Accomplishment Highlights**

- Completed Y2K testing for both systems and environment software for AIX, TRUE-64 (Compaq), and Solaris systems. This includes OS infrastructure as well as compilers, debuggers and parallel tools.

- Installed and brought into production Compaq ES40 nodes for B program standalone special use environment.

- Completed tri-annual shutdown and facilities refurbishment. This included a demonstration of emergency stand-alone environment for priority calculations that will be available during Y2K shutdown period.

- Upgraded the File Interchange Service (FIS): Completed phase 1 capacity expansion and conversion to DCE centralized authentication, i.e. eliminated Kerberos.

- Several new milestones/deliverables arising from ISecM requirements were completed, including:
  - Instituted scans of closed PI=1 systems
  - Moved thousands of Web pages into DFS behind firewall
  - Completed participation in ISecM summer study.

- **Milestone Status**

Classified Environment Q4FY99 Milestones

Web account generation and change forms automatically fed into the accounting database – Status: delayed due to having to divert manpower to other tasks.

Expected Completion Date: Q2FY00
The impact of the delay: Minimal. Current system and procedures are capable of handling current load.
Remediation plan: Manpower has been redirect back to working on this.

Present "live" tutorials with interactive response. (Distance learning) – Status: Completed

NEWS Data Server installed – Status: Completed

Tape Archive: 450 TB – Status: Completed
- Upgraded to 970 TB

Unclassified Environment Q4FY99 Milestones

Tape Archive: 150 TB – Status: Completed
- Upgraded to 250 TB

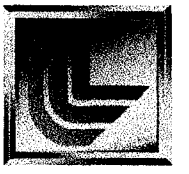
Retire Meiko – Status: Completed

- **Issues**

- Continued concern over the impact of ISecM, which requires redirection of key personnel away from programmatic deliverables.

- Potential polygraph testing and PSAP requirement are impacting staff morale.

Institutes



LLNL Progress Report for CASC Algorithms

R&D - 4Q FY99

- **Principal Investigator – Steve Ashby**
- **Project Description –**

.1 Scalable Linear Solvers

Investigators: Andrew Cleary, Peter Eltgroth, ***Robert Falgout****, Van Henson, James Jones, Mike Lambert*

CASC is developing portable, parallel, and reusable linear solvers for use in the stockpile applications codes. The emphasis is on preconditioned Krylov iterative methods for the solution of the linear systems arising from the spatial discretization of radiation transport problems. The CASC strategy is based on a two-pronged approach. In the near term (i.e., moderate problem sizes), incomplete factorization-based preconditioners are being combined with conjugate gradient methods to provide robust and efficient solution algorithms. In the long term (i.e., huge problem sizes), scalable multigrid methods are being investigated. CASC is investigating both geometric and algebraic multigrid methods, for structured and unstructured meshes, respectively. The geometric multigrid methods are being developed primarily for use within ARES, and the algebraic multigrid methods are being developed primarily for use within Kull and ALE3D.

.1.1 Accomplishment Highlights

This quarter was devoted to integrating *hypre*, CASC's parallel linear solver library, into the two ASCI codes, Kull and ALE3D. (Integration into ARES was completed some time ago, parallel testing was done on up to 1000 processors and 15 million spatial zones, and continues. See Q3-FY99 progress report for details.) This code integration involved a significant amount of work developing two new interfaces for *hypre*, appropriate for unstructured-grid problems: a linear-algebraic interface needed by Kull, and a finite-element interface, called the FEI, needed for ALE3D. As a result, *hypre* is now available in all three of the major ASCI codes at LLNL, and we are now beginning to test its solvers in the context of large-scale parallel physics simulations in both Kull and ALE3D (preliminary, small-scale tests are encouraging). Note that the solvers themselves have already been tested in parallel on up to 1000 processors. We detail this integration work below.

Matrix Interface for Unstructured Grid Problems

We have developed and implemented a new interface appropriate for unstructured applications such as Kull (in contrast to the structured-grid interface to *hypre* that is used in the ASCI code ARES). The application code sets up its linear algebra problems through interface calls based on row and column numbering for the linear system; these calls are similar to those made to set up a linear system in PETSc. This new linear algebraic solver interface, coined IJ interface, currently allows application codes to use CASC's parallel algebraic multigrid solver, BoomerAMG, and CASC's parallel incomplete factorization preconditioner discussed in the next subsection. This same interface will also allow access to future unstructured grid solvers developed in CASC, such as the sparse approximate inverse code (ParaSails) mentioned in the FEI subsection below, and even other libraries (a PETSc implementation is underway).

Parallel Incomplete Factorization Preconditioner

Integration of CASC's PILUT (Parallel Incomplete LU with Thresholding) preconditioner into the unstructured ASCI code Kull was completed. This required that PILUT was made compatible with *hypre*'s native ParCSR matrix format by implementing the GetRow interface (which PILUT uses) for the ParCSR matrix format. This new version of PILUT was then made an official part of *hypre* by meeting *hypre*'s software quality assurance standards, including testing, source code format, passing through Purify, etc.

The PILUT algorithm is a domain-partitioned variant of the established "dual-threshold" incomplete factorization methods of Saad. The original algorithm is based on mimicking Gaussian elimination, and thus retains some of the robustness properties of that algorithm, while greatly reducing the computational and memory complexity by systematically dropping small elements of the factors. The user can control both the amount of memory used by the preconditioner and the quality of the preconditioner through two parameters. ILUT methods have proven particularly effective for difficult anisotropic and convection-dominated problems. They are not completely algorithmically scalable, however, and lie between multigrid methods and simple iterative methods in terms of performance and cost, much like sparse approximate inverse methods. The parallel code PILUT achieves parallelism in the usual domain-partitioned approach: each processor performs ILUT on its local domain, which is completely parallel, and then they cooperate in a more tightly coupled way to factor the remaining boundaries. The resulting algorithm retains much of the numerical qualities of ILUT, and in particular, it is a *global* preconditioner and thus avoids the parallel convergence problems of true domain-decomposition algorithms. The parallel efficiency is reasonably good, though it depends on the "surface-to-volume" ratio of the problem, i.e., the size of the local problems versus the size of the boundary problems.

Detailed testing remains to be done, but preliminary testing on problems from Kull indicates some strengths and some weaknesses:

- Convergence is, as expected, slower than multigrid but faster than iterative methods. On these problems, it is also better than sparse approximate inverse methods.
- PILUT does not take advantage of symmetry, and this hurts it compared to solvers that do.
- Drop thresholds of zero, which are sometimes necessary for very hard problems, cause an unacceptable explosion in factorization time. Work is needed on this problem.
- Local reordering needs to be implemented to help further accelerate convergence.

Finite Element Interface (FEI)

In collaboration with Alan Williams and Robert Clay at Sandia National Laboratories and Kyran Mish at Lawrence Livermore, we have implemented a finite element solver interface for the unstructured preconditioners in the CASC preconditioner library. The finite element interface (FEI) gives finite element codes interchangeable access to a variety of solvers when they adopt that interface. This interface is currently undergoing a standardization process, and is being used by ALE3D. Our current efforts are in providing and testing CASC unstructured preconditioners linked directly to ALE3D through the FEI. This currently gives ALE3D access to BoomerAMG and PILUT, and will give access to a new symmetric, positive

definite version of ParaSails, currently being tuned and integrated. In the longer term, the FEI will provide the interface for other advanced solvers such as AMGe. The CASC implementation of the FEI builds on the linear algebraic solver interface discussed in the first subsection above.

hypre parallel AMG, AMG-GMRES and PILUT-GMRES in Kull

Using the IJ interface, we have added the capability to call *hypre* solvers from the ASCI code Kull. Currently, parallel Algebraic Multigrid (AMG), AMG-preconditioned GMRES, and ILUT-preconditioned GMRES solvers are accessible to the Kull user as input options. These *hypre* options are in addition to previously implemented PETSc calls. All of these solvers have been tested separately on up to 1000 processors, and parallel testing within Kull will begin as soon as Kull's parallel discretization routine is completed. However, initial testing has indicated that the addition of *hypre*'s parallel AMG code will prove particularly fruitful. In these tests, the PETSc ILU(0) preconditioned GMRES solver (Kull's native solver) has taken 200 iterations on some problems and still not converged, while AMG-GMRES consistently took 8-10 iterations. Furthermore, AMG is a scalable algorithm and ILU(0) is not, suggesting that the large-scale parallel results we hope to obtain shortly will prove even more dramatic.

.1.2 Milestones Status

.1.2.1 *Implement new sparse approximate inverse (SPAI) preconditioner into ALE3D and run a series of experiments to determine the method's algorithmic and parallel scalability, as well as it efficacy on ALE3D problems. [Delayed from Q2]*

Status: Completed

.1.2.2 *Conduct a full scalability study of our various geometric multigrid solvers on all three ASCI platforms. Run a variety of test problems, as well as real problems derived from ARES. Compare these solvers to our SPAI and ICT/CG solvers, as well as to other preconditioned iterative methods available in PETSc. [Delayed from Q2]*

Status: Delayed (in part)

Expected completion date: Q1 FY00

Explanation: Given in QPR Q3FY99.

.1.2.3 *We will work with the Kull team to get our various linear solvers into that code, and then we will conduct numerical experiments to determine the best solver.*

Status: Completed

.1.3 Issues

The design of a scalable multilevel solver is highly problem dependent. In particular, it depends on the nature of the underlying partial differential equations, the discretization scheme, and the grid on which the equations are being solved. Applications that employ unstructured meshes are particularly difficult, and the development of a robust algebraic multigrid solver is a long term research effort.

Interactions with non-LLNL (both U.S. and foreign) researchers are necessary to make the algorithmic development strides demanded by ASCI. Travel restrictions and policies that "frown on" foreign-national interactions could severely impact the quality of this research.

The development of efficient libraries is extremely difficult when the programming model is a moving target. Having **one** model available (e.g., message-passing with MPI) on all machines that provides access to the whole machine with adequate efficiency would be extremely helpful.

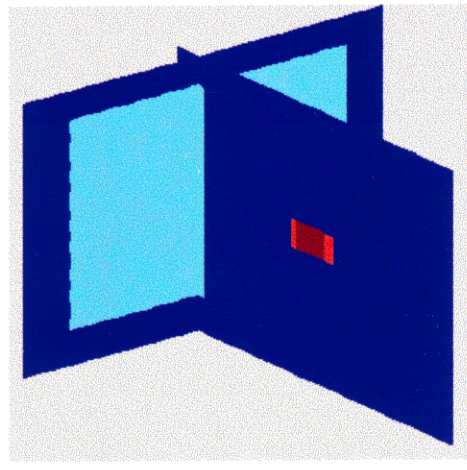
.2 Nonlinear and Differential Equations

Investigators: ***Peter Brown****, Britton Chang, Alan Hindmarsh, Carol Woodward*

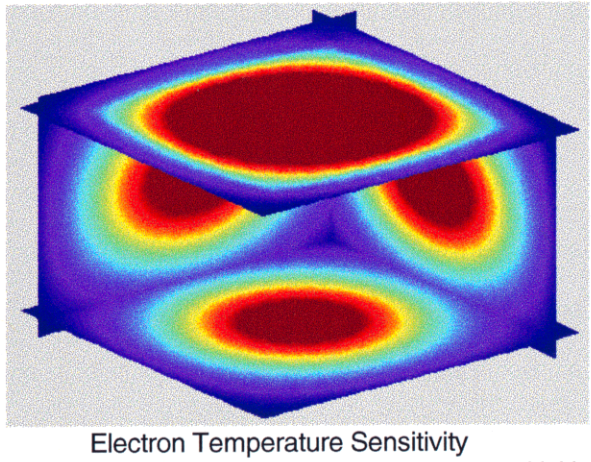
Many of the problems of interest to ASCI involve nonlinear processes, both time-dependent and steady state. We began work on nonlinear solvers in FY98 and have expanded our efforts in FY99. Our approach is based on Newton-Krylov methods, which only approximately solve the Jacobian linear systems, and leverages the linear solvers work described above. We are also considering Newton-Krylov-Schwartz methods and full approximation scheme (FAS) methods.

.2.1 Accomplishment Highlights

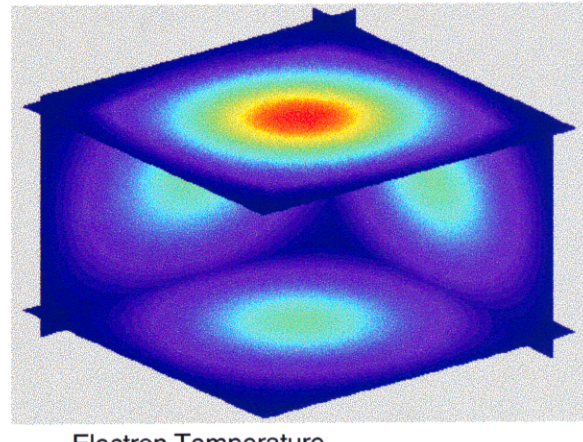
During the last quarter we have added a sensitivity analysis capability to our nonlinear radiation transport solver. The figures below describe an example problem containing a nickel source emitting radiation with a Planckian energy spectrum into CH foam and a rectangular silicon detector at a distance from the source. The slice plots show a snapshot of the electron temperature with a corresponding plot of the *sensitivity* of the electron temperature with respect to the source strength. An interesting output from this calculation is to calculate the detector response function along with its sensitivity to the source strength as a function of time.



Problem with nickel source and silicon detector



Electron Temperature Sensitivity



Electron Temperature

We will soon add the capability to calculate sensitivities with respect to other parameters such as material cross sections, as well as other output quantities.

.2.2 Milestones Status

.2.2.1 *We will develop a preliminary quasi-Newton nonlinear solver that uses multigrid to update the Jacobian systems. We will evaluate the scalability of this novel solver and then test the algorithm in ARES. [Q4]*

Status: Completed

As noted in last quarter's report, this milestone has been reworked under the title of "Fully Implicit nonlinear radiation solver in ARES" as part of the Transport Methods project. It was decided to pursue the use in ARES of the fully implicit nonlinear solver used in the ODE time integrator PVODE. This approach essentially replaces the time integration algorithm and adds a nonlinear solver to ARES all at once. This accomplishes what the above milestone was intended to do. We report progress in the Transport Methods section.

.2.2.2 *We will initiate a new effort in sensitivity analysis, the goal of which is to quantitatively measure the quality of large-scale ASCI simulations. Specifically, we will leverage our PVODE work to develop a capability to measure the sensitivity of a given output variable to various input parameters. [Q4]*

Status: Completed

We have completed a sensitivity analysis version of the ODE solver PVODE, referred to as SensPVODE. With this modified solver, users of PVODE can easily adapt their codes to perform sensitivity analysis. The current version of SensPVODE uses finite differences to obtain the sensitivity equations, which can sometimes be inaccurate. Thus, we are also developing a variant of SensPVODE that uses automatic differentiation to obtain the sensitivity equations analytically. To illustrate how easily SensPVODE can be used, we have modified our radiation-diffusion solver that uses PVODE for the time integration to also calculate sensitivities, and have done some preliminary calcuations as shown in the above figures.

.2.3 Issues

The SensPVODE solver performs what is referred to as forward-in-time sensitivity analysis, and is most appropriate for calculating solution sensitivities with respect to a few parameters. If one is interested in the sensitivity of only a few output quantities with respect to many input parameters (e.g., initial conditions), the backward-in-time or adjoint sensitivity methods are more appropriate. This approach is best done using automatic differentiation, but is much harder to use than the forward-in-time techniques, and this is a concern. Another concern is that for many ASCI problems, sensitivities with respect to many input and many output quantities are desired, and for these types of problems neither approaches are really suitable.

.3 Adaptive Mesh Refinement

Investigators: Suzanne Caffee, Milo Dorr, Richard Hornung, ***Scott Kohn****, Rick Pember, Steve Smith, Andrew Wissink*

SAMRAI is an object-oriented software framework that enables the development of parallel computational physics application codes using structured adaptive mesh refinement (SAMR). The SAMRAI effort focuses on the needs of large-scale, three-dimensional problems important to the ASCI program. Often, these applications encompass a wide range of physical, temporal, and physical scales. Thus, they require sophisticated computational approaches that combine diverse numerical solution methods, dynamic local mesh refinement, and massively parallel computing resources. The primary goals of SAMRAI are to support SAMR applications that require sophisticated solution algorithms for complex, coupled physics models and high-performance parallel computing hardware, and to explore the mathematical, computational and software engineering issues central to these problems.

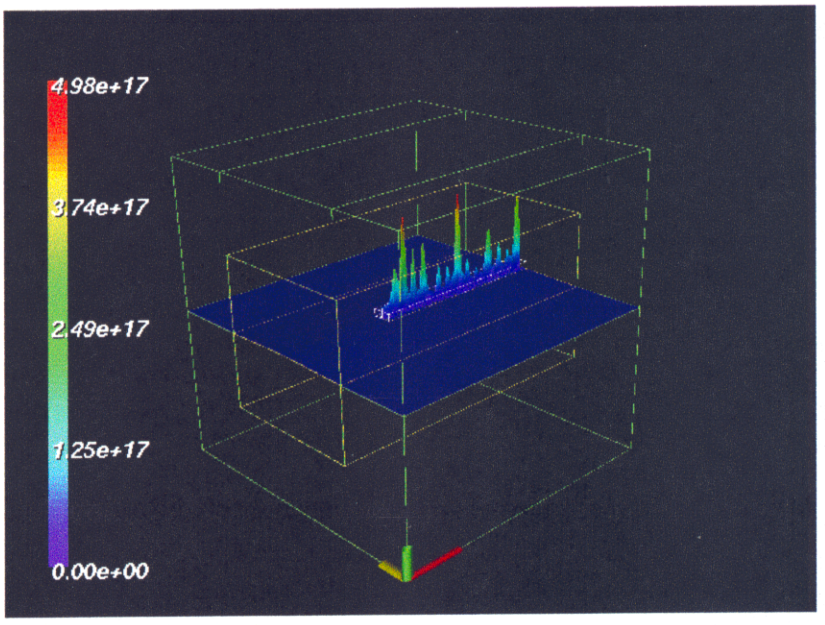
The SAMRAI team engages in close collaborations with application experts to apply SAMR technology to new problem domains and to motivate development of the software framework. Most notably, the University of Utah and University of Chicago ASCI Alliance Centers use SAMRAI. SAMRAI is also employed by the ALPS and ALE-AMR projects at Lawrence Livermore National Laboratory. The ALPS (Adaptive Laser-Plasma Simulation) project investigates SAMR methods to study the interaction between intense laser light and plasmas, which is a critical concern in the design of laser-driven fusion experiments. The ALE-AMR effort researches the combination of SAMR and ALE methods, which are used in ASCI application codes to simulate shock hydrodynamics. Overall, these efforts utilize coupled physics packages, hybrid solution methods (e.g., continuum and discrete models), linear and nonlinear solvers, large-scale parallelism, and complex data structures on SAMR meshes. The research program in SAMR methods and applications will guide the development of local refinement capabilities in future ASCI application codes.

.3.1 Accomplishment Highlights

Major accomplishments for FY99 Q4 include the following:

- We have developed a "remap" advection capability and combined it with a single grid Lagrangian gas dynamics method as part of the ALE-AMR effort. The Lagrangian plus remap combination is a crucial fist step necessary to proceed to a fully adaptive Lagrangian gas dynamics calculation. The code has been verified against several hydrodynamics test problems, including Sod shock tube, Colella-Woodward blast wave, Sedov blast wave, and the Noh problem.

- Two important solution algorithm enhancements have been made to the laser-plasma model in the ALPS code. First, we have reformulated the hydrodynamics method used in the plasma model to conserve total energy. Second, the light propagation model has been improved to interpolate the light intensity in Fourier space instead of "real" space. This adjustment was needed to remove spurious oscillations at coarse-fine grid interfaces when using adaptive mesh refinement.

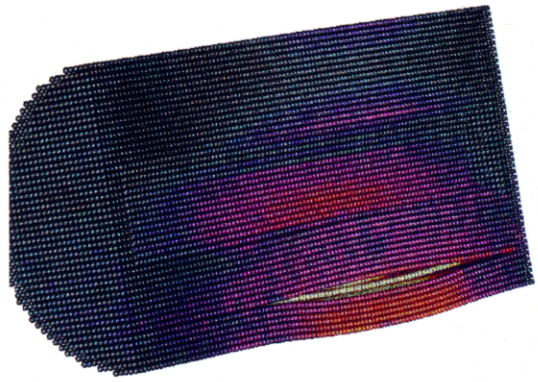


ALPS laser-plasma simulation of a filamentation instability. Boxes indicate local refinement around regions of high light intensity.

- More detailed testing has been performed to validate the ALPS code with the F3D code used in the Plasma Physics Group in X Division at LLNL. Several of these tests have demonstrated successful implementation of SAMR capabilities in the laser-plasma model. Preliminary studies have also demonstrated the potential advantages of using SAMR over single grid methods: adaptive speedups of 3 to 4 times and memory savings of two orders of magnitude have been demonstrated.

- Several new capabilities have been added to "Vizamrai", an interactive data visualization and animation tool for SAMRAI. These additions include isosurfaces, volume rendering, and bounding box calculations for a structured adaptive grid hierarchy. The tool is regularly used by ALPS and is currently being explored by the University of Chicago ASCI project.

- We are continuing our close collaboration with the University of Utah ASCI Alliance effort. We actively contributed to several aspects of the effort in preparation for the October TST site review. Specifically, we were involved in: 1) the coupling of PETSc (ANL) solvers with SAMRAI to develop parallel nonlinear solution methods on SAMR meshes, 2) the development of parallel MPM capabilities for container dynamics (see Figure), and 3) porting of the SAMRAI code to the ASCI Blue Mountain platform at LANL. Also, a summer student from the University spent the summer at LLNL working with us to develop a non-uniform load balancing capability in SAMRAI. This is currently employed in the particle-based container dynamics code developed in SAMRAI at the Center.

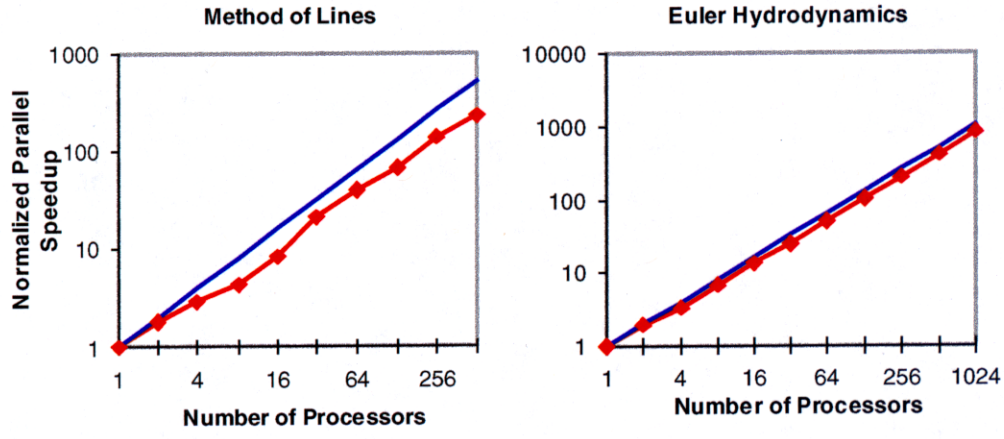


MPM container dynamics model written by the Utah ASCI Centere using SAMRAI. The particles, extracted from the computational mesh, represent a steel container filled with another material and extracted from the computational mesh. Note the debonding of the two materials near the bottom of the figure.

- We began a much closer collaboration with the University of Chicago ASCI effort than had existed previously. We were directly involved in the development of a parallel adaptive MHD simulation capability, the initial results of which will be presented at the October TST site review. While this code is a prototype, it has demonstrated the ability of SAMRAI to support rapid application development and is responsible for the growing interest in SAMRAI at the Center.

- We have begun a new collaboration with Alej Garcia, a faculty member at San Jose State University, and Nick Hadjiconstantinou, a faculty member at MIT, to develop a hybrid continuum-particle application to study Richtmeyer-Meshkov instabilities. This work will be of potential interest to scientists at LLNL studying inertial confinement fusion (ICF).

- The SAMRAI code has been ported to each of the three ASCI platforms and has been run on 1024 processors on each machine on a couple of different problems. Preliminary parallel performance analysis and scalability studies have begun. See Figure.



- We have developed a hierarchical keyword-value input database facility for SAMRAI and have begun to develop parallel restart and visualization file capabilities using HDF5. The input database substantially reduces user effort in dealing with application specific input files. The input and restart capabilities will be delivered to users in the next release of SAMRAI later this year.

- We have hired one new person to help with SAMRAI framework and application development. The additional developer will help SAMRAI address its growing customer needs.

.3.2 Milestones Status

.3.2.1 *Begin development of ALE-AMR shock hydrodynamics capability: one that marries tried-and-true ALE technology with the promise of AMR efficiencies [Delayed from Q2]*

Status: Completed

Development of Lagrangian hydrodynamics with remap step underway (see accomplishments above).

.3.2.2 *We will release version 1.0 of the SAMRAI code framework for structured adaptive mesh refinement applications. This framework will allow application code groups to rapidly build parallel AMR applications and experiment with various numerical methods.*

Status: Completed.

Distribution of SAMRAI began in Q2.

.3.2.3 *We will collaborate with the Utah Center of Excellence on the use of SAMRAI as the code framework for their fire simulation code.*

Status: Completed.

We are continuing our close collaboration with the Utah ASCI center. See accomplishments above.

.3.3 Issues

Development and support of a large C++ library across the three ASCI platforms as well as a large number of local development platforms for our collaborators is difficult and very time-consuming.

SAMRAI collaborators often do not have experience developing SAMR applications and the associated numerical and computational methods. As a result, successful application development requires members of the SAMRAI team to work closely with customers to provide the necessary expertise in SAMR, parallel computing, numerical methods, etc. These interactions, which go beyond the development of the basic software framework, can be very time-consuming. It is often difficult to schedule and plan for these interactions in advance so that they are easily coordinated with regular framework development tasks.

We continue to struggle with the definition of "scalability" in the context of SAMR applications. Since SAMR places computational effort only where it is needed to resolve specific features of the numerical solution, it is difficult to arbitrarily scale problem sizes as is typically done with non-adaptive applications.

Memory and performance restrictions are an increasing concern as we attempt to visualize data sets from larger and larger problems. While some progress has been made to cut memory usage (we have done so roughly by a factor of ten) in our Vizamrai tool, interactive processing of large data sets in the future will be difficult.

We have still not found a suitable postdoctoral candidate to work with us on the ALE-AMR effort. Progress on the effort, while steady, has been slower than expected due to this lack of resources.

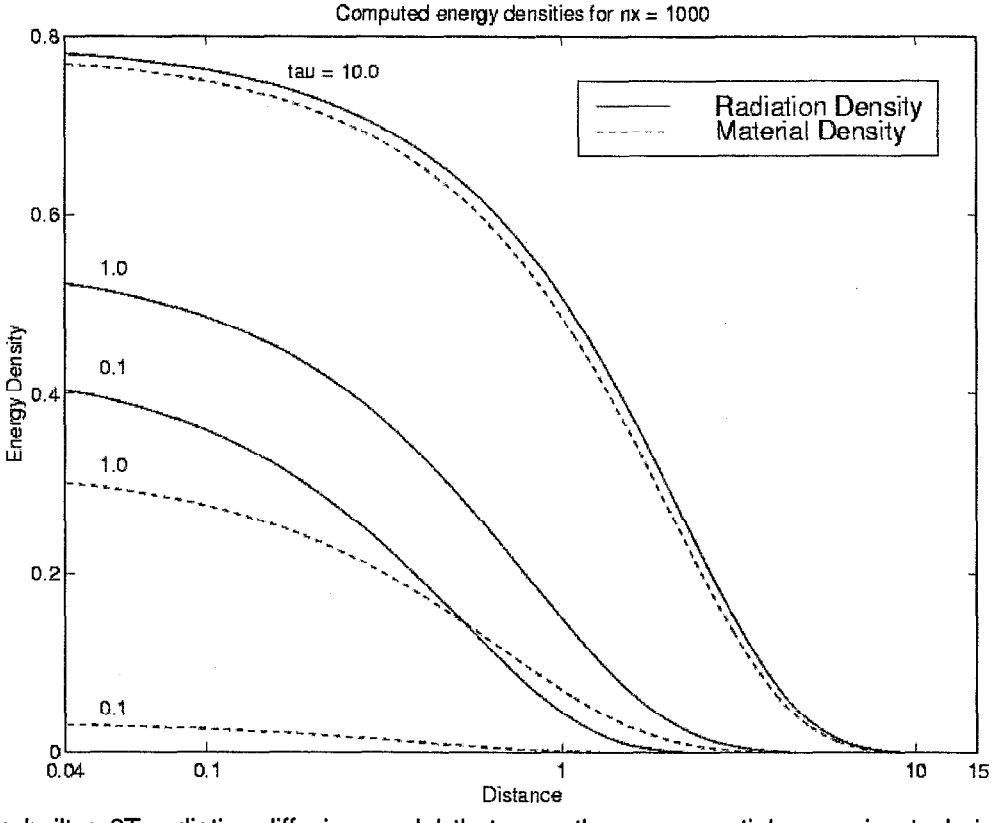
.4 Novel Transport Methods

Investigators: ***Peter Brown,*** *Britton Chang, Keith Grant, Carol Woodward*

The focus of this research effort is to explore novel parallel methods for neutron and radiation transport. This project leverages our linear solvers work to develop scalable preconditioners for use in solving to transport problems. For example, we have sped up the standard source iteration scheme by two orders of magnitude via the use of our Schaffer multigrid method as a preconditioner. We also are exploring a FOSLS (first order system, least squares) approach to formulating and solving the neutron and radiation transport problems of interest to ASCI. This novel approach avoids many of the numerical difficulties associated with current discretization schemes, and is designed to allow use of scaleable multigrid and/or adaptive mesh refinement methods. We are collaborating with Tom Manteuffel (University of Colorado), Paul Nowak (A Division), Frank Graziani (B Division), and Jim Morel (LANL); and we are leveraging LDRD funding.

.4.1 Accomplishment Highlights

In order to perform a precise comparison of our radiation transport solution approach to that used in the ARES code, it was necessary to build a modified version of our original multigroup radiation-diffusion code.



We have built a 2T radiation-diffusion model that uses the same spatial averaging techniques as in the ARES radiation solver. This new model has been verified against an analytic test problem due to Olson and Su. The above figure showing plots of radiation and material densities matches exactly with the results of Olson and Su. We have also interfaced our radiation-diffusion solver to a sophisticated geometry package allowing us to perform simulations with complex geometries.

We have also generated a parallel time-dependent Boltzmann transport solver that uses the IDA differential algebraic equation solver for the time integration. It also interfaces to the same geometry package, and we will soon perform a large multiprocessor run with this code similar to that done earlier with our steady-state Boltzmann solver.

.4.2 Milestones Status

.4.2.1 *We will demonstrate "full system" run of Ardra on ASCI Blue Pacific SST. [Q1]*

Status: Completed.

.4.2.2 *We will evaluate the FOSLS approach to radiation transport by implementing it in our Ardra research code. The idea behind this approach is to reformulate the transport equations in such a way that a standard discretization yields a system of equations that can be solved quickly using multigrid methods. [Q4]*

Status: Delayed

Expected Completion Date: Q1 FY00

Explanation:

We have completed an initial FOSLS-based solver for radiation transport. This code uses piecewise linear finite elements in space and an arbitrary order spherical harmonics approximation. We are currently using a conjugate gradient iteration with a block-diagonal preconditioner, where the blocks are based on the spherical harmonics moments. Each block is basically a Laplacian operator, and we invert these blocks using the multigrid solvers from the hypre library in the linear solvers project. Our initial tests with this preconditioning approach are somewhat disappointing, as we are not seeing good scalability of the overall iteration. This has lead us to conduct some theoretical analyses that has resulted in a new formulation of the FOSLS transport discretization. With this new approach, we intend to implement a block-based multigrid solution approach, wherein the blocks consist of all the moments at a spatial zone coupled together. The current multigrid solvers in the linear solvers project (hypre) do not yet handle systems, and so we are pursuing a multigrid solver for our specialized system, working closely with the hypre team. We have begun preparing a report on the nonscalability of our initial FOSLS approach, entitled "Space-Angle First-Order System Least Squares (FOSLS) for the Linear Boltzmann Equation."

.4.2.3 Fully implicit nonlinear radiation solver in ARES (Q4 FY99).

Status: Delayed

Expected Completion Date: Q1 FY00.

Explanation:

We have made considerable progress towards this milestone. In order to make a precise comparison with the 2T radiation-diffusion solver in ARES, it was necessary to significantly rework (i.e., rewrite) many of the inter-zonal averaging schemes used in our solver, as well as add a flux limiter and interface to the LEOS opacity library. This has taken considerable work, but is now almost completed. The above figure shows a plot of radiation and material densities that we have used to verify our new 2T code on an analytic test problem due to Olson and Su. We still need to add preconditioning to our 2T model, but this is a simple modification of that used in our

multigroup radiation-diffusion code. Once this is done, we will be able to complete this milestone by comparing our results with the radiation solver used in ARES.

.4.3 Issues

As noted in last quarter's report, an important issue in our codes is per processor performance, and we are have been investigating ways to improve our current performance statistics. We have been investigating the performance of our code on the IBM ASCI Blue machine at LLNL, and have written a report on our findings that will be presented at an upcoming conference entitled "Investigation of Realistic Performance Limits for Tera-Scale Computations," available as LLNL Technical Report UCRL-JC-135745.