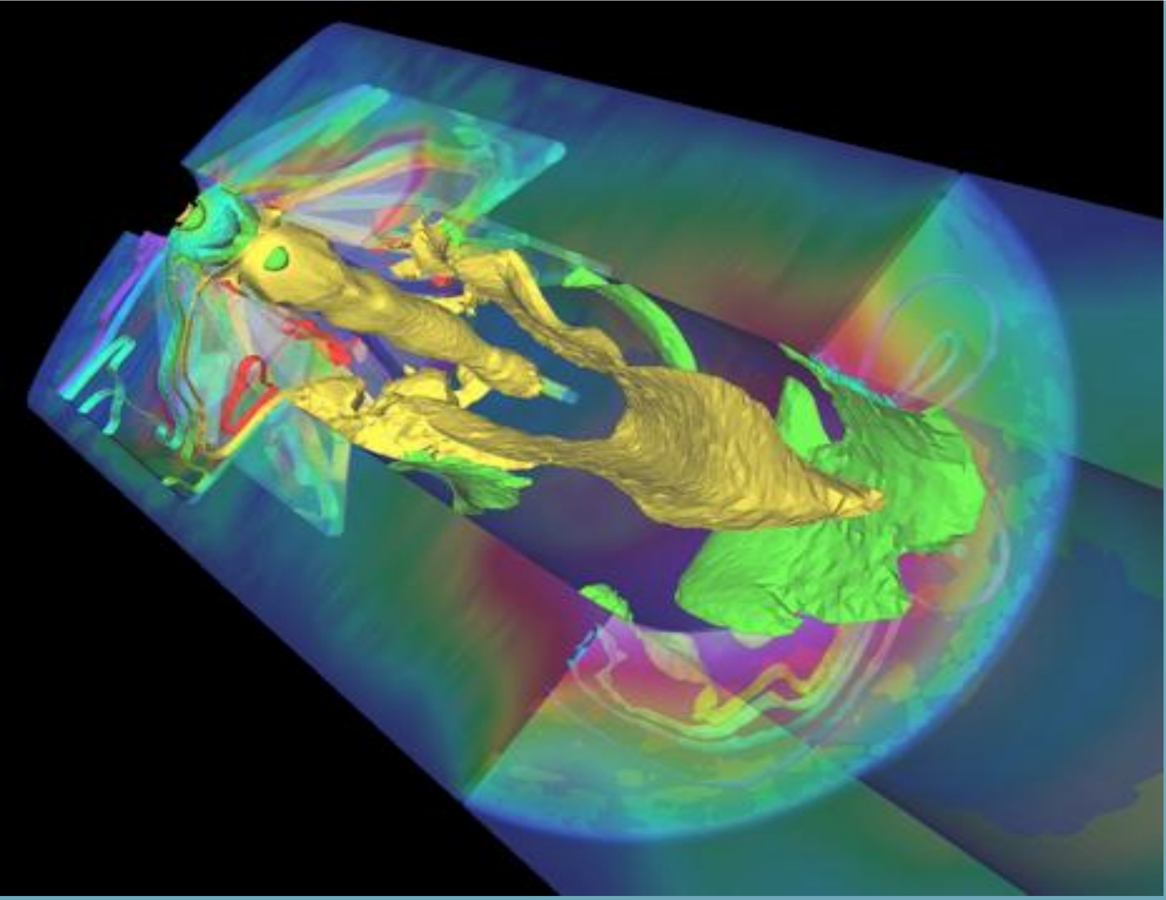

Advancing Simulation Science: The Legacy of the ASC Academic Strategic Alliance Program

Sandia National Laboratories

ON THE COVER:

Hot gas flow field and propellant stress in propellant of Titan IV rocket motor. Fully coupled "fluid-structure interaction" simulation performed using CSAR *Rocstar Simulation Suite."*

University of Illinois at Urbana-Champaign: Center for Simulation of Advanced Rockets (CSAR)

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Advancing Simulation Science:

The Legacy of ASC Academic Strategic Alliance Program

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- *California Institute of Technology: Center for Simulating the Dynamic Response of Materials*, led by Professor Daniel Meiron;
- *Stanford University: Center for Integrated Turbulence Simulation*, initially led by Professor William Reynolds (deceased), and later Professor Parviz Moin;
- *University of Chicago: Center for Astrophysical Thermonuclear Flashes ("FLASH"),* initially led by Professor Robert Rosner, and later Professor Donald Lamb;
- *University of Illinois at Urbana-Champaign: Center for Simulation of Advanced Rockets (CSAR),* led by Professor Michael Heath; and
- *University of Utah: Center for Simulation of Accident and Fire Environments (C-SAFE)*, led by Professor David Pershing.

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Advancing Simulation Science:
The Legacy of the ASC Academic Strategic Alliance Program

1. Introduction

1.1 Background

The Accelerated Strategic Computing Initiative (ASCI) was established in 1995 in the Office of Defense Programs (DP) of the Department of Energy (DOE), and incorporated into the National Nuclear Security Administration (NNSA) when the NNSA was created in 2000. The three NNSA national laboratories – Lawrence Livermore (LLNL), Los Alamos (LANL), and Sandia (SNL) – were funded to advance leading edge computational modeling and simulation capabilities in support of the DOE Stockpile Stewardship Program (SSP). The SSP, which is charged with maintaining the safety and reliability of the nation's enduring nuclear weapons in the absence of underground nuclear testing, depended, in part, upon ASCI's advanced computational capabilities to shift from underground test-based certification to science-based certification, employing a tool suite of computational modeling, scientific/engineering testing and experimentation capabilities. Since FY2002, ASCI matured into an ongoing, sustained program under the name Advanced Simulation and Computing (ASC).

For the NNSA and its laboratories, making the shift to simulation-based methods was a major challenge because it changed the way it certifies the performance, safety, security, and reliability of nuclear weapons. High performance computational modeling and simulation had to become an accepted, viable tool for stockpile certification. To help meet this immense challenge, ASCI's Academic Strategic Alliance Program (ASAP) was formed in 1997 to engage the U.S. academic community in advancing science-based modeling and simulation technologies. The ultimate goal of selected universities (known as ASAP Centers) was to demonstrate the power and validity of using large-sale, multi-physics, integrated, three-dimensional computer modeling to advance understanding of a challenging, critically important scientific or engineering problem of national interest. The specific problem chosen did not have to be of direct relation or interest to the NNSA laboratories. The unclassified research conducted through these partnerships has contributed to the knowledge base required to develop and demonstrate the powerful capabilities of modeling and simulation across a broad spectrum of science and engineering applications of national importance, using the largest massively parallel computers in the world.

Although the ASAP Centers' computational simulations did not involve nuclear weapons research, they contributed to SSP by furthering the following goals:

1. Establish and validate large-scale modeling and simulation as a viable methodology across complex scientific and engineering applications.
2. Solve science and engineering problems of national importance through the use of large-scale, multidisciplinary modeling and simulation.

3. Enhance the overall ASCI effort by engaging academic experts in computer science, computational mathematics, and numerical simulations of science and engineering problems.
4. Leverage relevant research in the academic community, including basic science, high-performance computing systems, and computational environments.
5. Strengthen education and research in areas critical to the long-term success of the ASCI and the Stockpile Stewardship Program.
6. Strengthen ties between the NNSA national laboratories and participating U.S. universities.

Achieving these goals required that each ASAP Center successfully develop an integrated, large-scale, three-dimensional, scalable simulation capability for their multi-physics problem, validate their model, run full system simulations, and report their results widely in the appropriate scientific and engineering literature, conferences, and through other contacts with industry and the scientific and engineering communities of interest. They also were charged with improving their computational science educational programs based on their ASAP experience. During the program, beneficial collaborations were developed between the ASAP Centers and the NNSA laboratories. Furthermore, more than fifty personnel from ASAP Centers, consisting of graduate students, postdoctoral researchers, and research staff, found employment at NNSA laboratories subsequent to their time at the Centers. A small subset of these is named in the following pages.

1.2 Strategic Alliance Centers of Excellence

The complexity of what was expected of the Centers necessitated a program with unusual characteristics. Based on NNSA laboratory experience, it was clear that the Centers would require significant, long-term, stable funding if they were to reach the goals set out for them. In particular, the normal academic mode of a single professor with a couple of graduate students and a post doc, with two or three years of funding, was unlikely to accomplish the goals above. The Centers needed significant time and support to create teams of people from disparate technical disciplines who could work together to achieve the common goal of solving an overarching application problem via building, running and validating the required complex computational models. This understanding led to an unusually high level of funding (approximately $4.5 M per Center per year) committed for five years, with possible renewal for another five years.

Because of the size of the commitment, its duration and the difficulty of the goals, it was necessary to set up a mechanism for close monitoring of progress, annual peer review of such progress for each Center, and interaction with the NNSA laboratories. The ASAP program was managed by the Alliance Strategy Team (AST), which was led by an NNSA manager and included one representative from each of the three NNSA laboratories. The AST was also responsible for setting up and managing the peer reviews, including selecting the independent review panels, whose members were drawn from the NNSA laboratories, other government agencies, and academia. Additionally, each ASAP Center was supported by its own Tri-Lab Sponsor Team (TST), which consisted of two technical staff members from each of the NNSA laboratories. One TST member from a given laboratory had expertise in the subject matter of the particular ASAP Center and the other had expertise in high performance computing. The stability of significant long-term funding, the close interaction with the laboratories, and the annual reviews were major factors in the success of the program.

In 1996 a request for pre-proposals was issued, resulting in about 80 responses. In 1997 these were reviewed over a two-day period by a team from national laboratories, private industry and academia. As a result, 48 of the pre-proposal responders were encouraged to submit full proposals. Again, these were reviewed over a two-day period by a review team of internal and external experts, resulting in seven proposals selected for site visits. Five university Centers of Excellence were ultimately chosen. Multiple disciplines and departments were engaged at each of the Centers. The TSTs helped the ASAP Centers understand the interests and experience of the NNSA laboratories in their ASCI work and fostered communication and interaction between the Centers and the laboratories. This close association with the three NNSA laboratories provided an unprecedented opportunity for collaboration in areas of common interest. Through their shared experiences using massively parallel computers, and their workshops and technical exchanges, the NNSA laboratories and the universities formed active exchanges and collaborations that were mutually beneficial. Each Center supported around 70 people each year. The total number involved over the life of the program was considerably larger due to a wide variety of interactions with the broader scientific community, as well as individual transitions in and out of the Centers. Thus a large number of faculty, research staff, postdoctoral researchers, and students were exposed over the life of the program to the methodologies, opportunities and challenges of applying numerical simulation to a large, complex, multidisciplinary application.

The five Centers created by ASAP were:

- California Institute of Technology: Center for Simulating the Dynamic Response of Materials, led by Professor Daniel Meiron;
- Stanford University: Center for Integrated Turbulence Simulation, initially led by Professor William Reynolds (deceased), and later Professor Parviz Moin;
- University of Chicago: Center for Astrophysical Thermonuclear Flashes ("FLASH"), initially led by Professor Robert Rosner, and later Professor Donald Lamb;
- University of Illinois at Urbana-Champaign: Center for Simulation of Advanced Rockets (CSAR), led by Professor Michael Heath; and
- University of Utah: Center for Simulation of Accident and Fire Environments (C-SAFE), led by Professor David Pershing.

As the Centers began operation, the scale of interdisciplinary team research employing large scale, high performance computing required by ASAP was uncommon in academia owing to technology limitations, education and research funding practices, and academic tenure policy. Computing systems available to the academic community had a peak performance of about half a teraflop, while ASCI systems available at the NNSA laboratories had only recently reached peak performance of slightly more than one teraflops (ASCI's Red machine at SNL in 1997). In the pre-ASCI environment, models of complex phenomena were normally built in one or two dimensions and were, at best, loosely coupled through shared files. The rare three-dimensional simulations were considered heroic calculations and were conducted primarily on government facilities. Even though the applications of interest frequently involved the interaction of multiple physics over large length and time scales, simulations were normally restricted to a single discipline or the physics was greatly simplified. In addition, the simulations only covered a narrow range of length and time scales.

In anticipation of the computing requirements necessary to meet the demands of the complex simulations that the Centers were asked to perform, the NNSA laboratories gave the Centers access to a significant fraction of the resources that were available in the non-classified computing environment. In addition, to facilitate access and usage of these facilities, the Computer Resource Team was established consisting of a representative from each of the laboratories and the Centers.

As mentioned above, the prevailing situation for science and engineering research at universities was one of single-researcher or small-group projects on narrowly focused topics. Tenure reviews emphasized a strong record of sole or primary authorship of high-quality research articles in peer-reviewed journals as the preferred metric of achievement for a research professor. This latter emphasis had the consequence of discouraging interdisciplinary collaborations, especially in large research groups because at the time there were fewer journals for publishing interdisciplinary research and because the value of each participant's contributions could be hard to assess in collaborative work. Further, significant funding and time were required to develop large scientific codes and the supporting infrastructure, resulting in fewer papers. Such large-scale projects also required significant full-time research staff, such as post docs and research faculty and staff. The prevailing pursuits of focused, single-researcher projects at universities necessarily impacted the educational practices. Graduate students were trained to work in the existing academic environment and had little opportunity for participating in large, interdisciplinary collaborations that could better prepare them for work in project teams involving large codes and associated software engineering practices, as were common at the NNSA national laboratories. Thus, for ASAP to be successful it required not only significant scientific and computational advances but also major organizational innovations.

California Institute of Technology—The Caltech Center had the goal of developing a Virtual Test Facility (VTF), a suite of codes that could be integrated in different ways to provide diverse means to simulate the dynamic responses of solid or fluid materials loaded by an impactor or explosively driven pressure. The emphasis was to understand how intense loadings affect materials by utilizing simulations based on explicitly modeled deformation mechanisms. Driver applications for these developments included automobile crash; gas pipeline explosions; aircraft structural fatigue; laser fusion; hypersonic combustion; design of metal components that operate beyond the elastic range (*e.g.*, munitions, armor, energy absorbers); designing systems that operate in the presence of fluid turbulence (*e.g.*, aircraft wings, reentry parachutes on spacecraft); and tailoring metal properties by controlling microstructure.

At the time ASAP began, computational modeling of the dynamical behavior of materials was largely phenomenological. Typically the constitutive properties of the material, such as the detonation speed of an explosive or the stress response of a solid, were provided by parameterized expressions whose parameter values were determined from specific calibration experiments. The experiments provided limited amounts and kinds of information. While these computational models did a good job reproducing the calibration data, they could not be relied on for extrapolation. Often the parameter values needed to be recalibrated for a different material or even the same material in a different geometry, in order to obtain acceptable agreement between simulation and experiment.

University of Chicago—The primary focus of the FLASH Center at Chicago has been simulating the explosion of Type 1a Supernovae that are produced when an aging white dwarf star shrinks to the point at which the intense pressure at its core ignites a thermonuclear explosion releasing a flash of energy that heats the dying star's core to billions of degrees in a fraction of a second. Since the flash occurs in white dwarves that are always of nearly the same size and mass, Type 1a supernovae all have about the same peak brightness, making them effective "cosmic yardsticks" for studying the expansion of the universe.

At the time ASAP began, the international supernova community usually fit observations of Type Ia supernova light curves and spectra using a highly simplified model. In this approach, a one-dimensional white dwarf star was artificially expanded, after which an ordinary flame front was sent through it at nearly the speed of sound, i.e., a speed ~1000 times faster than is physically realistic. It was only beginning to be understood that the deflagration phase had to be followed by a detonation phase, in order to match spectroscopic observations. The first simulations of buoyancy-driven turbulent nuclear combustion had just been done. Simulations of the hydrodynamic explosion phase were almost exclusively two-dimensional, and ignition was almost always assumed to occur at the center of the star. Radiation transfer calculations were always done in one dimension.

University of Illinois, Urbana-Champaign—At Illinois, the Center set out to perform high-fidelity, three-dimensional, fully coupled simulations of solid rocket motors, with specific emphasis on the Reusable Solid Rocket Motor (RSRM) that provides 80% of the lift to place the U.S. Space Shuttle into orbit. Specific goals were to simulate a full two-minute burn of the RSRM and to understand failure modes such as the O-ring failure that caused the loss of the Challenger shuttle in 1989.

Even though a solid rocket motor involves a number of interacting components, the industry and NASA standard at the time was to model the individual components with relatively low fidelity simulations in one or two dimensions, thus ignoring the complex component interactions. High fidelity three-dimensional simulations were viewed as too costly and not feasible in the rocket design and analysis process.

Stanford University—The Stanford Center had the goal of modeling a complete jet engine involving three components: the compressor, the combustor and the turbine. The key was to link the three components together in a seamless simulation even though different models were used in each component. Additionally, modeling the combustion itself presented a complex, multi-physics challenge.

Industry viewed high-fidelity three-dimensional, end-to-end, full jet engine simulations as too costly and not feasible in the engine design process. The individual components were modeled with relatively low fidelity one-dimensional simulations. The design of new jet engines was heavily based on experience and engineering intuition with components built and tested individually, and assembled and tested as a whole system only at the full production stage.

The Stanford Center was unique in that it also performed research on compilers and supercomputer architecture at several levels, using feedback from work on the engine simulation to demonstrate the value of the new computer science approaches developed.

University of Utah—At Utah, the Center was focused on accidental fires and explosions, particularly in the context of handling, transporting, and storing highly flammable materials. The particular problem was to simulate the explosive response of a canister containing an explosive material embedded in a jet fuel pool fire, from initial heating to ignition and explosion of the container.

The state of the art at the time was to simulate the pool fire with low-fidelity, reduced dimensional models with no explicit time dependence to obtain initial conditions for the heating of the canister. A completely separate simulation was then used to determine the response of the canister and the explosive material; thus the dynamic impact of the fluctuating nature of the fire was completely lost.

1.3 Summary of Results & Accomplishments of the ASAP Program and the ASAP Centers

At the completion of the ASAP program, all five centers had made major advances on the goals outlined in Section 1.1. Details of their accomplishments are summarized in the sections to follow. Perhaps most significant is that all had developed full-scale, integrated, multi-physics, multi-scale, three-dimensional simulations of their chosen system, and the organizational and software infrastructures that supported these simulation capabilities. The simulations were demonstrated to run efficiently on a variety of multi-teraflops platforms provided by the Centers' local computing laboratories, NNSA, and the DOE Office of Science. In many cases their simulations represented a capability that was not available anywhere else for their chosen applications. The accuracy of their simulations, resulting from the multi-scale models' ability to track events at the relevant scales, has clearly demonstrated the value of the latest ASC supercomputers for advancing science and engineering. The Centers have also established and demonstrated approaches for validating simulation codes against experiments, which was an essential advance needed to make high performance computer modeling viable for scientific and engineering applications. Such efforts led to enhanced collaboration between experimentalists and computational modelers for simulation validation. The technical achievements of the ASAP Centers have led to thousands of publications, invited presentations and special sessions at prestigious technical conferences. Key publications are listed at the end of this report. In addition, the Centers' powerful software infrastructures built to support the simulations were made available to the scientific and engineering community.

At the beginning of the program, the University of Illinois was the only institution of the five Centers to have a formal program in computational science. By the end, all had a formal program in place that provided an augmentation to the more standard disciplinary degree. Through these programs and other Center activities, many hundreds of students and post docs were exposed to the power of team research and multidisciplinary modeling and simulation. The Centers convincingly demonstrated the importance of having a critical mass of full-time research associates as a new paradigm in academic research, working closely with graduate students and faculty. As mentioned above, many of these researchers accepted positions at NNSA laboratories, or went on to research positions in industry, other government agencies, or to faculty positions in many universities. Although the overarching applications chosen by the Centers were not directly connected to the NNSA, collaborations between Center and NNSA laboratories' personnel evolved from specific research topics pursued by the Centers.

2. Center Accomplishments

2.1 California Institute of Technology

2.1.1 Evolution of Large-scale, Multidisciplinary Modeling and Simulation

Simulation State of the Art—When the Caltech's Center for Simulating the Dynamic Response of Materials (CSDRM) was first established, it had long been known that a hierarchical multi-scale approach that represented the actual mechanisms underlying the observed behaviors was the preferred way to achieve a predictive simulation capability. At the time, however, this was almost impossible to carry out in a practical way for two reasons. First, the understanding of such multi-scale effects was incomplete. More importantly, even if one knew all the relevant interactions, it would not be possible to carry out a simulation because such multi-scale models required the use of many internal degrees of freedom for each computational cell, which made the simulations into prohibitively large computational challenges.

The advent of massively parallel computation made it possible to overcome both of these limitations. It was conceivable to use high performance computing (HPC) to investigate interactions on the microscopic scale that could, ultimately, inform engineering scale, continuum models. Secondly, it was possible to consider performing the very large simulations that utilized these more detailed, mechanistic models.

Results and Payoffs—Making predictions for the targeted driver applications required the ability to understand, at the most fundamental level, the dynamic response of materials to strong insults. The approach was to develop a Virtual Test Facility (VTF), a set of computer simulation codes that could be integrated in different ways to provide a means to simulate the dynamic response of solid, fluid, or combined solid and fluid bodies subjected to some strong dynamic mechanical loading. Application of the VTF resulted in several breakthroughs:

- Demonstration of the importance of impulse effects on the deformation of metals loaded by high explosive blasts was achieved through simulations in which both fluid and solid effects were calculated simultaneously and self-consistently.
- Coupled fluid-solid simulation of reentry parachutes for spacecraft revealed mechanisms and interactions leading to observed instabilities in parachute performance.

- Simulation of hypersonic combustion provided a means of validating the Center's fluid turbulence models and demonstrated the viability of their approach to structure-based turbulence modeling.

In the course of developing the VTF and the component multi-scale material models, the Center achieved the following:

- Developed numerical methods in solid mechanics for bridging length scales;
- Achieved new innovations in first principles-based computation of material properties such as ReaxFF inter-atomic potential that enables simulation of chemistry in a classical molecular dynamics (MD) method;
- Developed a multi-scale modeling method for investigating polycrystalline plasticity of metals (Cu, Ta, Fe);
- Developed structure-based modeling for large eddy simulation of turbulent flows;
- Achieved new insights into the behavior of converging shock waves through synergistic use of experiments and simulations;
- Developed a deeper understanding of metal deformation behavior through multi-scale modeling that is anchored in fundamental, atomistic scale simulations. In particular, Caltech identified the origin of differences between the predictions of the Taylor hypothesis for deformation of polycrystals and experiment.

The Center's efforts in HPC and multi-scale modeling also produced advances in computer and computational sciences:

- Extended the ghost fluid method to couple Eulerian and Lagrangian codes;
- Developed efficient, fast algorithms for generating level sets;
- Advanced software integration through development of a Python scripting framework, called Pyre, for coupling solver routines within the VTF in a scalable manner. This is used to drive coupled simulations, in a transparent way, across multiple computing platforms.

Additionally, advances were made on methodology and approaches to validating a large-scale, integrated, multi-physics code ensuring that the simulations were solving the equations that correctly described the physical phenomena of interest:

- Coupled experimental capabilities with the advanced VTF simulation capabilities to validate the CSDRM's models for turbulence and the multi-scale models of material behavior;
- Demonstrated the value of coordinated development of numerical simulations and experiments. Experimental results were used to validate and sharpen the simulations, and simulations were used to design new integrated experiments.

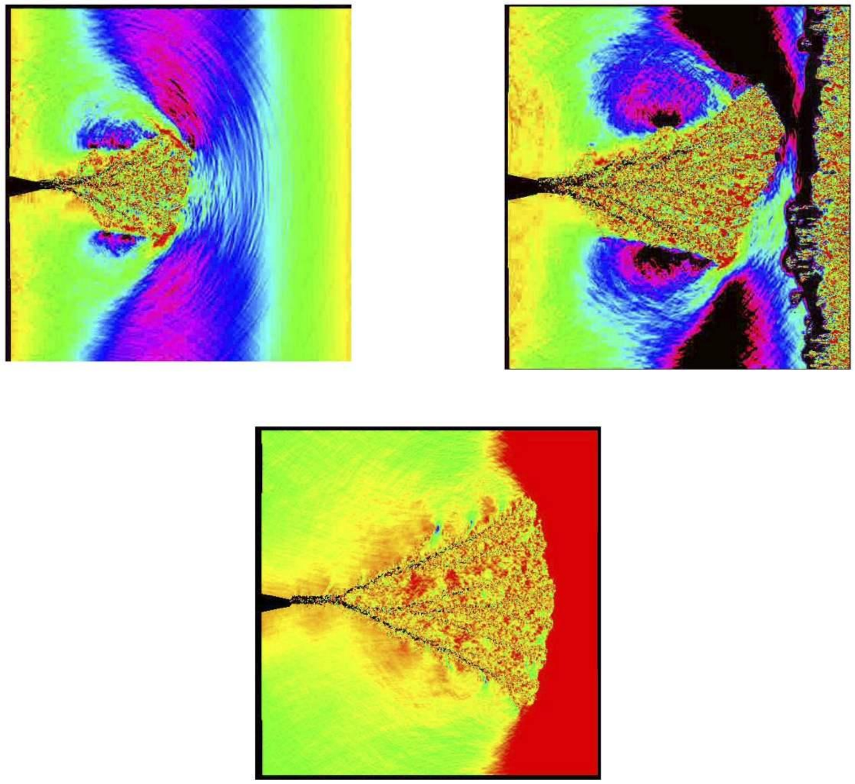

Figure 2.1-1—An image of a branching crack colored by strain rate.
The images show the stochastic nature of branching crack growth and the importance of precursor elastic waves that can be seen propagating ahead of the cracks. The calculations are performed using the Adlib solid mechanics solver of the VTF with a cohesive finite element capability allowing the mesh to separate when a critical tensile loading is exceeded at an element boundary.

Software available as a result of the program—Software integration through the Pyre Python scripting framework served as an example of a successful development activity that was emulated by different groups at the NNSA laboratories, as well as elsewhere. The other software product from the CSDRM that was picked up by the NNSA laboratories is the ReaxFF reactive inter-atomic potential model. ReaxFF, developed by A. van Duin and W.A. Goddard, permits simulation of chemistry (making and breaking of bonds) in a classical MD simulation. ReaxFF was adopted by researchers at both LANL and SNL. At SNL, Aidan Thompson incorporated ReaxFF into his massively parallel MD code, GRASP, producing the first freely available parallel implementation of the reactive potential. It was later migrated into SNL's widely used massively parallel MD code, LAMMPS.

2.1.2 Impact on NNSA Laboratories, Other Agencies, Scientific and Engineering Communities, and Industry

The experience and successes of Caltech's CSDRM significantly contributed to the selection of a new team, which drew heavily from the ASAP team, for funding under the NNSA Predictive Science Academic Alliance Program (PSAAP), the follow-on to ASAP. This stands as a substantial impact on the NNSA laboratories and the wider community as it continues Caltech's developments, presentations, and publications in multi-scale simulation of material response using HPC. Specific impacts from CSDRM include:

- A number of applications of MD and quantum mechanics with LANL and LLNL including Van Duin and Goddard's ReaxFF reactive interatomic potential (described above);
- Creation of a discrete differential geometry and geometrical calculus as a new approach for solving problems in solid mechanics simulation and visualization of simulation results;
- Adoption by SNL and LANL of the philosophy, ideas, and software capabilities to develop and promote advanced classical MD simulation methods that are informed by high accuracy quantum calculations and can capture chemical events;
- Follow-on applications of the VTF and the resulting capability in forming high performing interdisciplinary research teams include those working on the DANSE (Distributed Data Analysis for Neutron Scattering Experiments) project and on earthquake prediction;
- Continuing support by LANL for the turbulence modeling work; in particular, the use of Caltech's Large Eddy Simulation (LES) approach as a kind of "ground truth" for their Reynolds-averaged Navier-Stokes (RANS)-based approach;
- Improvements in the ghost fluid and level set methods used in the detonation shock dynamics work at LANL;
- Collaboration with LLNL on the use of the porous plasticity model to model spall;
- Investigation with LANL of the use of laminate methods to understand sub-grain structures and their evolution;
- Integration of the quasi-continuum approach with the ParaDis dislocation simulations at LLNL;
- Exchange of the AMROC class library with SNL collaboration of load balancing strategies.

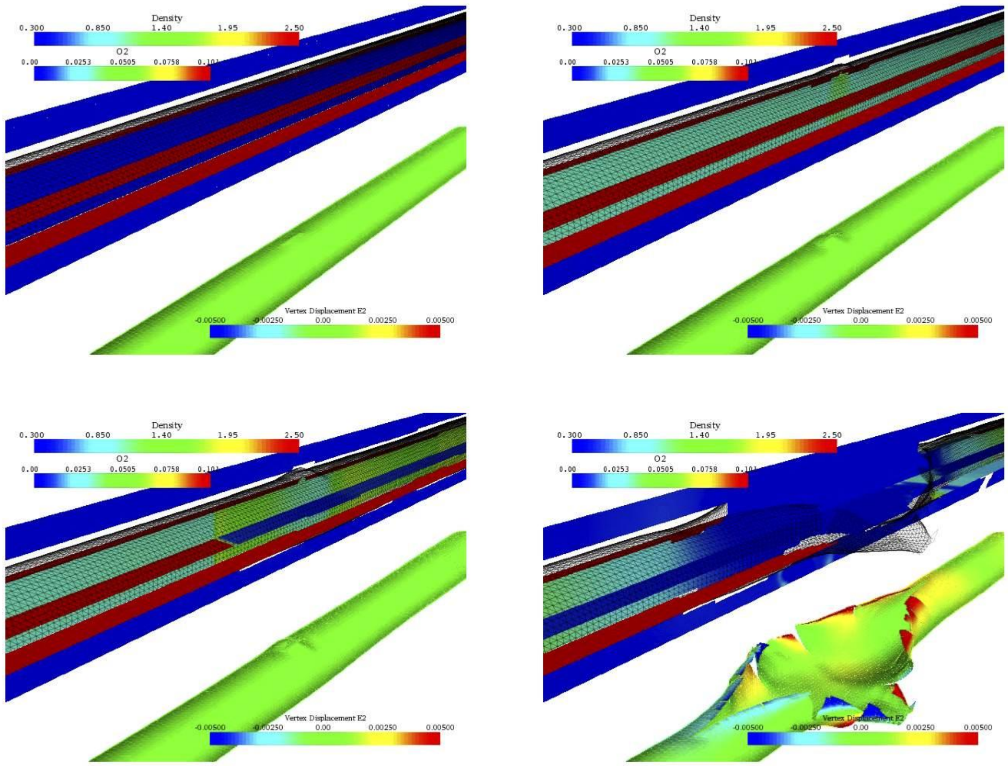

Figure 2.1-2—A calculation of a detonation wave propagating in an aluminum tube using the solid fluid coupling capability of the VTF.

The tube has been scored so as to nucleate a crack in the tube. Once the detonation passes over the crack it loads the metal shell, and a running crack then ensues. The detonation waves are produced by the combustion of ethylene. The fracture capability uses the cohesive shell elements integrated into the SFC shell solver.

2.1.3 Impact on Education and Research in Academia

ASAP increased the visibility of computational science at Caltech and was the impetus for the development of the Computer Science and Engineering minor that is now in operation. Not only is the integrated, multi-scale approach the basis of Caltech's follow-on PSAAP Center, it has also been adopted by groups at NASA and MIT. The ASAP effort developed a culture of interdisciplinary research that integrates modeling, computational science, and experiment. This approach has been used repeatedly in research programs that Caltech has engaged in since the original ASAP Center. Caltech is reorganizing to merge programs from applied math, computer science, information science, and controls into a department of Information Science and Computational Mathematics. This will be one of the few large-scale research thrusts of the Engineering division.

A legacy of the CSDRM is the education in dynamic response of materials of a group of researchers who are producing important work in academia and at the national laboratories. Another is having a group of faculty, at Caltech and at other institutions, who understand the research issues of the NNSA and other agencies and can respond appropriately in support of future initiatives. The VTF software framework continues to be supported and used productively, even after key staff departed.

Publications are another enduring part of the legacy of CSDRM. The Center made available on their web page over 300 journal publications, proceedings papers, theses, and reports spanning computational and computer science, solid dynamics, compressible turbulence fluid dynamics, atomistic methods for material property prediction, and validation experiments.

2.1.4 Connections among the NNSA Laboratories and Participating U.S. Universities

A member of the TST, Peter Schultz (SNL), spent a year at Caltech in Prof. W. Goddard's Materials and Process Simulation Center (MSC) learning their approach to multi-scale materials modeling and providing them his code and expertise in quantum density functional theory (DFT) calculations. Several staff and students who were key to the atomistic multi-scale effort from the CSDRM Center have been hired at the NNSA laboratories and other universities: R. Muller (SNL); A. Strachan and M. Koslowski (both previously at LANL but now Professors at Purdue involved in that university's PSAAP Center project); R. Deiterding was hired by Oak Ridge National Laboratory. Collaborations and interactions continue between SNL and Prof. W. Goddard's MSC and with alumni of his laboratory, including Tahir Cagin, Marcus Bueler, Timo Jacob, A. Strachan and M. Koslowski. Interactions with NNSA laboratories are continuing under the ASC PSAAP program.

2.2 University of Chicago

2.2.1 Evolution of Large-scale, Multidisciplinary Modeling and Simulation

Simulation State of the Art—Prior to the ASAP program, simulations of Type Ia supernovae were highly simplified, as described in Sec. 1.2. By the end of the program, however, the University of Chicago Center had developed the FLASH code, a widely used, open-sourced, extensible, modular, massively parallel block-structured adaptive mesh refinement (AMR), three-dimensional community code for astrophysical simulations, and had carried out the first three-dimensional simulations of the deflagration and detonation phases of Type Ia supernovae. The simulations showed that the outcome of this phase is dramatically different if ignition occurs at a point or at a cluster of points that are even slightly off center in the white dwarf star. Most simulations of the explosion phase of Type Ia supernovae now take ignition to occur at a point or at a cluster of points that are off center or are randomly distributed around the center. Chicago's FLASH simulations led to a variety of scientific advances, discussed below.

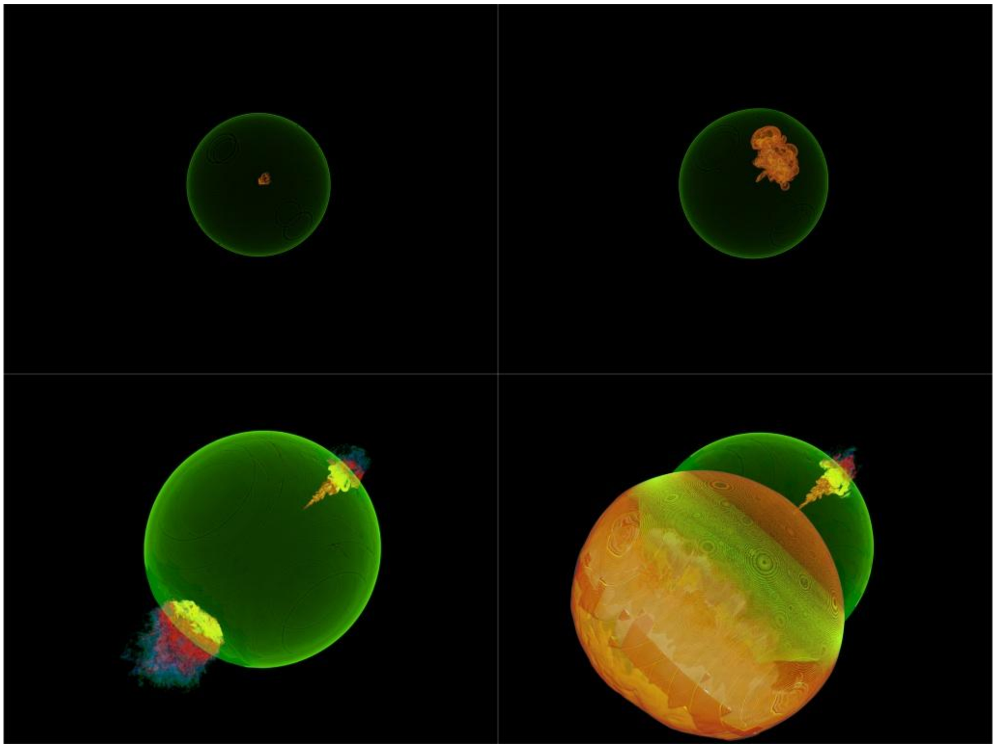

Figure 2.2-1—Flash Center Simulation of GCD Model of Type Ia SNe for Multiple Ignition Points.
Images showing the gravitationally confined detonation (GCD) model of Type Ia supernovae at four key moments: (a) 0.25 s, soon after the bubble becomes Rayleigh-Taylor unstable and develops into a mushroom shape, (b) 0.7 s, shortly before the bubble breaks through the surface of the star, (c) 3.9 s, when the hot ash has flowed over the surface of the star and has begun to collide, and (d) 4.2 s, as the detonation wave sweeps through the star. The surface of the star is shown in green and the extremely hot matter (ash or unburned fuel) is shown in red and yellow. The simulation began with 30 hot, burning, 16-km radius bubbles randomly distributed within an 80-km sphere that is offset 100 km from the center of the star. This large-scale 3D numerical simulation showed that the GCD model can account for the full range of observed luminosities. It was carried out using the FLASH code on the Intrepid machine at Argonne National Laboratory under the INCITE program.

Results and payoffs—The FLASH code led to the discovery of a completely new mechanism, known as Gravitationally Confined Detonation, to account for Type Ia supernovae (Calder et al. 2003; Plewa, Calder, and Lamb 2004). This mechanism is the only one so far in which initiation of a detonation does not have to be put in by hand. It accounts for the observed range of nickel masses and peak luminosities, and shows scaling behavior suggesting that all initial conditions lead to a one-parameter (e.g., mass of nickel) family of outcomes. In current work, researchers are extending these results to spectral predictions via two-dimensional radiative transfer calculations, and have begun the first comprehensive, systematic validation of several current models of Type Ia supernovae, using a large suite of three-dimensional simulations and high-quality light curves and spectra obtained by the SDSS-II Supernova Survey team and its collaborators. This work is important because the intrinsic luminosity of Type Ia supernovae is a key factor in interpreting cosmological expansion and the properties of dark matter. The goal of the Center's simulations is to reduce the scatter in the calibration of Type Ia luminosity permitting more reliable conclusions about the properties of dark matter.

In addition, FLASH has led to:

- Discoveries and demonstrations in isotropic homogeneous weakly compressible turbulence, including:
  - Scaling behavior for density and temperature fluctuations (Benzi et al. 2008);
  - Universality of statistical properties of particle trajectories (Lanotta et al. 2008).
- The demonstration that wind-wave mixing can explain carbon enrichment necessary for novae (Alexakis et al. 2005, 2007);
- The elucidation of differences between buoyancy-driven and fully developed turbulent nuclear combustion (Townsley et al. 2009);
- Other important three-dimensional simulations include:
  - Galaxy cluster mergers (Zu Hone et al. 2009a, 2009b, 2010);
  - Rayleigh-Taylor instability (Dimonte et al. 2007).

FLASH also has been applied to other important problems, including:

- Relativistic accretion onto neutron stars;
- Helium burning on neutron stars;
- Nova outbursts on white dwarfs;
- Gravitational collapse/Jeans instability;
- Laser-driven shock instabilities;
- Flame-vortex interactions;
- Richtmyer-Meshkov instability;
- Cellular detonation;
- Magnetic Rayleigh-Taylor instability;
- Orzag/Tang MHD vortex.

Software available as a result of the program—One of the chief legacies of the Chicago FLASH Center is the FLASH code, a widely deployed community code for astrophysics, CFD, MHD, and eventually HEDP. It is extensible, modular, and massively parallel, with block-structured AMR. FLASH includes a built-in unit test framework. The code team adheres to a rigorous software maintenance process, and conducts annual tutorial sessions, for which the slides are posted on the FLASH web site. The code has been downloaded more than 2000 times, and more than 700 licenses have been granted for its use. More than 370 scientific papers have been published for which researchers used FLASH, including more than 650 scientists as co-authors.

2.2.2 Impact on NNSA Laboratories, Other Agencies, Scientific and Engineering Communities, and Industry

The FLASH Center's outreach to Argonne National Laboratory (ANL) in computer science led to a strong program of interaction in the general area of computational science between the two organizations. Of particular importance was the application of ANL's work in visualization to FLASH simulations.

Also, Professor Robert Rosner, the founding director of the Center, became chief scientist and then, for five years, director of ANL. This led to increased engagement between ANL and the University of Chicago in computational science.

The FLASH Center has attracted significant support from other agencies. Examples include:

- NASA Applied Information Systems Research: probabilistic modeling of dynamic spectra and other data ($118K for 2010-2012);
- NSF Office of Cyber infrastructure PetaApps: petascale algorithms for multi-body fluid-structure interactions ($2.25M for 2010-2013, $450K of which comes to the FLASH Center);
- NSF Physics at the Information Frontier: implicit solver on parallel block-structured AMR grid ($400K for 2010-2012);
- NSF Astronomy and Astrophysics: petascale simulations of supernovae, including light curves and spectra ($2.25M for 2010-2014);
- Others:
  - Argonne's LDRD project;
  - Chicago-Fermi Lab's strategic initiative grant;
  - NNSA and DOE Office of Science/ASCR's partnership for HEDP capability.

2.2.3 Impact on Education and Research in Academia

The FLASH Center's work led to the creation of University of Chicago's Computation Institute in 2000. The result was a university faculty structure for training students and postdocs in computational science. Computational science faculty is now in the Departments of Astronomy & Astrophysics, Biological Sciences, Computer Science, Mathematics, and other departments. Other legacies include the Toyota Technical Institute-Chicago, dedicated to basic research and education in computer science, including scientific computing. This institution was founded in 2003 and has close ties with University of Chicago's Computer Science Department.

Furthermore, the FLASH Center transformed the University of Chicago's interactions with ANL. As noted above, Robert Rosner recently served as director of ANL, which has led to increased engagement of its staff at the University of Chicago.

Finally, FLASH Center personnel helped found and participated in three NSF Physics Frontier Centers: the Joint Institute for Nuclear Astrophysics, the Center for Magnetic Self-Organization in Laboratory and Astrophysical Plasmas and the Center for Cosmological Physics (now the Kavli Institute for Cosmological Physics).

2.2.4 Connections among the NNSA Laboratories and Participating U.S. Universities

The FLASH Center has trained 29 students, 43 post docs, and many staff researchers, of whom 12 went directly to NNSA laboratories after leaving the FLASH Center. Other impacts of the Center include:

- Two students who were key FLASH developers (Paul Ricker and Michael Zingale) won Presidential Early Career Awards in Science and Engineering.
- Twenty-six Center students and post docs went on to faculty positions, taking with them their expertise in computational science, spreading an appreciation of its importance and its use in the academic community.
- There have been several collaborations between FLASH personnel and NNSA researchers. Collaborators include Guy Dimonte (with Calder), Chris Fryer and Aimee Hungerford (with Heger, Lamb, Jordan, Townsley), and Chris Tomkins (with Weirs, Dwarkadas, Plewa) at LANL; and Chris Mauche (with Plewa and Truran) at LLNL.
- FLASH is being used to conduct simulations of Rayleigh-Taylor mixing by Guy Dimonte at LANL.
- Frank Timmes and Bruce Fryxell, former members of the FLASH Center who went to LANL, played key roles in designing and implementing the Tri-Laboratories Test Suite, which was based on FLASHTest, the Center's test suite. More recently, Fryxell moved to University of Michigan to lead the V&V task of the PSAAP project there.

2.3 University of Illinois at Urbana-Champaign

2.3.1 Evolution of Large-scale, Multidisciplinary Modeling and Simulation

Simulation State of the Art—Prior to the ASAP program, high-fidelity, three-dimensional, end-to-end, full rocket engine simulations were not available to researchers and design engineers. The Illinois center, known as the Center for Simulation of Advanced Rockets (CSAR), set out to demonstrate that such simulations were not only possible but also desirable. To this end they developed a software infrastructure called Rocstar, which is the only full-system, three-dimensional simulation capability in the US for solid rocket motors. No such capability exists in NASA or DOD. Significant capabilities of Rocstar include:

- Turbulent, reactive multiphase flow;
- Materials modeling;
- Propellant combustion;

- Component oriented software architecture to facilitate adding additional physics modules or other capabilities.

Running on state-of-the-art computing systems, CSAR has simulated the full two-minute burn of the solid rocket booster engine (RSRM) that powers the U.S. Space Shuttle. This involved integrating multiple disciplines and treating time scales from microseconds to minutes.

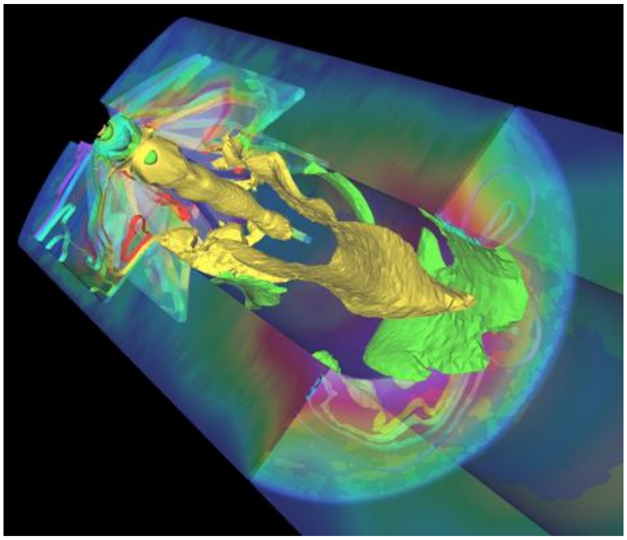

Figure 2.3-1—Hot gas temperature field and propellant stress in NASA RSRM rocket motor. *Fully coupled "fluid-structure interaction" simulation performed using CSAR Rocstar Simulation Suite.*

Results and Payoffs—Using the Rocstar suite, Illinois was able to model and analyze several different aspects of solid rocket motors in addition to a complete two-minute burn of the RSRM:

- Analysis of the propellant slumping problem that led to failure in the Titan IV rocket;
- Full simulations of small rockets, such as the attitude control motors;
- Simulation of turbulence around the flexible inhibitor in the RSRM that can be a contributor to power fluctuations;
- Simulation of impingement of unburned aluminum fuel particles on the nozzle of the RSRM;
- Simulations showing a connection between resonant acoustic modes in rocket motors and propellant morphology.

In addition, demonstrating its flexibility and utility, the CSAR simulation technology has been applied to other significant problems:

- Analysis of helicopter blade performance, particularly for noise suppression;

- Analysis and modeling of the exhaust from naval ship stacks to determine the thermal impact on nearby structures;
- Investigation of the structural impact of atmospheric flow around tall buildings;
- Study of injury mechanisms in kidneys due to cavitation bubble dynamics;
- Use of the shock interface capability to study volcanoes on Io.

CSAR has made significant science and engineering advancements in pursuit of its goals:

- Developed the first three-dimensional packing code for propellants capable of packing spherical and generic (non-spherical) particles at realistic packing densities. It is now used for general packing problems in addition to energetics.
- Conducted constitutive and damage modeling of heterogeneous propellants and metallic components.
- Modeled crack propagation particularly for burning and pressure-driven scenarios.
- Characterized material property of *in situ* materials from tomographic imaging and analysis.
- Conducted multi-scale materials modeling and molecular-level modeling of material interfaces.

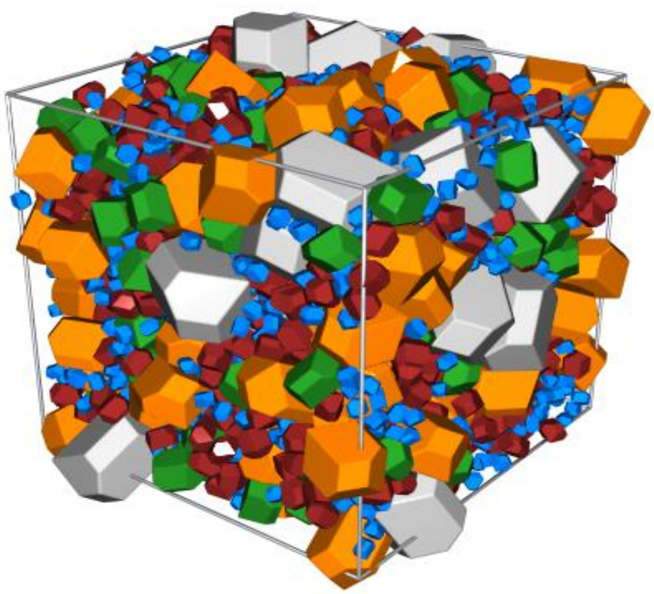

Figure 2.3-2—Crystal packing morphology simulation of energetic material using CSAR Rocpack code.

Pursuit of CSAR goals led to significant advances in computer science via the development of a multi-physics integration framework to support:

- Parallel programming environments Charm++, AMPI, and ParFUM;
- Parallel I/O (Panda);
- Parallel performance monitoring and modeling;
- Visualization.

A number of computational mathematics advances were made in support of CSAR's goals:

- Space-time discontinuous Galerkin methods;
- Time zooming to support simulations across broad ranges of time scales;
- Original LES turbulence modeling;
- Accurate and conservative data transfer methods based on common refinement and stable and efficient explicit surface propagation;
- Mesh smoothing, repair and re-meshing with quality metrics.

Software available as a result of the program—CSAR developed Rocstar, an object-oriented integration framework with flexible parallel orchestration, stable component coupling and time-stepping. The university has spun off IllinoisRocstar as a company to perform engineering analysis and to customize and support the simulation software. Rocstar code is now available as open source.

2.3.2 Impact on NNSA Laboratories, Other Agencies, Scientific and Engineering Communities, and Industry

Over its lifetime, CSAR has supported over 160 graduate students, of which about 40 have taken positions at the NNSA or other DOE laboratories.

The US space program and the role of rockets in DOD are dependent on the design of efficient, effective and safe solid rocket motors. NASA and the DOD have requested specific simulations be run by CSAR:

- Analysis of the RSRM V, the proposed follow-on to the RSRM rocket motor;
- Analysis of the Orion Launch Abort System, the new system intended to safely propel the crew vehicle away from the rest of the rocket in case of emergency.

The solid rocket motor industry requires cost effective designs that meet government requirements. With this in mind, Illinois is investigating erosive burning, a major unknown in solid rocket motors. This involves:

- Cross-flow velocity,
- Particle size,
- Pressure,
- Initial temperature.

Illinois' science and technology capabilities that have contributed to US industry:

- ATK (Alliant Techsystems, Inc.) has utilized the simulation capability to validate its own low-fidelity design codes.
- Boeing uses the meshing technology and the Rocstar framework for fluid-structure interaction.
- Caterpillar has incorporated the meshing and parallelization technology into its own in-house software capabilities.

As recognition of its simulation capabilities, the University of Illinois has received support from a number of organizations. Two CSAR spinoff companies (IllinoisRocstar, LLC and Buckmaster Research) have received Department of Defense's (DOD's) small business technology transfer (STTR) and small business innovation research (SBIR) sub-awards to study how rockets behave in fires, and the chemical, mechanical and thermal effects on nozzle erosion. Other STTR/SBIR awards have come from DOD and NASA. A recent NASA Jet Propulsion Laboratory (JPL) project through IllinoisRocstar provides support to implement CSAR efforts in reduced order clustering for UQ.

CSAR has received funding from ATK and NASA to study the impact of grain-size, material behavior and mechanics on combustion, acoustics, and thermo-mechanical properties of rocket motors. In addition, Illinois was the only academic member of the Integrated Product Team for the five-year USAF Solid Propellant Performance Project (now complete).

Finally, the broad science and engineering communities have benefitted from the more than 1200 journal articles published by CSAR faculty, staff and students.

2.3.3 Impact on Education and Research in Academia

The Computational Science and Engineering (CSE) program at the university is the home of CSAR and is the model for university multidisciplinary centers at Illinois. As a result of the ASAP award for CSAR, the CSE program has grown in size and influence with 17 participating departments (up from eight departments at the time the ASAP program began) and 140 affiliated faculty. Because of CSAR's demonstration of the value of multidisciplinary, cross-departmental research, the university has developed new multidisciplinary centers such as the Midwest Structural Sciences Center (AFRL), the MURI Center for Stress Wave Mitigation (ARO) and the now completed Center for Process Simulation and Design (NSF and DARPA).

2.3.4 Connections among the NNSA Laboratories and Participating U.S. Universities

CSAR science and technology that have come to the NNSA laboratories include:

- Interaction with Dan Hooks (LANL) on the use and capabilities of the CSAR packing code, Rocpack.
- Demonstrations of the packing of the energetic materials HMX, PETN and RDX.
- Potential integration of some key Rocstar features with SNL Sierra toolkit.

2.4 Stanford University

2.4.1 Evolution of Large-scale, Multidisciplinary Modeling and Simulation

Simulation State of the Art—Prior to the ASAP program, engine researchers and designers did not perform high-fidelity, three-dimensional, end-to-end, full jet engine simulations. Jet engine components were/are built and tested individually and assembled and tested as a whole system only at production. Nothing like Stanford's full system three-dimensional simulations had ever been attempted. The Stanford Center, known as Center for Integrated Turbulence Studies (CITS), set out to demonstrate that such simulations were not only possible but also desirable. To this end a general high-fidelity simulation environment was developed for multi-physics and geometrically complex turbulent flows. Specifically, this is the only full system, three-dimensional, unsteady, integrated simulation capability in the US for jet engines; no such capability exists in NASA, DOD, or industry.

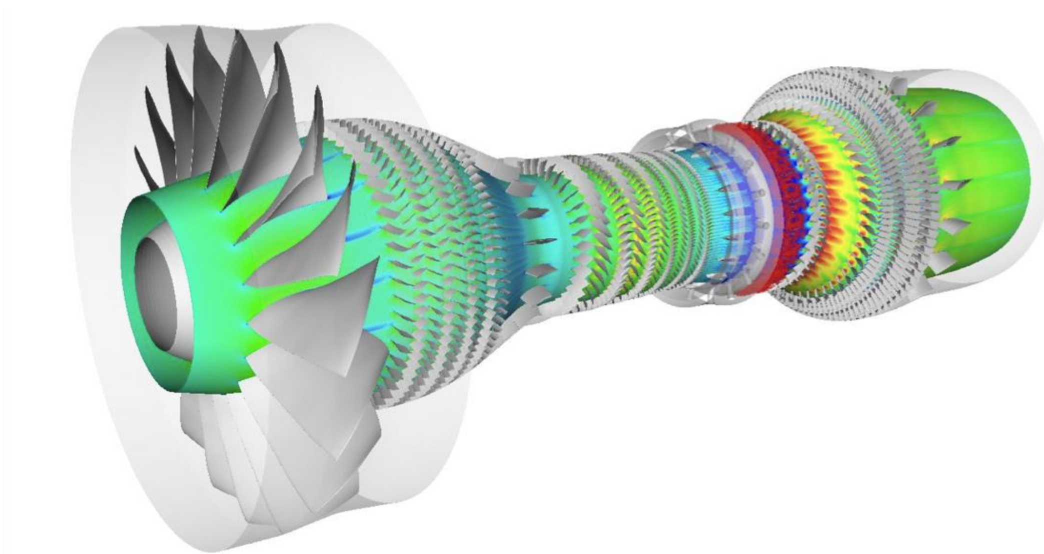

Figure 2.4-1—The overarching problem for Stanford's Center for Integrated Turbulence was the integrated simulation of the Pratt & Whitney commercial jet engine.
This image shows the instantaneous flow field on a surface through the engine. The integrated simulation included the fan, compressor, combustor, turbine, and nozzle.

Results and Payoffs—The payoff for significantly improved jet engine designs, even given the current mature state of the art, will be enormous, particularly for those who live within earshot of an airport or are affected by poor air quality due to engine emissions. In addition, better understanding of how jet engines work will allow the industry to improve performance, fuel-efficiency, and reliability. Another advantage will be for engine manufacturers that spend upwards of $1 million for each engine performance test to significantly reduce these costs by being able to do virtual full engine testing in the computer. When testing a new engine or concept, it is essential to approximate conditions at cruise altitude, which is expensive. Being able to simulate these conditions would allow testing during the design process and eliminate a lot of the guesswork.

Using state-of-the-art computing systems, CITS has simulated the full flow path of a jet engine. This involved integrating compressor, combustor and turbine. These models encompass multiple scales and physics. Stanford's integrated system-level simulations identified three coupled effects that had never been seen before in simulations, which led United Technologies Research to import the following Stanford work:

- Integrated fan/compressor simulations that revealed the remarkably long persistence of fan wakes into the low-pressure compressor.
- Integration of the combustor with the upstream high-pressure compressor that identified potential sensitivity of diffuser performance and separation to inflow wakes.
- High-fidelity reacting-flow simulations of the combustor that identified a potential mechanism for hot-streak formation and migration to the inflow turbine blades.

Stanford's studies of supercomputer software and hardware architecture within the Center have also had significant industry impact:

- The research on virtual operating systems led to the spin-off of the VMware Corporation, which is now close to $2B/year in revenue.
- Significant work in streaming supercomputer architectures, influencing work on a possible emerging exascale system path.
- Promising work on programming languages for large-scale scientific computing.

Software available as a result of the program—Stanford developed three key pieces of software:

- A Python based framework for integrating multidisciplinary codes called the Coupler for High-performance Integrated Multi-Physics Simulation (CHIMPS).
- A Reynolds Averaged Navier Stokes (RANS) fluid flow code.
- A LES combustor code, which was the first multi-physics large eddy simulation software technology for complex domains.

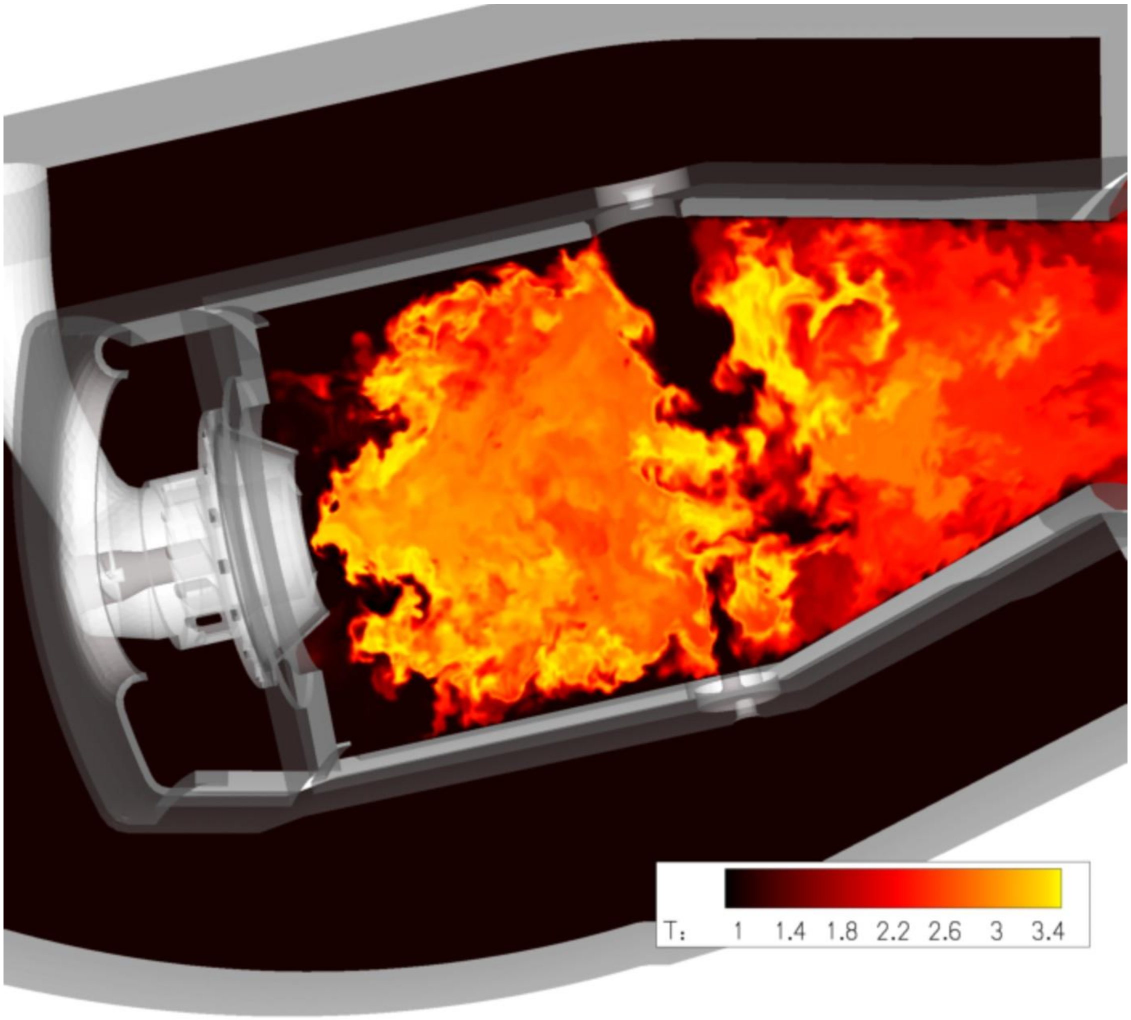

Figure 2.4-2—Instantaneous temperature on the mid-plane of a Pratt & Whitney 6000 combustor operating at cruise conditions.

2.4.2 Impact on NNSA Laboratories, Other Agencies, Scientific and Engineering Communities, and Industry

- The scientific areas below are examples of research that had impact on NNSA laboratories through collaborations:
  - High-fidelity multi-physics Large Eddy Simulation (LES) on unstructured meshes and the parallel, scalable LES solver CDP.
  - Fundamental mechanism developed for bypass laminar/turbulent transition.
  - Large eddy simulation of combustion to predict pollutants.
  - Numerical Analysis of Multi-code Coupling using summation-by-parts approaches.

- Significant computer science advances include:
  - High-speed signaling technology developed in the early years of the program. This technology now forms the basis for data communication in almost all high-performance computers.
  - High-radix interconnection networks. Technology was transferred to Cray for use in their latest supercomputers.
  - Streaming supercomputer architecture legacy: the adoption of stream processors for scientific computing has been significantly sped up by CITS research efforts.
  - Static program analysis methods for detecting bugs in software commercialized by Coverity, Inc.
  - Affine loop analysis methods used in all vectorizing compilers.
  - Work on virtual machines and virtual clusters commercialized by VMWare.
  - Work on parallel graphics, Chromium, set world rendering record and is widely used in DOE laboratories.
  - Stream Programming Models such as StreamC and KernelC, Brook and BrookGPU, Sequoia, CUDA and Cg (NVIDIA).

- The CITS simulation technology has been applied to other significant problems which have attracted funding from other agencies:
  - The prediction and control of helicopter noise.
  - The analysis and modeling of the mixing characteristics of buoyant plumes and fires.
  - The investigation, in collaboration with LANL, of the mechanism of tsunami wave generation due to landslides.
  - Extension of flamelet-based chemistry to include heat losses (DOE).
  - Pollutant predictions in real combustors including the effects of radiation (DOE).
  - Computing wall pressure fluctuations on airfoils using immersed boundary methods (Navy).
  - Conjugate heat transfer in turbulent flows (DOE).
  - Synthetic jet control of airfoil flows at high angle of attack (Industry).
  - High-lift multi-element airfoil simulations (Industry).
  - Airplane contrail simulations to improve contrail sub-grid modeling in global climate models (FAA, NASA).
  - Coral reef nutrient transport and response of coral morphology to flow (NSF).
  - Polymer-induced turbulent drag reduction (DARPA).
  - Urban environment dispersion (Army).

  - Low-Mach number noise prediction (cooling fans, car mirrors, trailing edge noise) (Navy, Industry).
  - Compressible jet noise prediction (NASA).
  - MHD simulations with application to metal casting (Industry).
  - Particle deposition in human respiratory system (EU).
  - Race car aerodynamics (Industry).
  - Science and technology advances generated at Stanford that have benefitted the NNSA laboratories include:
    - Dynamic subgrid turbulence models (LLNL);
    - Soot and combustion models (SNL);
    - Reynolds averaged turbulence models (SNL);
    - Streaming programming (LANL);
    - MMS for variable density flows (SNL);
    - Low dissipation discretization schemes (SNL).
  - Exposure to Brook prototypes helped understanding of GPU languages (CUDA, OpenCL, Brook+) at SNL, now being used to investigate improvements in combustion modeling.
  - Open source graphics libraries and standards have had a major impact on the national laboratories' Powerwall developments.

2.4.3 Impact on Education and Research in Academia

The impact of CITS research and development has been varied and wide spread. Some highlights include:

- Demonstration of the value of the multidisciplinary, cross-departmental model of CITS as shown in the creation of a new Institute for Computational and Mathematical Engineering at Stanford. The Institute has a broad graduate curriculum with focus on scientific computing and is training a new generation of modern computational engineers.
- Brought to Stanford and affiliated research communities a multidisciplinary "National Lab" culture in scientific computing used in studying large-scale problems, including:
  - A multidisciplinary task force mentality to resolve problems and focus on integration;
  - A focus on a multidisciplinary, multi-scale, project structure; software engineering; code-integration; V&V for other research activities, e.g. DARPA Helicopter Quieting, NASA Research Agreements.
- Establishment of the Pervasive Parallelism Laboratory, largely an industry-funded Center, whose existence can be linked directly to the investment in the Computer Science component of Stanford's ASAP project.

- Increase in the number of courses in computational science; for example in UQ, Parallel Computing, Computational Fluid Dynamics.
- Growth of on-campus computing resources, (e.g. in Mechanical Engineering alone 10,000+ CPUs and over 50K GPUs are now available for research use).
- Significant increase in industrial collaborations/affiliates.
- An anticipated increase at Stanford of involvement of the Statistics and Applied Mathematics community owing to the interest in probabilistic methods for UQ, which are expected to grow and spread to other fields such as bio-medical engineering.

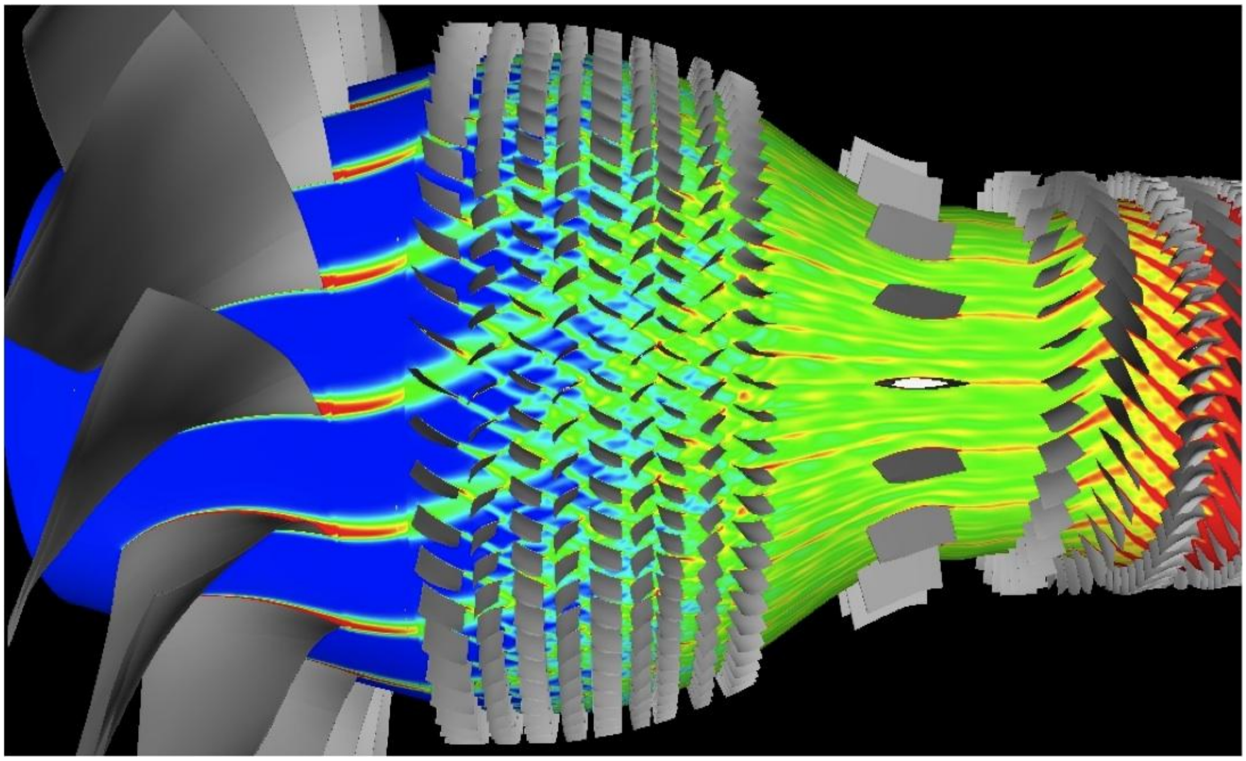

*Figure 2.4-3—**Persistence of entropy wakes from the upstream fan well into the compressor.** This work led to the identification of several important coupled effects.*

2.4.4 <u>Connections among the NNSA Laboratories and Participating U.S. Universities</u>

Collaborations with the NNSA laboratories included:

- Combustion and turbulence modeling with SNL.
- Turbulence modeling of truck aerodynamics with LLNL.
- Visualization with all three laboratories.
- Programming environments with LANL.

- Tsunami modeling with LANL.
- Energy-conservation in numerical discretizations with SNL.
- Verification using MMS with SNL.
- Buoyancy-driven instabilities modeling with SNL.
- LES simulations in models of buoyant plumes with SNL.
- Multiple convection operators for each transport PDE with SNL (SIERRA/Fuego).
- Parallel I/O (UDM) with LANL.
- Parallel global solvers with LLNL (Hypre).
- Parallel grid generator with SNL (Cubit).
- Python-based code-to-code interfaces with LLNL/LBNL/Caltech.

2.5 University of Utah

2.5.1 Evolution of Large-scale, Multidisciplinary Modeling and Simulation

Simulation State of the Art—C-SAFE started with two legacy codes that were not integrated with each other: (1) a Reynolds-Averaged Navier Stokes (RANS) combustion code (Banff) that solved for the equilibrium state-space distribution in a gas-fired furnace, and (2) the SCIRun scientific problem-solving environment that contained components for visualizing static problems. Neither code had any time-dependent components and neither was capable of describing the dynamics of fire, reaction of energetic materials, solid mechanics, fluid-structure interactions or explosions. Neither code had any capability to deal with adaptive mesh refinement. The Banff code ran only on single-processor machines; SCIRun ran only on parallel computers with shared-memory architectures.

By the end of the program, the C-SAFE fire model was the highest fidelity fire model in the world for the simulation of large, jet-fuel fires because it:

- Is LES-based;
- Contains detailed soot sub-models based on molecular fundamentals;
- Uses parameterization as the methodology for including first principle chemistry in the simulation;
- Employs a surrogate fuel formulation developed by C-SAFE to accurately represent the chemical and physical characteristics of complex jet-fuel;
- Calculates radiation, including the effect of soot, using a discrete ordinates method so the directional-dependence of radiation can be included;
- Utilizes robust nonlinear and linear solvers for large-scale, nonlinear sets of PDEs;
- Has been rigorously verified and validated against extensive experimental measurements, and

- Captures a wide range of length scales (e.g. fires from centimeters to meters and explosions from micrometers to centimeters) and time scales (e.g. fires from milliseconds to minutes and explosions from microseconds to milliseconds);
- Exhibits excellent parallel scaling to run on platforms as small as a laptop or as large as 100,000 processor cores.

Results and Payoffs— One of the major results of C-SAFE was a study of the effect of four parameters (fire size, container location, wind speed and fuel evaporation rate) on the incident heat fluxes on a container filled with an energetic material. The study included 16 full-scale simulations focusing on time to ignition and the kinetic energy of the container explosion. The results confirmed intuitive understanding based on experiments. For example,

- The slower the heat-up, the more violent the explosion;
- The most dangerous location for high-energy explosives in an accidental fire is adjacent to the fire, *not* in the middle of the fire.

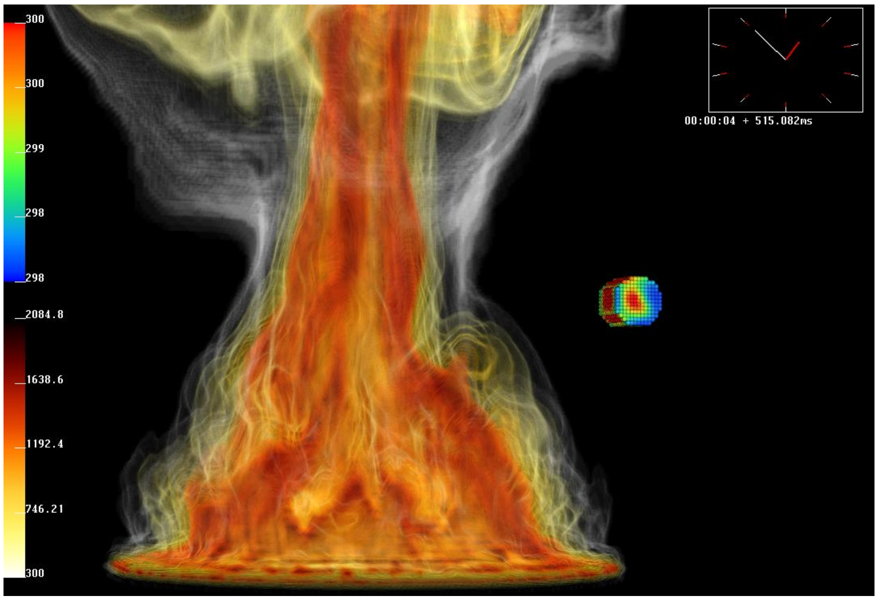

Figure 2.5-1—Heat Flux Validation – Container Near Large Pool Fire.

Other simulation and validation experiments have revealed the basis of interesting behavior of damaged explosives. If a completely filled container of explosive is heated externally, the resulting combustion normally is confined to a small volume just inside the container wall, and the velocity of the steel fragments is low (about 100 m/s) as a result of rapid depressurization of this small combustion volume. However, if a smaller amount of explosive is used by incorporating a hollow bore (like a rocket motor), the explosive can be damaged by collapse of the hollow bore. The combustion can then spread to a large volume of explosive before the container breaks, and the kinetic energy of the steel fragments can be up to ten times higher. The site of maximum heating turned out to be counterintuitive, i.e., hotter on top than bottom.

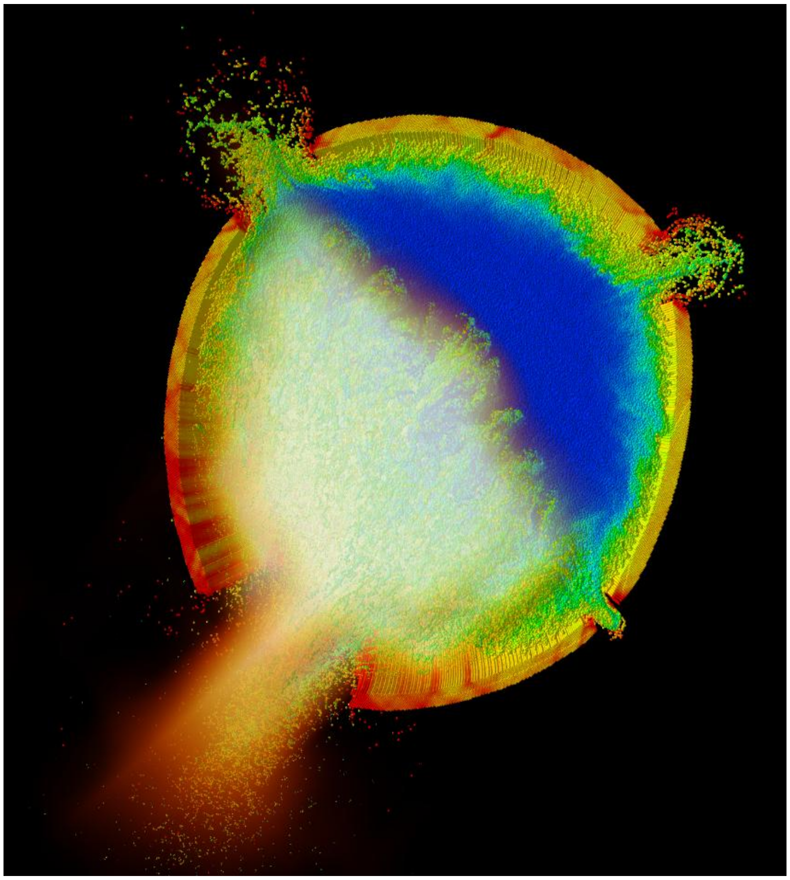

Figure 2.5-2—Exploding Container.

Working in collaboration with the SCI Institute, C-SAFE scientists have produced major, new visualization techniques with broad impact, including:

- New, high-speed, real-time ray tracing,
- New volume rendering algorithms,
- New AMR visualization techniques,
- New methods for realistic rendering of luminous flames.

The resulting three-dimensional volume-rendered images of fires and of explosives have enhanced understanding of the structure and physics in these systems where experimental data are difficult to obtain.

C-SAFE pioneered work in the material point method (MPM). The motivation was to find a technique for treating the canister dynamics. In the beginning, various aspects of the method such as convergence were not well understood. Through years of research, publications and workshops, C-SAFE staff has evolved the method into the Generalized Interpolation Material Point Method (GIMP). It is now the *de facto* standard and is a smoother, more stable and accurate version of MPM. It is viewed as a robust technique for a broad range of problems including for example, micro vessels, foam, snow, powdered metals and rock, and PBXs.

Software available as a result of the program—Work at the Center culminated in Uintah, a set of libraries and applications for simulating and analyzing complex chemical and physical reactions. In particular, Uintah:

- Allows engineers to transform existing serial codes into high-speed parallel codes without being bogged down by parallel programming details;
- Balances computational loads across thousands of processors;
- Provides high-speed graphics interfaces;
- Allows integration of components developed by third parties including non-linear and linear solvers designed for solving complex-flow problems (e.g. PETSc and Hypre).

2.5.2 Impact on NNSA Laboratories, Other Agencies, the Scientific and Engineering Communities and Industry

Over its lifetime, C-SAFE has supported over 100 graduate students who have gone on to promote computational science in university, industrial and government laboratory positions. Integrated simulations using the C-SAFE code have enabled the solution of real problems of national interest:

- Rapid analysis of terrorism threats;
- Design of large-scale fire experiments;
- Developing protocols for transportation classification of hazardous materials;
- Protection of the environment through proper flare design;
- Investigation and analysis of an extremely violent transportation accident leading to new approaches to storing and transporting explosive material;
- Uintah is being used at the University of Arizona to model the transport of oxygen and other tissue-building blocks in order to optimize the design of the engineered specimens, allowing them to achieve functionality more quickly.

Accomplishments of C-SAFE have led to contributions to and from industry:

- Comparison of two- and three-dimensional simulations convinced Schlumberger of the power of three-dimensional simulations leading to support for planning explosive bore holes in sandstone.
- ATK/Thiokol Propulsion sets up and ignites actual explosives intended to generate data needed to validate the predictions of C-SAFE's simulations.

- C-SAFE faculty member, Steve Parker, formed a company known as RayScale, which then was bought by Nvidia resulting in an Nvidia Research Office in Salt Lake City and the Ray Tracing Center of Excellence, both led by Parker.
- Another C-SAFE faculty member, Grant Smith, formed a startup research company, Wasatch Molecular, Inc., to carry out SBIR- and STTR-funded projects with Uintah and other software products.
- Additional funding comes from John Zink, Chevron, Praxair, and CH2M Hill.

As a result of C-SAFE's accomplishments, Utah also receives support from NIH, NSF and DOE including:

- The DOE SciDAC Center for the Visualization and Analytics Center for Enabling Technologies;
- Awards from the NSF Petascale Applications program for enhancing Uintah and porting it to the NSF Teragrid;
- Within the DARPA Virtual Soldier project, Utah used MPM to simulate a penetrating wound with a comprehensive cardiac/torso model to understand the mechanics of wounding in an effort to improve the chances of recovery from such wounds;
- Under NIH support, the Uintah fluid-structure interaction component, known as MPMICE, is currently being employed in a study of phonation, or the production of sound, in human vocal folds;
- NIH support for an interdisciplinary effort to study the growth of blood vessels.

One of the biggest success stories is the Institute for Clean and Secure Energy, led by Phil Smith. There are about 60 projects and 28 faculty members in the Institute; work is on clean coal, carbon sequestration, oil shale tar sands, heavy oil, and the quantification of combustion hazards. This is a direct result of C-SAFE with funding from a number of different sources, including DOE Office of Fossil Energy and NNSA (for a new project on Predictivity of Carbon Management).

University of Utah faculty, students and staff have published more than 170 scientific articles based on C-SAFE supported research in computer science, mechanical engineering, chemical engineering, chemistry, and applied math.

2.5.3 Impact on Education and Research in Academia

Utah now has a formal computational engineering and science program that initially started as a certificate program and transitioned in early 2000 to a Masters degree in Computational Engineering and Science. This has led to the initiation of a Computing Ph.D. in the School of Computing with multiple tracks (scientific computing, computer graphics and robotics).

C-SAFE has helped to provide an environment in which various disciplines (biomedical engineering, chemical engineering, chemistry, computer science, materials, and mechanical engineering) interact. Students have grown up in the C-SAFE interdisciplinary environment and leave with the benefit of understanding interdisciplinary research. The university has an evolving culture of UQ in a broad spectrum of application areas.

C-SAFE success has led to growing on-campus computing resources, such as the Updraft Cluster that was deployed in 2008 with 256 dual-quad core nodes producing 22 teraflops. Parallel computing is now viewed as the preferred approach for high accuracy simulations.

Multi-authored papers are now the norm and contribute to faculty advancement.

2.5.4 Connections among the NNSA Laboratories and Participating U.S. Universities

At LANL Uintah has been used to model the dynamic compaction of foams, such as those used to isolate nuclear weapons components from shock loading. The Material Point Method component was used to carry out these simulations, which allowed for compression of the foam to full densification.

Visualization technologies, including ray tracing, have been exchanged with all three NNSA laboratories. Collaboration on combustion modeling with LANL and SNL is ongoing.

One of the legacies of CSAFE is the lasting strong and deep collaboration between the Combustion and the V&V/UQ groups at SNL and the Combustion Simulation Group at the University of Utah. This collaboration includes the Fire Science & Technologies group, the Thermal/Fluids Computational Engineering Sciences group, the V&V group (all at SNL-Albuquerque), and the Combustion Research Facility (CRF) at SNL-Livermore. There are numerous examples of such collaborations:

- Dr. Jackie Chen (SNL-Livermore) holds an adjunct appointment at the University of Utah and shared graduate students (James Sutherland and David Lignell) with Prof. Philip Smith. Each of these students spent two years of their Ph.D. studies working at the CRF in Livermore. After receiving their Ph.D. degrees, each went on to tenure-track faculty positions (James Sutherland at the University of Utah and David Lignell at Brigham Young University).
- Other SNL staff members have served on Ph.D. advisory committees at the University of Utah, including Alan Kerstein (SNL-Livermore) and Rod Schmidt (SNL-Albuquerque).
- The SNL fire simulation software development is led by Stephan Domino, who graduated from Utah with a Ph.D. and was supervised by Prof. Smith.
- For ten years, SNL and Utah held an annual "Soot Workshop," which brought together leading soot researchers from around the world. The focus of this group evolved to include not only issues of soot formation, but many other issues related to heat transfer in pool fires, notably V&V.
- The collaborative efforts in Verification, Validation and Uncertainty Quantification (V&V/UQ) between Utah and SNL grew to include two joint workshops on V&V/UQ. Relationships that developed through these meetings with both Sheldon Tieszen (SNL-

Albuquerque) and Chris Shaddix (SNL-Livermore) have resulted in a variety of technical exchanges involving students and faculty at the University of Utah.

- A One-Dimensional Turbulence (ODT) workshop was held that brought in researchers from around the world interested in pursuing the ODT model formulated by Alan Kerstein (SNL-Livermore).
- SNL experimental data have played a key role in the validation of the Utah fire models.

3. Summary

The aforementioned accomplishments demonstrate that ASAP met the goals for which it was established:

1. Establish and validate large-scale modeling and simulation as a viable methodology across complex scientific and engineering applications.
2. Solve science and engineering problems of national importance through the use of large-scale, multidisciplinary modeling and simulation.
3. Enhance the overall ASCI effort by engaging academic experts in computer science, computational mathematics, and numerical simulations of science and engineering problems.
4. Leverage relevant research in the academic community, including basic science, high-performance computing systems, and computational environments.
5. Strengthen education and research in areas critical to the long-term success of the ASCI and the Stockpile Stewardship Program.
6. Strengthen ties between the NNSA national laboratories and participating U.S. universities.

ASAP also demonstrated the impact of an interdisciplinary research model that required building a large multi-science/engineering computational simulation. By providing sustained multi-year funding over a significant time period the universities were able to assemble the required multidisciplinary research team and develop the computational model that enabled the science/engineering advancements. The research model also involved close interaction between the Centers and the NNSA laboratories. Keeping a focus on both integration of the research team and the science and engineering led to a new computational science methodology within the universities. Further, increasing the emphasis on V&V added to the value of the program. Finally, in addition to the literally thousands of peer reviewed publications produced by the Centers, one of most significant contributions is the number of students and postdocs trained in research and development of large-scale modeling and simulation.

Appendix A: Publications

The Centers produced literally thousands of publications in refereed journals and conference proceedings. Rather than attempt to list all of the publications (which are available on the Centers' websites), each Center was asked to provide a list of the twenty most significant publications.

California Institute of Technology - Center for Simulating the Dynamic Response of Materials

"Fundamental Structure of Steady Plastic Shock Waves in Metals," A. Molinari and G. Ravichandran. Journal of Applied Physics 95(4), 2004, 1718-1732.

"Fracture response of externally flawed aluminum cylindrical shells under internal gaseous detonation loading," T.W. Chao and J.E. Shepherd. International Journal of Fracture 134(1), 2005, 59-90.

"Planar Shock Cylindrical Focusing by a Perfect-gas Lens," P.E. Dimotakis and R. Samtaney. Physics of Fluids 18, 031705-1.

"Thermal Equation of State of bcc Tantalum to High Pressures and Temperatures," R.E. Cohen and O. Gulseren. PHYSICAL REVIEW B Volume: 63 Issue: 22 Article Number: 224101 Published: JUN 1 2001.

"A Detailed Model for the Decomposition of Nitramines: RDX ad HMX," D. Chakraborty, R. Muller, S. Dasgupta, W. Goddard III. JOURNAL OF COMPUTER-AIDED MATERIALS DESIGN Volume: 8 Issue: 2-3 Pages: 203-212 Published: 2002.

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"Large-eddy simulation and multiscale modeling of a Richtmyer-Meshkov instability flow with reshock," D.J. Hill, C. Pantano, and D.I. Pulllin. Journal of Fluid Mechanics 557, 2006, 29-61.

"Large-scale fluid-structure interaction simulation of viscoplastic and facturing thin shells subjected to shocks and detonations," F. Cirak, R. Deiterding, and S.P. Mauch. COMPUTERS & STRUCTURES Volume: 85 Issue: 11-14 Special Issue: Sp. Iss. SI Pages: 1049-1065 Published: JUN 2007.

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