Accelerated Strategic Computing Initiative
--
alliance pre-proposal conference

December 5-6

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U.S. Department of Energy
President Clinton’s Vision:

“...we can meet the challenge of maintaining our nuclear deterrent under a [comprehensive test ban] through a stockpile stewardship program without nuclear testing.”
Create leading-edge computational modeling and simulation capabilities critically needed to promptly shift from nuclear test-based methods to computational-based methods, to integrate stockpile stewardship elements and provide an integrated nuclear explosion testbed.
Simulation Tools Provides Integration of Great Science, Experimental Facilities and Archive Data for Confidence in the Stockpile

1. Full scale or full energy-density studies & experiments

2. Computation & Modeling

3. World-class & forefront, academic & lab scale scientific studies & experiments

Confidence

Virtual Testing

• Safety
• Reliability
• Performance
We are focused on Nuclear Weapons Simulation

Simulation
“digital proxy for physical”

National Labs
applications
weapon science
simulation & AGEX
adv. computation

Computer Co’s
computers
software & OS
prog. support

University & other Lab
science
collaboration
applications & prog. tools
### The Mechanics of Crash & Burn for Non-Nuclear Safety

<table>
<thead>
<tr>
<th>Structural Impact</th>
<th><img src="image1.png" alt="Image" /></th>
<th><img src="image2.png" alt="Image" /></th>
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<tbody>
<tr>
<td>Fuel Dispersal</td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
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<td>Fire Dynamics</td>
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<td>Thermal Insult</td>
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<td>Chemical Decomposition</td>
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<td>Pressurization</td>
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<td>Fracture</td>
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<td>Gas Expansion</td>
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<td>Electrical Insult</td>
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ASCI produces and supports simulation capabilities for designers who make critical decisions about the enduring stockpile.

- Core Science Base & AGEX
- Underground Test Archive
- Experiments Data
- Archival Data
- ASCI & Stockpile Computing
- Designers
- Simulation for Assessment, Certification, & Predictive Surveillance
- 3D, Full Physics Simulation Capability
- Enduring Stockpile

Stockpile Requirements

W87 W88 B61 W76 B83 B53 •••
There Are Five ASCI Strategies

**Applications**
- Focus on 3-D, “full-physics”, full-system applications

**Computers**
- Focus on the high performance end of computing

**PSE Infrastructure**
- Use, develop, leverage, and adapt HPC and NII technologies to create problem-solving environments

**Alliances**
- Encourage Openness, Teaming and Collaboration

**Pgm-3Labs Team**
- Execute ASCI as a 3-Lab, single-program activity
Applications focus on 3D, “full-physics”, high fidelity simulation, have key milestones tied to the stockpile, and require unprecedented application and computer speed increases.
ASCI Success Depends upon Balanced Growth across all Strategies

- Memory
- Computing Speed
- Parallel I/O
- Application Speed Increase
- Archival Storage
- Network Speed

Platforms

PSE

- 50 Terabytes
- 130 Petabytes
- 500 Gigabytes/sec
- 5000 Gigabits/sec
- 130 Gigabits/sec

- Flops $10^{14}$
- $X10^5$
- '96 '98 '00 '02
- 2003/2004

Comparison chart of memory, computing speed, parallel I/O, and network speed across different years.
High Speed Storage and I/O

SecureNet and Distributed Computing

Problem Generation and Visualization

Interactive Vis. of TB data sets

Volume Rendering, Real-time Visualization

Integrate with Scientific Data Management

Inter-Lab Distributed File System

1 Gb/sec

Secure Collaboration Environment

10 Gb/sec

Integrate Archival Storage and I/O

1 GB/sec

Problem Solving Environment

100 MB/sec

Application Speed

100x 1,000x 10,000x

Year

96 97 98 99 00 01 02

6 yr

Integrated Set of Scaleable Tools

2D Vis
Manual Gridding

100 Mb/sec

8 yr to MPP prod. code

Production Quality Scaleable Tools

Accelerate Application Development

Problem Solving Environment Roadmap

DOE12/96 ASCI-APPC Dec.5-6
ASCI Computing Systems Roadmap
-- working with industry to reach unprecedented computer performance --

<table>
<thead>
<tr>
<th>Time (CY)</th>
<th>Capability</th>
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<tr>
<td>1995</td>
<td>1+ T flop / 0.5 TB</td>
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<tr>
<td>1996</td>
<td>3+ T flop / 1.5 TB</td>
</tr>
<tr>
<td>1997</td>
<td>10+ T flop / 5 TB</td>
</tr>
<tr>
<td>1998</td>
<td>30+ T flop / 10 TB</td>
</tr>
<tr>
<td>1999</td>
<td>100+ T flop / 30 TB</td>
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- Option Red
- Option Blue

- Intel selected August 1995
- RFQ announced - February 1996
- IBM system selected - July 1996 (2.5 TB)
- SGI/Cray system selected - Sept. 1996
- Plan
- Develop
- Use

mid life “kick”
Option Red -
General System Characteristics

- 4536 Two Processor Nodes - 9072 P6 200 MHz Processors
- 64 MBytes per Node
- OS Capability to treat two nodes as one node with 128 MBytes
- 2.42 TBytes/sec Aggregate Memory Bandwidth
- 10 GBytes/sec Aggregate Disk System I/O Bandwidth
- 38 x 32 x 4 Communication Logical Mesh Size (Topology)
- 800 MBytes/sec Bi-Directional B/W per Link
- 512 GBytes/sec Bi-Directional Cross Section B/W
- 32 Service Nodes
- Ethernet, FDDI, ATM (OC-12)
- Full Unix (OSF/1) Running on the Service Nodes
- Light Weight Kernel (LWK) Running on Compute Nodes (Puma Based)
ASCI-Blue:
A single system composed of commercial multiprocessor computers linked with a high speed interconnect.

- 3 Peak Teraflops
- 1.5 Terabytes Memory
- 75 Terabytes Disk

- A single system allows both parallel and serial software to be used
- A single system view reduces operational complexity
IBM Approach:
Large Number of Nodes then SMP

IBM SP-3

- 3.23 TF Peak + 0.855 sPPM TF Sustained
- 512 SMPs, 2.5 TB Memory, 76 TB Disk
  - Each SMP 8 way PPC 630 @ 400 MHz
    (option for 16 way)
  - Each SMP 3 GB Memory
  - UMA Memory Architecture

- Colony Switch and Adapters
  - Baines Network (like Meiko)
  - MPI Delivered Performance
    - 22 microsec latency
    - 850 MB/s bandwidth (17GB/s bi-directional)
SGI Approach:
Big SMP Node First, then More Nodes

SGI Scaleable Node-1 (SN-1)

- 24 logical SMPs, 15 TB Memory, 76 TB Disk
  - Each SMP 128 way H1 microprocessor @ 500 MHz
  - Each SMP 62.5 GB Memory
  - DSM (NUMA) Architecture over 3072 nodes

- Distributed Shared Memory Architecture
  - Cache coherent shared memory over 4096
  - Fat hypercube with multiple 1-D torus connections
  - 5 microsec MPI Delivered Performance
Alliances Strategy

- **Motivation**
  - ASCI simulation and computing problems are so hard that labs cannot solve them alone
  - Develop a broad consensus that simulation is an appropriate means of ensuring confidence in the safety, performance and reliability of the stockpile
  - Help train the next generation of stockpile stewards

- **Three Levels**
  - Strategic Alliances
  - Strategic Investigations
  - Task Oriented Collaborations
Major Goals and Objectives

- Establish and validate the practices of large scale modeling, simulation, and computation as a viable scientific methodology in key scientific and engineering applications that support DOE science-based stockpile stewardship goals and objectives.

- Accelerate advances in critical basic sciences, mathematics, and computer science areas, in computational science and engineering, in high performance computing systems and in problem solving environments that support long-term ASCI needs.

- Establish technical coupling of Strategic alliances efforts with ongoing ASCI projects in DOE laboratories.

- Leverage other basic science, high performance computing systems, and problem solving environments research in the academic community.

- Strengthen training and research in areas of interest to ASCI & SBSS and strengthen the ties among LLNL, LANL, SNL and Universities.
Academic Strategic Alliances

- Large, long term relationships to achieve broad milestones
- Support confidence in Simulation
- Multidiscipline, coordinated effort
- 4 - 5 alliances (single institution...collaboration with other key researchers and industry partners are ok)
- $4-$5M/yr each for up 10 years
Examples of Potential Research Topics

- Physical Sciences/Mathematics
  - Hydrodynamics
  - Transport
  - Material Modeling (including aging)
  - Turbulence
  - Numerical Methods
  - Applications & Computer Algorithms

- Computer & Computational Science
  - Petaop Systems & Software
  - Scaleable Architecture
  - Scaleable I/O
  - Visualization
  - Data Management
  - Tools
  - Libraries for Scaleable Systems