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ASCI Applications

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ASCI Blue Pacific
A White Paper

4. ASCI Applications

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ABSTRACT: *ASCI applications codes are key elements of the Department of Energy's Stockpile Stewardship and Management Program (SSMP). They will provide the*

simulation capabilities needed to predict the performance, safety, reliability, and manufacturability of the U.S. nuclear deterrent.

1. Introduction

The Accelerated Strategic Computing Initiative (ASCI) is a key element of DOE's Stockpile Stewardship and Management Program (SSMP), which is charged with the responsibility to maintain the safety, reliability, and effectiveness of the U.S. nuclear deterrent without the use of underground nuclear testing. The ASCI vision is to shift promptly from nuclear test-based methods to computation-based methods for fulfilling the requirements of stockpile stewardship. To achieve that shift, ASCI will create the leading-edge computational modeling and simulation capabilities that are essential for maintaining the safety, reliability, and performance of the U.S. nuclear stockpile. The SSMP Plan describes the ASCI strategies to realize this vision and achieve the specific program objectives in the areas of performance, safety, reliability, and renewal. Among these key strategies, ASCI Applications projects will develop the high-performance software needed to support SSMP objectives (see Fig. 1).

Figure 1. The Applications effort is one of several elements of the integrated program established to address the ASCI challenge.

While the DOE national laboratories have always been at the forefront of scientific computing, many of the calculations conducted as part of the nuclear design process have had to reflect gaps in our understanding of the detailed physics of nuclear weapons. Of course, these calculations have always had the final arbiter of underground nuclear tests to validate the results. In the post-nuclear-testing environment, the laboratory's application development must support capabilities in three main thrusts:

- Produce full-system, high-fidelity physics, 3D simulations
- Validate simulations with nonnuclear experiments and archival nuclear test data
- Accelerate code performance for ongoing stockpile investigations

These full-system, high-fidelity physics, 3D simulations must fully cover the most important events affecting nuclear and nonnuclear performance through the complete stockpile-to-target sequence and affecting safety through a combination of hypothetical, complex, accident scenarios. These events are then related to critical theoretical, computational, and experimental issues. For reliability, the critical issues are associated with the most critical materials present in weapons and, for renewal, the issues are associated with weapon components that can be expected to require refurbishment or remanufacture.

In the future, scientists will rely primarily on the use of validated advanced computational modeling capabilities to simulate the performance of aging and remanufactured nuclear weapon components and systems, and to support weapon certification. Rudimentary versions of this capability exist today. For example, it is now possible for an experienced scientist to perform routine two-dimensional simulations of the response of a weapon in certain abnormal environments using detailed geometries and relatively high resolution, based on empirical models. However, to meet the future needs of stockpile stewardship, applications must achieve higher-resolution, three-dimensional, high-fidelity, full-system capabilities.

The term "high fidelity" is meant to imply a reliance on a suite of capabilities with a firm theoretical and mathematical basis that accurately capture the phenomena of interest, as opposed to capabilities based on empiricism. It refers to the fundamental scientific and engineering modeling that must be incorporated in the application codes; it includes physics, chemistry, materials science, and engineering sciences. It will be a formidable challenge to replace the codes normalized to test data with integrated predictive physical models.

The combination of fundamental physics models, advanced 3D numerical methods, and new, powerful computer platforms will require substantially more complex application codes than any that have been developed to date. These applications will integrate 3D capability, finer spatial resolution, and higher fidelity physics to meet SSMP needs in the absence of new underground nuclear tests or extensive prototype performance validation tests. The performance applications will be verified and validated using experimental results from historical underground tests along with data from a range of nonnuclear test facilities, such as advanced hydrodynamic capabilities at Los Alamos and Lawrence Livermore National Laboratories and LLNL's National Ignition Facility.

Section 2 of this chapter will provide a brief overview of the ASCI Applications effort. Section 3 will discuss some of the initial applications work performed on the ASCI Blue Pacific Initial Delivery (ID) system in Livermore and will take a brief look at the future of that system.

2. ASCI Applications

Integrated Codes

LLNL's strategy for our integrated codes is based on an analysis of the requirements for high-fidelity simulations across the full set of problem domains, ranging from manufacturing and safety issues on one end to weapon performance on the other. The problem domain also includes the physics required to simulate experiments on key aboveground experimental (AGEX) facilities (e.g., NIF, AHF), since modeling of these experiments will play an important role in the validation and verification of these codes. For each major problem class, we determined the physics/algorithms, spatial resolution, and spatial dimensionality required to achieve high-fidelity results (see Fig. 2). Of course, this analysis is based on our current understanding — we will surely discover new factors as we eliminate known inadequacies in our codes. We determined that we can cover our problem space with two classes of codes: one that spans the space from manufacturing to one-point safety and another that spans the space from one-point safety to full-system performance.

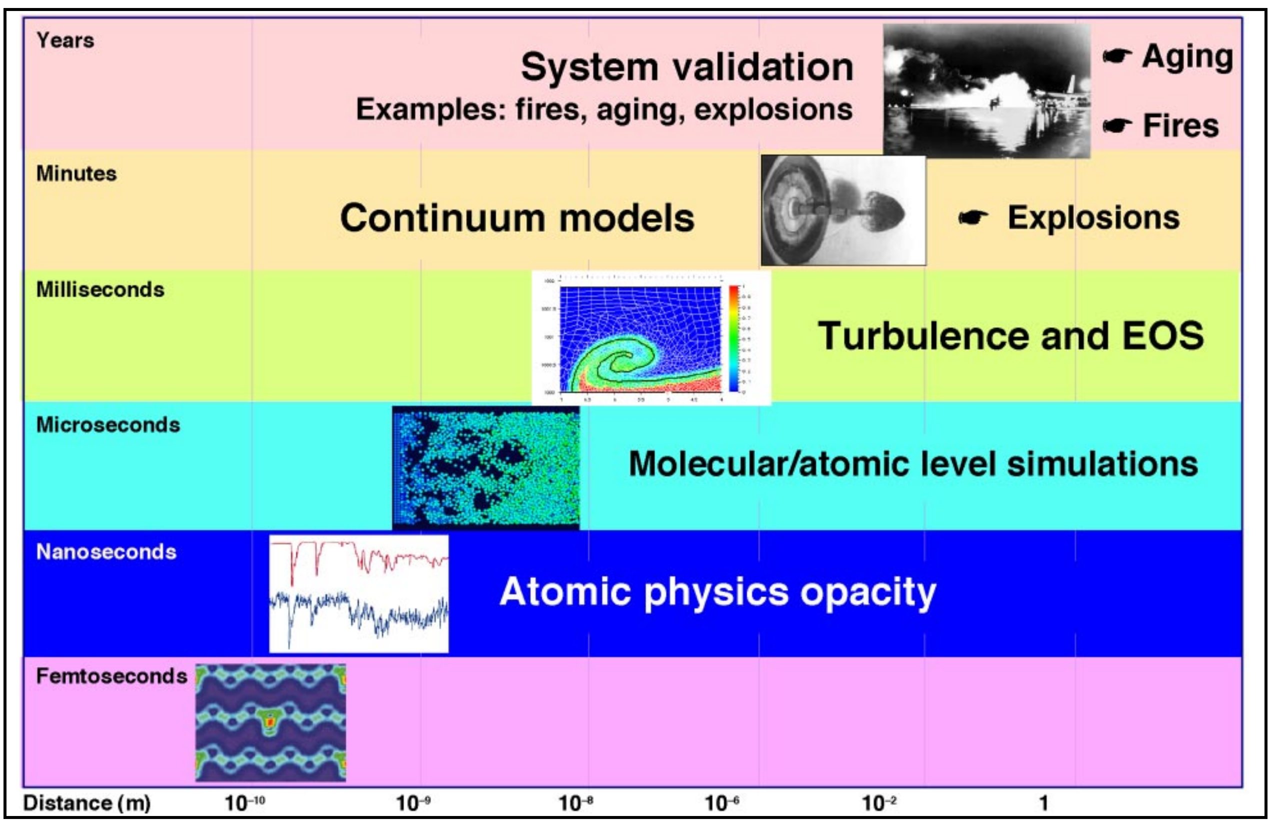

Figure 2. Some important physics issues remain outside the realm of numerical simulation. We need a hierarchy of models and modeling methods to enable predictive capability for all processes relevant to weapon performance.

Of course, our principle objective is to transfer the developments from the broader scientific community to development of full-system performance codes that will:

- Predict normal performance of full weapon systems from high-explosive detonation to total system energy output
- Predict effects of aging defects and manufacturing processes on weapon performance
- Predict results of complex integrated AGEX experiments (e.g., NIF)
- Predict behavior in some abnormal environment scenarios (e.g., one-point safety)

Improving the Scientific Basis for Weapons Simulation Codes

Accurate material properties are essential to high fidelity simulations; uncertainties in many key material properties are known to be a major source of error in simulating weapon behavior. Our ASCI Applications program is directly supporting a broad-based effort to develop much improved values for a variety of material properties important to the accurate prediction of weapon behavior. In particular, it is supporting a major new thrust to the use of high-end computing to enable microscopic-level simulations as a tool to develop predictive models for use in continuum codes.

The ASCI Materials Modeling and Simulation effort focuses on the development of predictive, physics-based models to determine the effects of materials properties, as derived from processes such as aging and manufacturing, on stockpile performance. Innovative materials simulations will serve as the basis to the development of these predictive, physics-based materials models. The strategy is to enable materials simulations as a research tool for the development of predictive, physics-based materials models to be inserted within full-scale simulation codes. Moreover, these projects are fully aligned with the overall ASCI objectives to develop predictive, three-dimensional, high-fidelity physics applications leveraging the utilization of emerging high-performance computer architectures.

ASCI Materials Modeling and Simulation projects are organized in terms of:

<u>*Materials properties*</u>:

- **Thermodynamic properties** as they relate to issues of stockpile performance, safety, and reliability: Equation-of-state (EOS) for thermodynamic variables and their derivatives, phase diagrams and structures, high-pressure phase transitions, melting, etc.

- **Mechanical properties and aging** as they relate to issues of stockpile performance, safety, and reliability as well as materials strength, aging, and failure: Constitutive materials models, deformation and plastic flow, void formation and spall, ejecta from shock-loaded surfaces, etc.

and

Materials systems:

- **Metals and alloys:** Actinides, hydrogen, simulants, etc.
- **Energetic materials, high explosives (HE), and organics:** TATB- and HMX-based HE, polymers, binders, etc.

Turbulence

The ASCI shift to high-fidelity 3D simulations requires accurate modeling of subgrid-scale turbulent mixing effects. The development of subgrid-scale models is a particularly challenging task for ASCI code developers. These models will be validated through a combination of experiments and high-resolution 3D direct numerical simulation. These direct numerical simulations are being performed on LLNL's ASCI Blue Pacific initial delivery system as well as the ASCI Red machine at Sandia.

The LLNL ASCI Applications program supports full-scale simulations as well as the development of improved micro-scale, zonal physics models. Foremost among these micro-scale models is the development of improved physics-based materials and turbulence models. Consequently, the LLNL ASCI Applications program forms the basis of a balanced, broad-based program addressing the need for improved, physics-based micro-scale subgrid zonal physics, as well as integrated, full-scale applications.

External Contributions – Strategic Alliances

Because materials science forms the basis of modern science and technology, the ASCI Materials Modeling and Simulation program offers unprecedented and wide-ranging opportunities for technical exchanges with the academic community. Moreover, because the development of predictive materials models encompasses only unclassified research activities, productive scientific interactions and personnel exchanges with the academic community are greatly facilitated and have been pursued aggressively.

Toward this end, the ASCI Academic Strategic Alliance Program (ASAP) has established university partnerships, at three finding levels, to make use of a wide range of scientific expertise in a number of important research areas.

Level One — Strategic Alliance Centers

Alliance "Level One" partnerships (ten-year, $3M to $5M/year projects) have been formed with five major American universities:

- The Center for Integrated Turbulence Simulations at Stanford University
- A Computational Facility for Simulating the Dynamic Response of Materials at the California Institute of Technology
- Center for Astrophysical Thermonuclear Flashes at the University of Chicago
- The Center for Simulation of Accidental Fires and Explosions at the University of Utah/Salt Lake
- The Center for Simulation of Advanced Rockets at the University of Illinois at Urbana/Champaign

These high-end applications research thrusts include areas of general scientific interest. The Strategic Alliance projects, of course, do not include the work of building the design codes that will simulate the operations of nuclear weapons or their components. They will, however, assist the wide scientific community in creating the scientific and computational tools that will contribute to the shift from a test-based environment to a simulation-based approach to addressing a broad list of challenges in the national interest, including national security issues.

Level Two — Strategic Investigations

The Academic Strategic Alliance Program also has established smaller-scale "Level Two Strategic Investigations." These will consist of collaborations in the approximately $100K to $400K/year range with overall funding starting at $3M in FY1997 to about $5M in the out years. The focus of these efforts is more discipline- and individual-project specific than that of the Level One projects. The following broad categories characterize the areas targeted by the ASCI program for Level Two Strategic Investigations:

1. Data manipulation, visualization, and their integration to enable "end-to-end" solutions for managing, assimilating, and delivering tera-scale scientific data to desktops of scientists, analysts, and code developers. Examples of potential topics of interest include:
- Scientific data management for tera-scale data
- Visualization of multi-dimensional tera-scale data

2. Scalable parallel computational algorithms for teraFLOPS systems (1000s of processors). Topics in computational mathematics, software, and algorithms in computational physics/engineering (for example, radiation diffusion/transport and mechanics) of interest to ASCI include:
- Parallel algorithms for the solution of sparse systems of linear and nonlinear equations arising on structured and unstructured meshes, as well as for gridless methods.
- Uncertainty quantification methods
- Mesh generation, mesh partitioning, and dynamic load balancing tools, such as parallel mesh generation for complex geometries, mesh partitioning algorithms for block-structured and unstructured meshes, and techniques for adaptive load balancing of applications.

3. Scalable parallel software tools for effective use of massively parallel teraFLOPS computing systems. Categories of tools of interest include:
- Tools, compilers, and technologies for optimizing the use of deep memory hierarchies in clustered SMP systems
- Performance monitoring, profiling and analysis tools at micro to macro levels
- Scalable debugging technology, integrated with other tools as appropriate
- Run-time tools for managing and optimizing the performance of parallel applications

4. Software tools and algorithms for achieving tera-scale performance through distance computing in the form of heterogeneous distributed computing systems with thousands of commodity SMPs (with 2-16 processors/node) and commodity high-speed interconnects (SAN, LAN, WAN). Topics of interest for such systems include:
- Algorithms for fault detection, recovery and containment in parallel heterogeneous clustered computing systems
- Latency-tolerant algorithms for deep memory hierarchies for such distributed computing systems
- Computer simulation models for evaluating total system performance (from hardware architecture to applications).

- Resource management techniques, (e.g., CPU, memory, network input/output).

Level Three — Individual Collaborations

Individual collaborations, primarily between one laboratory and one university researcher, will be awarded in the $50K to $100K range for short-term projects out of laboratory programmatic funds. Each laboratory will establish its own selection criteria for these projects.

Manufacturing

We are at the beginning of a multi-year, multi-code effort to acquire capability for analysis of complex 3D stockpile manufacturing issues. The intent is to describe a set of manufacturing issues that have high priority that can be related to particular issues on particular weapon systems. Of those, we initially chose a subset of six problems that intersect with the need for full 3D simulations that cannot be credibly run with converged finite-element meshes on today's single-processor computers. These were chosen to act as a challenging set of programmatic drivers. The five problems that will proceed into FY98 and beyond under the current plan are these:

1. Thermal Forming and Joining - solid phase emphasis
2. Welding and distortions
3. Spin Forming in 3D
4. Pit Manufacturing Simulation Tool--Coupled Fluid/Thermo/Mechanical
5. Gas Quench Model, Loosely coupled CFD/Thermal/Phase Transformation

The capabilities needed to carry out these simulations, both in algorithms and material models, are being directly incorporated into the ASCI codes themselves, either by the code group members themselves or by engineers working with closely with the code team. These capabilities will be available for use by any users of the codes as soon as they verified and validated.

ASCI Blue Pacific Accomplishments

IBM delivered the 512-node Blue Pacific computer system to Building 113 at LLNL on September 20, 1996. Within two weeks of delivery, the system was up and running — conducting significant stockpile stewardship-related calculations within the first month. Among the early ASCI applications-related accomplishments using this computer are the following:

- Advanced ASCI simulation codes are providing unprecedented capabilities to our scientists:
  - — 3D hydrodynamic and radiation-hydrodynamic calculations of actual weapons systems are being carried out with greater spatial detail than ever before
  - — Calculations of coupled, 3D, thermal/chemical/hydrodynamic calculations of weapon-safety (e.g., a weapon in a fire) are now possible for the first time
- ASCI simulation codes and algorithms can take advantage of large-scale parallelism:
  - — Hundred-fold speedups (relative to YMP speeds) were obtained for 3D hydrodynamics calculations
  - — Excellent parallel scaling of a deterministic radiation-transport package has been demonstrated
  - — A 900-million-zone 3D mesh was generated in less than ten minutes using a new parallel mesh-generation code — an operation that would take weeks using existing codes

• Atomic-scale material simulations on ASCI platforms have already led to breakthroughs in the understanding of the behavior of key materials (see Figs. 3 and 4):

— Prediction of the phase diagram of actinides using first-principles methods

— Atomic-level determination of materials failure under shock-loading conditions

— Establishment of a microscopic basis for prediction of mechanical failure of metals

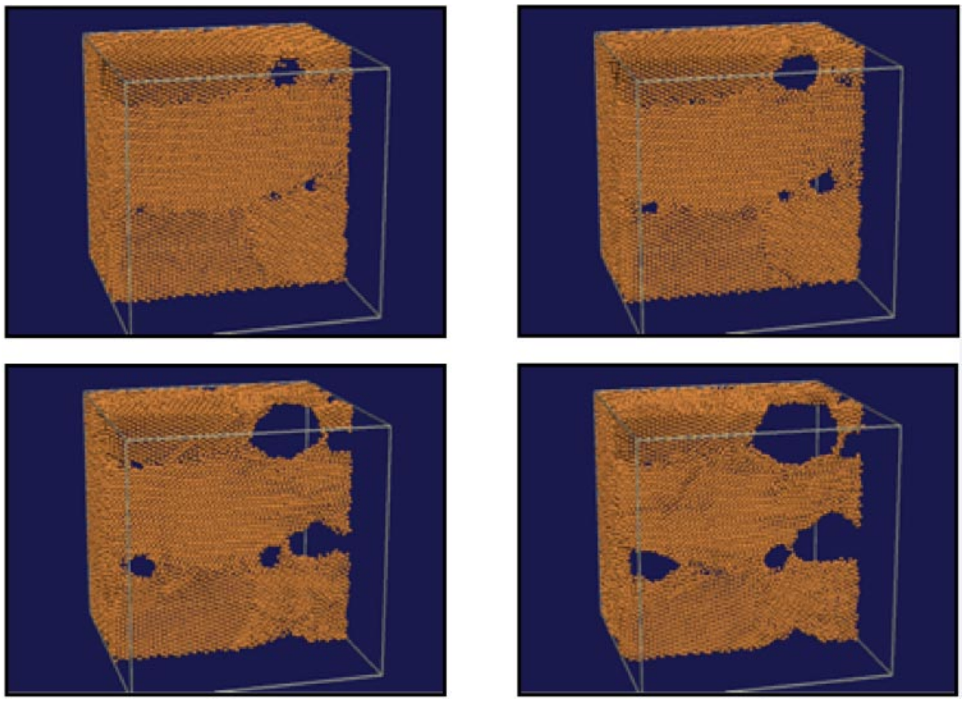

Figure 3. We have created a crystalline material model to predict microscopic failure processes of aging materials.

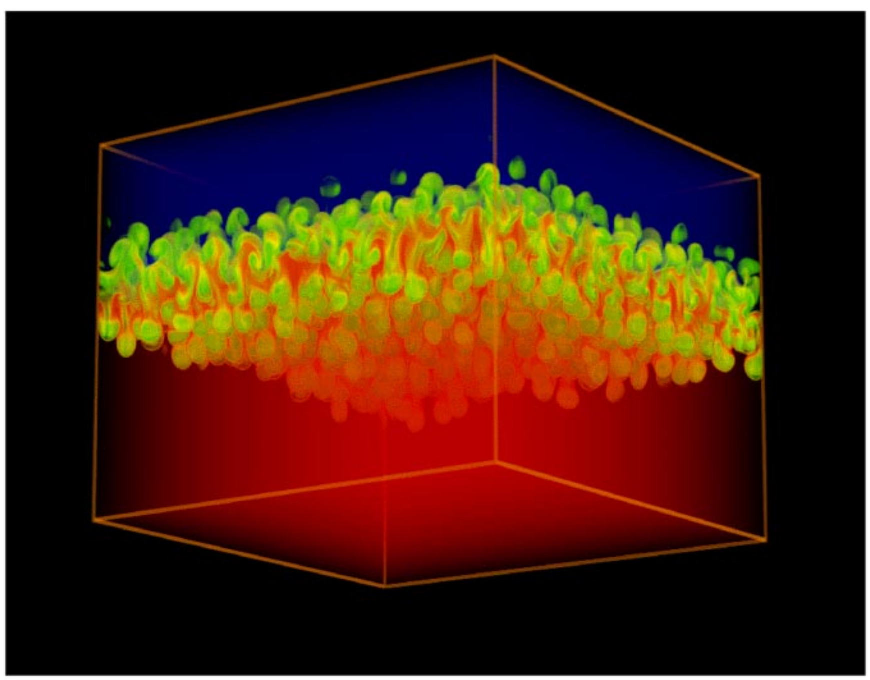

Figure 4. We have done pioneering calculations of 3D compressible turbulence. This simulation required over 130 million grid points, requiring 10^{15} operations, using 10,000 node-hours.

The Sustained Stewardship TeraFLOPS (SST) computer

The 100-teraFLOPS threshold is the entry-level computing capability for fulfilling the requirements of stockpile stewardship. Our primary goal is to achieve that level of computing capability in the 2003/4 time frame. The machine that will accomplish this milestone will require applications that work efficiently when distributed over approximately ten thousand processors. The Sustained Stewardship TeraFLOPS (SST) machine will give us the hardware power to make this a reality. The SST will be installed in Building 451 at LLNL in FY1999. Once we have done the applications work to achieve the 100-teraFLOPS milestone, we will be able to conduct 3D simulations at a level of complexity that matches our current physics understanding. The simulations we have accomplished in 2D on the ASCI Blue Pacific Initial Delivery system will be done in 3D on thousands of processors on the SST.

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