ACADEMIC STRATEGIC ALLIANCES PROGRAM

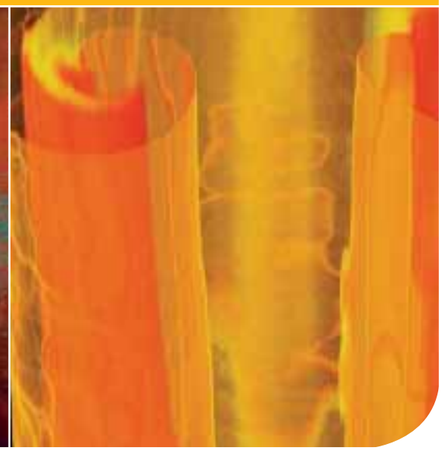
NNSA
National Nuclear Security Administration

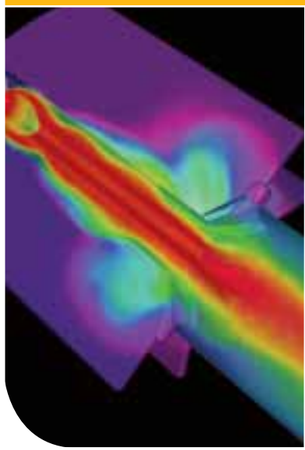
Los Alamos
NATIONAL LABORATORY

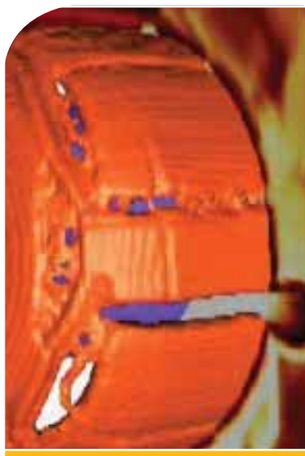
Sandia National Laboratories

University of California
Lawrence Livermore National Laboratory

DEPARTMENT OF ENERGY
UNITED STATES OF AMERICA







ASC™

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BACKGROUND

In order to provide leading edge computational modeling and simulation capabilities to support the Stockpile Stewardship Program (SSP) of the Department of Energy National Nuclear Security Administration (DOE/NNSA), the Advanced Simulation and Computing (ASC) program, historically known as ASCI, was developed in 1995. In its first ten years, ASC's strategic goals emphasized the development and use of high-fidelity, scalable, three-dimensional, multidiscipline codes to address stockpile issues, along with the creation and deployment of the required computational capabilities and supporting infrastructure at the three NNSA Defense Programs (DP) laboratories – Lawrence Livermore, Los Alamos, and Sandia National Laboratories.

In summer of 1997, the ASC program initiated the Academic Strategic Alliance Program (ASAP) by creating long-term strategic alliances with five U.S. universities (the Centers) to focus on high fidelity, scalable, three-dimensional, multidisciplinary computational science problems.

Computational science is the discipline of representing and simulating systems of real physical processes on computers. Research conducted through the university partnerships solves problems across a broad spectrum of science and engineering applications of national interest using some of the largest massively parallel computers in the world.

Although the computing problems tackled by ASAP do not involve nuclear weapons research, the computational science, computer science and computational mathematics methodologies and tools developed do provide benefits to the DOE Stockpile Stewardship Program, as well as to other national scientific, economic, and social needs. In addition, they demonstrate to a wide scientific community that such validated simulations can be carried out, using unclassified problems similar in complexity to what the national laboratories face for the SSP. Further, they provide training for graduate students and post doctoral fellows who are potential candidates for laboratory, teaching and industrial employment.

This program is unique in that each Center focuses on problems that support the ASC strategic goals. They:

- Involve complex simulations and supporting tools that require the integration of a number of academic disciplines and software components;
- Involve the integration of multiple scales in both time and space;
- Address the difficult problem of verification and validation of the simulations.

MULTIDISCIPLINARY APPROACH

One interesting and unique element of this program is the interdisciplinary approach all Centers must take to create simulations of their chosen problems. Typically, universities are structured along discipline lines (departments, schools) and seldom cross those lines in research projects. However, in ASAP the problems being addressed involve a number of disciplines ranging across science and engineering to computational mathematics and computer science. The multidisciplinary approach is essential to each Center's success as the complexity of their problems requires integrating shared knowledge, computer codes, supporting infrastructure and information across many areas of research.

MULTIPLE SCALES

The Centers are addressing problems with elements that occur at very small time and distance scales. For example, the small eddies in a river influence the flow pattern of the entire river. In order to model the larger river flow, the small eddies must be taken into consideration. Wide ranges of time scales present similar difficulties. Some problems may have processes that occur within short intervals, perhaps at the nanosecond level (one billionth of a second), while the timescale of the problem itself is measured in minutes or hours. Simulating multiple scales in time and space is an extremely difficult problem that the Centers are addressing within their research problems.

VERIFICATION AND VALIDATION

One of the major reasons the Centers were created was to demonstrate the power of verified and validated simulation. The process of verification and validation assures both that the writer's code does exactly what it was intended to do (verification) and also that the results produced by the code accurately represent the physical processes under study (validation). This is an extremely difficult problem that confronts not only the Centers, but also the DP laboratories in their challenge to use simulation as an alternative to nuclear testing while incorporating the results of focused single physics experiments. It is also an important element of each Center's work, and tackling the issues surrounding verification and validation requires the Centers to develop new approaches to problems and possibly to expand their research in unexpected directions.

FUTURE DIRECTIONS

Up until recently the ASAP program has been focused on strategic tasks similar to those being carried out within ASC, namely building large complex, integrated,

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parallel, multiscale simulations systems; providing the tools to support their building and integration; deploying large massively parallel computer systems on which to run these simulations; and beginning the process of their verification and validation. While continuing the above goals, the strategic focus of ASC has shifted to improving the confidence in scientific and engineering prediction through simulations. This requires:

- Integrating the ASC Program with certification methodologies;
- Developing the ability to quantify confidence bounds on the uncertainty in simulation results;
- Increasing predictive capability through tighter integration of simulation and experimental activities;
- Providing the necessary computing capability to code users, in collaboration with industrial partners, academia, and government agencies.

The work of the ASAP Centers is also evolving to emphasize support for these types of activities. Further, any future ASAP follow-on program will also focus on the science of prediction.

UNIVERSITY PARTNERS

Each of the five university ASC ASAP Centers focuses on developing one multidisciplinary application of national importance. In addition to leading to revolutionary advances in physical and engineering sciences, the integration of computer-based simulations from multiple disciplines provides unprecedented opportunities for major advances and discoveries in areas such as mathematical modeling, numerical mathematics, computer systems, computer sciences, and information science. The ultimate goal is to integrate large computer models from various disciplines into single, comprehensive models necessary to solve critical scientific and engineering problems.

The complexity of these problems requires computational power well beyond what is presently available anywhere. Thus, the DP laboratories have given the Centers unprecedented access to some of the most powerful unclassified computer systems available. Of significant value to the effort is the experience faculty and students gain using massively parallel computers, as well as their ability to help the labs identify problems in the hardware and software in these cutting-edge facilities.

Each Center is in the midst of its second five-year funding commitment and supports around 70 people each year. The total number involved is considerably larger, due to the broader involvement of the scientific community as well as individuals transitioning in and out of the Centers.

CENTER GOALS

CALIFORNIA INSTITUTE OF TECHNOLOGY

Center for Simulating the Dynamic Response of Materials

At Caltech, the Center has developed simulation codes for its virtual shock physics test facility (VTF). The VTF advances materials design through its capability to simulate the dynamic response of materials under intense loading conditions. Two important foci of the Center's research are the development of advanced multiscale material models and the integrated verification and validation of those models via in-house experiments. The Center's research has applications in areas such as geophysics, structural dynamics and materials design. Research areas include computational mathematics, chemistry, fluid dynamics, computer science, engineering, materials science, solid mechanics and physics.

STANFORD UNIVERSITY

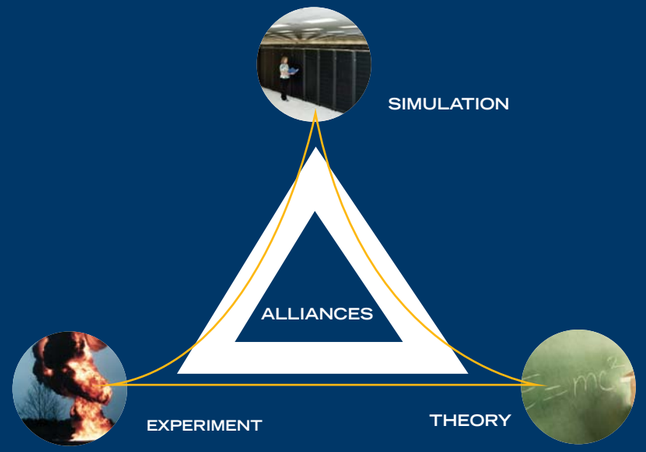
Center for Integrated Turbulence Simulations

The goal of Stanford's Center for Integrated Turbulence Simulations (CITS) is to build high-fidelity computational tools for the simulation of mutiphysics, multiscale problems in complex, industrial configurations. CITS general purpose codes combine accurate and scalable numerical algorithms and detailed physical models. The overarching problem is the simulation of a jet engine. CITS is working to establish a new paradigm that will shorten the design cycle, reduce testing expense, and improve the reliability and prediction of emissions, and noise from gas turbine engines. Research areas include fluid dynamics, computational mathematics, physics, chemistry and computer science.

ACADEMIC STRATEGIC ALLIANCES PROGRAM

INTEGRATING THEORY, EXPERIMENT AND SIMULATION

The development of the science of verified and validated computational simulations adds a powerful third methodology, when integrated with theory and experiment, for discovery and understanding in science and engineering.



UNIVERSITY OF CHICAGO

Center for Astrophysical Thermonuclear Flashes

Referred to as the FLASH Center, the Center at the University of Chicago is working to understand the physical problems of nuclear ignition, detonation, and turbulent mixing of complex multi-component fluids and other materials as represented by supernovae. Better understanding of the physics of supernovae will play a central role in answering fundamental cosmological questions such as the rate of expansion of the universe. Research areas include nuclear physics, astrophysics, fluid dynamics, mathematics, and computational science.

UNIVERSITY OF ILLINOIS at Urbana-Champaign

Center for Simulation of Advanced Rockets

The Center for Simulation of Advanced Rockets (CSAR) at the University of Illinois at Urbana-Champaign is using the NASA Space Shuttle booster and other rockets as the basis for a detailed, whole-system simulation of solid propellant rockets. CSAR research on the behavior of solid propellant rockets will have direct benefits for their design and testing and for closely related technologies, such as gas generators used for automobile air bags and fire suppression. Research areas include astrophysics, chemistry, computer science, fluid dynamics, materials science, numerical analysis, physics, structural analysis, and thermal sciences.

UNIVERSITY OF UTAH

Center for the Simulation of Accidental Fires & Explosions

The focus of Center for Simulation of Accidental Fires & Explosions (C-SAFE) is to provide state-of-the-art, science-based tools for the simulation of accidental fires and explosions, especially in the context of handling, transporting, and storing highly flammable materials. C-SAFE's simulations will help to better evaluate the risks and safety issues associated with fires and explosions in the aerospace, chemical, and petroleum industries. Research areas include computer science, materials science, chemistry, physics, and engineering.

MATERIALS UNDER STRESS

How do materials react to interactions that expose them to extreme environments, such as hard blows, explosions, and other shocks? An obvious way to find out is to carry out experiments that expose the materials to real shocks that cause waves of intense pressure to travel through the materials. In many situations, however, those experiments can be either overly simple or extremely expensive and time consuming. So research teams set out to simulate the impacts.

Why is that important? "Factors such as how alloys behave when a car crashes and how metal fatigues when a plane has flown for too long and has become exposed to the dynamics of flight through the atmosphere, are all aspects of our understanding of how materials behave under stress," Daniel Meiron, principal investigator at the Center for Simulating the Dynamic Response of Materials (CSDRM) explains. "To make predictions in these cases requires the ability to understand materials at the most fundamental level."

That is the basic mission of the CSDRM at the California Institute of Technology. "The Center has developed a virtual test facility (VTF), a suite of codes that can be integrated in different ways to provide a means to simulate the dynamic responses of solid or fluid materials loaded in some way under pressure or hit hard," says Meiron. "The emphasis is trying to understand how intense loadings affect materials."

The VTF itself permits researchers to simulate strong shock waves and detonations as they interact with solid and fluid targets. In that way it contributes to the Center's overall aim of using its simulation ability to figure out the ways in which the target materials respond to the collisions and to validate those computations against experimental data gathered from real collisions.

Scientists at the Center must deal with a wide range of material behavior. For solids, they want to simulate different forms of deformation – elastic, plastic, and the nonlinear responses known as shock waves, for example. Fluids – that is, liquids and gases – react differently, in that they respond to pressure without the back-reactions from the strength of solid materials. "But if you send high loading through them," Meiron says, "you'll generate shock waves that interact with any inhomogeneity and start turbulent mixing as a result of the compression. This mixing is a key process in many NNSA Advanced Simulation and Computing program applications."

IMPROVING CONFIDENCE IN PREDICTION VIA COUPLED EXPERIMENTS AND SIMULATION

In the first five years of its existence, CSDRM focused on developing the computational capability to perform large-scale integrated simulations of shock waves in solids and fluids. This involved deploying existing algorithms for compressible flow in fluids and high strain rate mechanics in solids on the ASC platforms, as well as developing new algorithms to enable the coupling required to do fully integrated simulations. This effort has resulted in a simulation capability that performs scalably on the ASC platforms and enables simulation involving calculations of unprecedented numerical resolution.

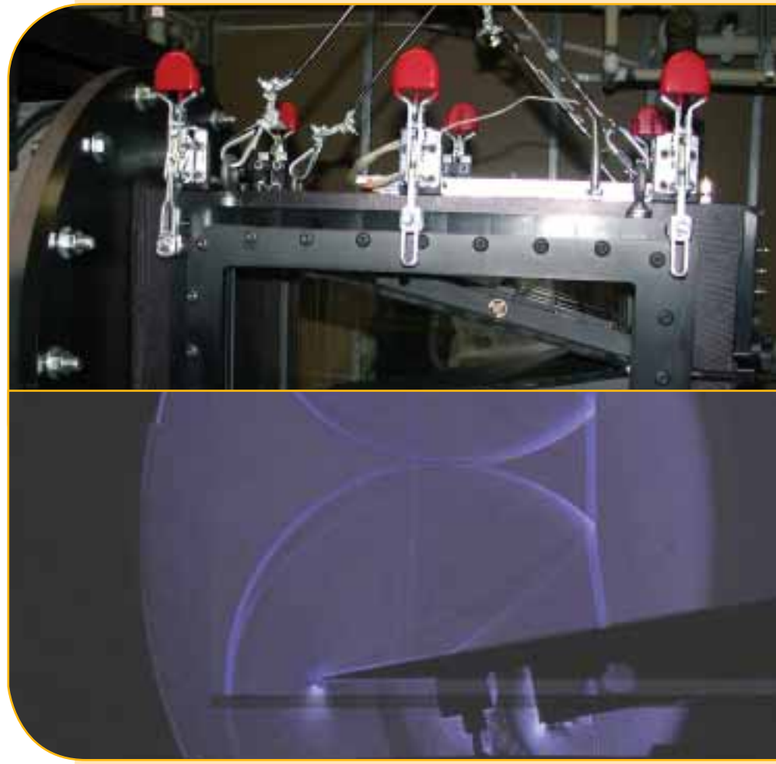
With this computational foundation in place, the Center increased its emphasis on validation. Several key experiments (two examples are discussed in the main text) were explicitly designed to couple the validation process directly to simulations using the Center's VTF software framework. For example, the converging shock simulations and experiments provide a unique testbed for validating the Center's work on turbulence modeling, while the experiments and simulations on dynamic deformation are used to validate the multiscale materials models that form the foundation of the Center's research activities. Because the relevant scales in a simulation are now tracked in an "intelligent" way via the Center's multiscale models, significant computational resources such as those provided by the unique ASC facilities are required to properly simulate the validating experiments. In addition, the new generation of validated models emerging from the Center's work provide important contributions to parallel basic research efforts in solid and fluid mechanics at the DP laboratories.

The use of well-instrumented "in-house" experiments to validate the models embodied in the VTF software ensures that experimental results can be properly compared with simulation and that the validation process provides a real but controllable challenge to simulation. The parallel development of integrated experiments and simulations is a unique feature of the Center's program; experimental results can be used to sharpen simulations and vice versa. In particular it becomes possible to diagnose the levels of uncertainty in the various stages of the multi-scale models used in the VTF and ultimately to quantify bounds on the predictive capability of the models. Most importantly, the predictive capability of the VTF software is strongly enhanced via this iterative validation process. This integrated approach to computation, experimentation, validation, and ultimately prediction is now a key feature of the process employed by CSDRM in training its PhD students who will comprise the next generation of computational scientists.

INFORMED MODELS

In the past, scientists have used engineering models to simulate the dynamic responses of different materials. Engineering models are phenomenological in character and are typically adjusted to mimic known experimental data; they are important tools in that they are designed to be simple to implement but they are generally not viewed as predictive. It has long been recognized that a more predictive approach is to develop models that couple the various length scales that are active when a material undergoes deformation. Such models are called "multiscale." For example, when a shock wave propagates through a metal it affects the material down to the atomic scale. "Our goal," Meiron says, "has been to engage the best work in multiscale models to build simulations to the extent possible based on first principles. We have constructed models that are based directly on the underlying microscopic materials physics and so the predictions are more trustworthy. Such models are generally more complex mathematically and require more intensive computation than engineering models, but this can be accommodated using the leading edge capability of the ASC computing facilities. Rather than interpolation, which is the hallmark of engineering models, we have produced a set of models endowed with information that comes from very small length scales starting at the atomistic." That type of modeling includes the plastic response of solids at extremely small scales and the mixing of fluids that takes place when vortices created by pressure waves interact with density interfaces and with each other.

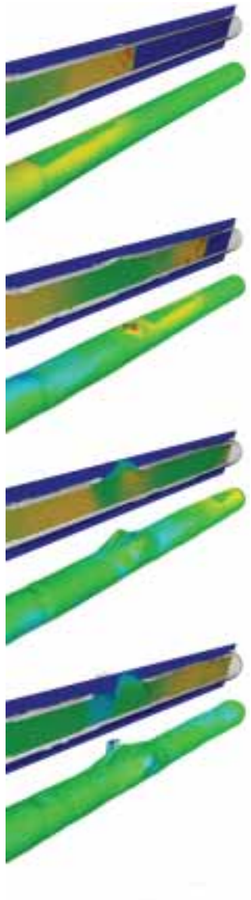
Tailored validation experiments
Shown in the figure is the converging shock experimental facility developed by Prof. Paul Dimotakis for the express purpose of validating the fluid mechanics simulation capability of the VTF. Shock waves are generated at the left via a standard shock tube and then enter the test section shown in the figure where they are made to converge and amplify. The resulting flow is then simulated using the VTF.



Integrated simulation and validation
Shown in the figure is a depiction of a converging shock wave using the Schlieren diagnostic technique. As the shock enters the test section, the convergence of the test section causes the formation of kinks on the leading shock wave as well as complicated wave patterns called Mach stems (seen behind the leading shock wave). The results of a corresponding VTF simulation are overlaid via a synthetic Schlieren image generated directly from the numerical results. The two patterns are nearly indistinguishable lending confidence to the fluid simulation capabilities of the VTF.

The natural differences between solids and fluids mean that scientists can't use a single approach to simulate both types of material. Indeed, they use entirely different types of algorithms to describe the effects of pressure on the two broad groups. In cases where both the fluid and solid need to be simulated at once (such as the flow of air over an airplane wing) these differing approaches need to be applied simultaneously. Hence, much of the Center's early work has involved the development of techniques that integrate computer codes that describe solids and fluids.

Technologies designed to deal with solids and fluids individually present their own challenges. For example, the fluid solver that the team uses must be able to handle shock waves, strong nonlinear jumps in fluid properties that occur over just a few Angstroms – the dimension across an atom. To incorporate those scales, researchers use modeling and a hierarchy of meshes – networks of minuscule shapes that represent the state of the fluid being simulated at each point in space and time. "In order to implement such a calculation on the ASC massively parallel computers, you must then distribute the meshes across many processors and make sure that the workload among the processors is balanced," says Meiron. "That's a big challenge that we have met through the use of a software framework developed by Center researcher Ralf Deiterding that facilitates the process of creating and distributing the meshes." Simulation of solid mechanics involves a similar meshing problem. "Our new multiscale models involve a significant amount of computation in each little cell being simulated," Meiron says. "The simulations may be carrying on the order of a billion variables at any one time." The result is the ability to model materials at levels of unprecedented fidelity. An example of the use of the VTF in a fully integrated mode is shown in the figure on this page where the rupture of a metal tube by a gaseous detonation wave internal to the tube is simulated.



Integrated simulation of fluid and solid mechanics via the VTF
Bottom: Recovered samples from the laboratory of Prof. Joe Shepherd displaying Aluminum tubes that have been ruptured due to the propagation of a gaseous detonation wave in the tube.
Left: Integrated simulations using the coupled fluid-solid mechanics capability of the VTF. Two distinct codes, an Eulerian fluid mechanics capability to simulate the detonation, and a Lagrangian shell solid mechanics code with fracture capability to simulate the tube, are coupled via the Center's unique level set coupling approach to generate the simulation of the fracturing tube.

TWO KEY EXPERIMENTS

Having developed their basic tools during the initial five years of the program, CSDRM's researchers are now testing and validating them. Two experiments – the creation of converging shock waves and studies of polycrystalline metals under strong loading – illustrate the way in which the Center's work closely couples simulation and supporting experiment. This direct connection of experiment to simulation is a relatively new approach to verification and validation.

"Converging shock waves in cylindrical or spherical geometry represent one of the most effective means of reaching very high pressures and temperatures – to stimulate laser fusion, for example," says Paul Dimotakis, Professor of Aeronautics and Applied Physics at Caltech. "Exploding supernovae, for example, work in similar ways."

Dimotakis theorized that sending a shock wave through a boundary between a fluid and a solid or two different fluids might cause the wave to converge in such a way that it creates ultrahigh pressures. "VTF simulations have confirmed that there exist particular solutions that lead to converging shocks," Dimotakis continues, "and we have confirmed the results experimentally." His team has fielded simple experiments and is developing more complex methodologies. "Our experiments could not be done without assistance from the VTF simulations," he adds. "And it would also be impossible to check the simulations without the experiments. This is a fully synergistic process where simulation and experiment mutually support each other: a very important model for scientific progress." While simulation and experiment have always been important tools for Caltech researchers, the close coupling of these approaches that is facilitated by the Center has allowed for additional insights that benefit both theory and design of future experiments. The insights into the behavior of shock waves in converging geometries as described above would not have been obtained without the close coupling of simulation to experiment. A comparison of the simulation and experiment for the converging shock can be seen on page 6.

Experiments overseen by Guruswami Ravichandran, Caltech Professor of Aeronautical and Mechanical Engineering, aim to validate predictions of VTF simulations on the behavior of polycrystalline metals under extreme strain rates. "We measure the stress-strain response and the temperatures at these very high strain rates," Ravichandran explains. So far, the team has compared experimental results with simulations for copper. The level of detail in simulation that can be achieved using the VTF is unprecedented and has provided important insights into how, for example, the individual metal crystallites comprising the solid interact with one another to determine the large scale response of the material. The VTF results have made it possible to understand the shortcomings of traditional models that do not take into account multiscale interactions and to then understand how to create models that do reflect the underlying microscopic interactions. "Now we're moving on to more complicated metals of more interest to the national laboratories," Ravichandran says. "We've worked on tantalum and, more importantly, on iron which is a very complicated material because it can change its crystalline structure as it responds to strain."

The Center is now well along in the next phase of operation: performing simulations with direct relevance to fundamental issues in the dynamic response of materials that are not only directly connected to the experiments in progress but are in fact influencing the design and operation of future experiments. "Without the VTF software and the interdisciplinary approach fostered by the Center, this simply would not have been possible," says Meiron.

ALTERNATIVE APPLICATIONS

The research has several potential applications. Most obviously, it will help to further computer-aided design of materials. But it also contributes, for example, to areas such as earthquake prediction and environmental analysis; astrophysics; inertial confinement fusion; and many others as the multiscale physics modules that have been developed as part of the Center's research program are useful in a wider setting. The Center has also made important contributions in the area of software integration though the development of a component framework used to couple the component solvers of the VTF. Using the object-oriented component-based semantics of the scripting language Python, the framework (called Pyre and developed by center researcher Michael Aivazis) can be used to drive coupled simulations in a transparent way across multiple computing platforms. The framework has now been adopted by other Caltech research groups to integrate solvers in other diverse disciplines ranging from geophysics to the data analysis of neutron scattering experiments.

The Center also makes a significant contribution to training the next generation of specialists in computer simulation and has initiated an interdepartmental program in Computational Science built around the ideas of integrated simulation and validation. "We'll start a graduate student on a fundamental problem that could become a thesis. But we don't necessarily tie them to our Center's deliverables," Meiron says. "We tie postdoctoral fellows more directly to the development of simulation methods." Even so, some graduate students end up playing a major role in the Center's work by contributing a core algorithm. For example, Sean Mauch developed in his PhD thesis a new fast level set algorithm, a core algorithm that makes the fluid-solid coupling capability of the VTF highly efficient. Overall, says Meiron, "We regard our students' work as long-term research that will ultimately be of great importance to us."

STANFORD UNIVERSITY

TAMING A JET ENGINE

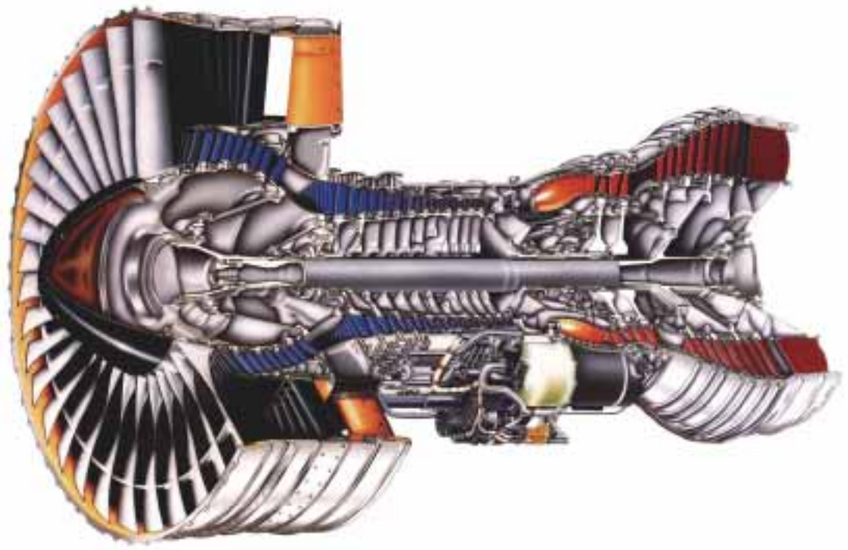
The inside of a jet engine is a violent world. Molecules of air are drawn into the fan and compressor where they are squeezed to 40-fold atmospheric pressure. Then they are spewn into a combustion chamber where they react with a swirling mist of highly flammable jet fuel and burn into a 3000ºF inferno of flames that accelerates into a whirling turbine where energy is extracted from the flow to drive the upstream fan and compressor, propelling the aircraft forward. This Hades is a place most people would never want to visit. But scientists at Stanford University's Center for Integrated Turbulence Simulations (CITS) are attempting to enter the violent, chaotic, and turbulent world of the jet engine to understand it and, just perhaps, to tame it.

The CITS research team, which includes researchers from the departments of Aeronautics and Astronautics, Computer Science, Mechanical Engineering, and the Institute for Computational and Mathematical Engineering (ICME), are all focused on the project's ultimate goal: a computer simulation of a working jet engine.

"Nothing like this has ever been attempted," says Parviz Moin, director of CITS. "Jet engine components are built and tested individually and assembled only at production. Calculating the flow and chemistry in a complete, integrated jet engine is an extremely challenging problem, but we have a team with broad expertise dedicated to making it happen."

The payoff will be enormous – particularly for those who live within earshot of an airport or are affected by poor air quality due to engine emissions, and that's most of us these days.

"Understanding better how jet engines work would allow us to improve performance, fuel-efficiency, reliability, and to create engines that make less noise and that emit fewer pollutants," says Frank Ham, an engineer in the Center's combustor group. "There is a push now for the next generation of jet engines to reduce the environmental impact of combustion by decreasing the amount of soot and particulates that contribute to air pollution."



Cutaway illustration of a gas turbine engine showing primary flow path through compressor (blue), combustor (orange with flame), and turbine (red).

But the immediate advantage would be for engine manufacturers that spend upwards of $1 million for each engine performance test.

"The design of new jet engines has been heavily based on experience and engineering intuition," says Moin. "When testing a new engine or concept, it is essential to approximate conditions at cruise altitude, and that's expensive. Being able to simulate these conditions would allow testing during the design process and eliminate a lot of the guesswork."

CITS has developed simulation tools that, for the first time, integrate all major engine components thus allowing engineers to evaluate performance of the entire system before it is physically assembled. In addition, fundamental work in combustion science in CITS has led to breakthroughs that in turn have substantially increased the accuracy in predicting engine emissions.

But actually doing what the Center has set out as its "grand challenge" means taking on a problem that has vexed scientists since Leonardo da Vinci first pondered the physics behind a turbulent river current.

"You have to understand that turbulence is a classic problem in physics, and one that many people consider unsolved," says Ham. Inside an engine, air and jet fuel flow under turbulent conditions, with little eddies and vortices that help mix the two components and maximize combustion. The simulation of an entire jet engine is what is called a multiscale problem, one that involves simultaneous calculation of events at the scale of the overall engine dimensions in meters, down to that of the smallest atomized fuel droplets in micrometers. Even on the world's fastest supercomputers, it remains impossible to perform engine simulations that resolve this full range of scales, and some approximation or modeling must be used.

THE MISSION

The mission of Stanford's ASC Center is to develop a verified and validated high-fidelity general-purpose computational fluid dynamics tool for multiscale, multiphysics flows in realistic configurations. CITS research is in basic physics, physical modeling and numerical algorithms blended with a unique effort in designing next generation of supercomputing architectures. CITS computational tools can tackle grand challenge problems never attempted before where turbulence, combustion, compressibility effects, high levels of heat release, phase interfaces in highly complex geometries, play a significant role. These goals are directly aligned with the ASC goal of "delivering increasingly accurate simulation tools to sustain the Stockpile Stewardship Program".

CITS tools have clearly demonstrated their superiority with respect to industry standards and the Center's first landmark simulations of the reacting multiphase flow in realistic jet engines have spurred the interest of aerospace giant Pratt & Whitney. In a fruitful collaboration, CITS has been granted access to a considerable amount of experimental datasets currently being used to certify the code's capabilities for Pratt & Whitney's in-house use. Current full-engine integrated simulations also have the potential to impact the design of future systems by answering several long-standing questions related to engine performance and stability.

In the past eight years, the multidisciplinary nature of the Center's research (a prerogative of the ASC Alliance program) resulted in the development of a parallel, scalable computational infrastructure that enables complex integrated simulations, but also guides the architectural design of a new class of streaming supercomputers. Scientific breakthroughs have been achieved by tackling the physical modeling in a truly multiscale fashion; as an example, detailed direct numerical simulations of the flow around one drop of fuel have been used to derive engineering models to be used in the full-scale engine simulation where millions of droplets interact, burn and evaporate. Turbulence/combustion interactions have also been addressed using a multiscale approach where a range of techniques with various levels of fidelity and computational cost are integrated in the simulation environment.

Several collaborations have been established with the NNSA national laboratories either through the use of CITS codes or specific technological components (numerical algorithms or physical models); as an example, the interaction with Sandia National Laboratories (SNL) on the modeling and prediction of fires and buoyant plumes is impacting one of SNL's legacy codes, FUEGO.

Since its inception, Stanford's group has been validating its models and simulation techniques using canonical and complex flows and combustion experiments. More recently, researchers at the Center are working on the incorporation of error estimation procedures into CITS codes with the objective of quantifying uncertainty bounds in the predictions in accordance with the current and future goals of the ASC program.

STANFORD UNIVERSITY

To address this restriction, fully a third of the engineers and computer scientists working in the CITS group are engaged in designing an entirely new scientific computer and accompanying software (see sidebar below).

COMBINING APPLES AND ORANGES

To solve the overall problem, the CITS staff has divided the engine into its three major components: the compressor, the combustor, and the turbine. The volume occupied by each component is covered with a series of regularly spaced points known as a computational grid. To simulate a working engine, the scientists must calculate flow at each grid point. The challenge is that the equations and models appropriate for each engine component are quite different.

In the compressor and turbine portions of the engine, the scientists use a mathematically simplified "average flow" that is much smoother than the actual flow. This dramatically reduces the simulation time and cost, while producing a quite accurate simulation.

In the combustor, however, this simplified approach is not accurate enough. The scientists have to resort to a more accurate description of turbulence because of the important role it plays in the mixing and combustion of the fuel.

These high fidelity predictions have led to a better understanding of the complex interactions between fluid flow, fuel evaporation and chemical reactions. For the first time, design engineers can observe the true dynamics of the combustion process instead of just the time averaged result.

For the complete simulation to work, these different mathematical descriptions of turbulence must be integrated, creating quite a computational challenge. Much of the research team's effort has been aimed at designing the computer codes that exchange the appropriate information regularly and efficiently as the flow evolves over time.

"These integrated turbulence simulations are multiscale problems that quickly exceed the computational resources of all but a handful of labs," says Moin. "That's why our partnership with the Department of Energy has been so fruitful. They have some of the fastest and largest massively parallel computers and have made those resources available to us. Our engine simulations help to test these systems, finding bottlenecks and reporting back to them. We both have an interest in large-scale computations and there is a lot of cross fertilization between our groups."

SEEING THE LIGHT

The team has been working to develop the software to perform large-scale multicode, multiphysics flow simulations on the massively parallel computers at Los Alamos, Lawrence Livermore and Sandia National Laboratories.

"This is a major accomplishment," says Moin. "We've been able to model the complex geometry and physics of flow of both gas and liquid fuel. This tells us the larger goal is within reach."

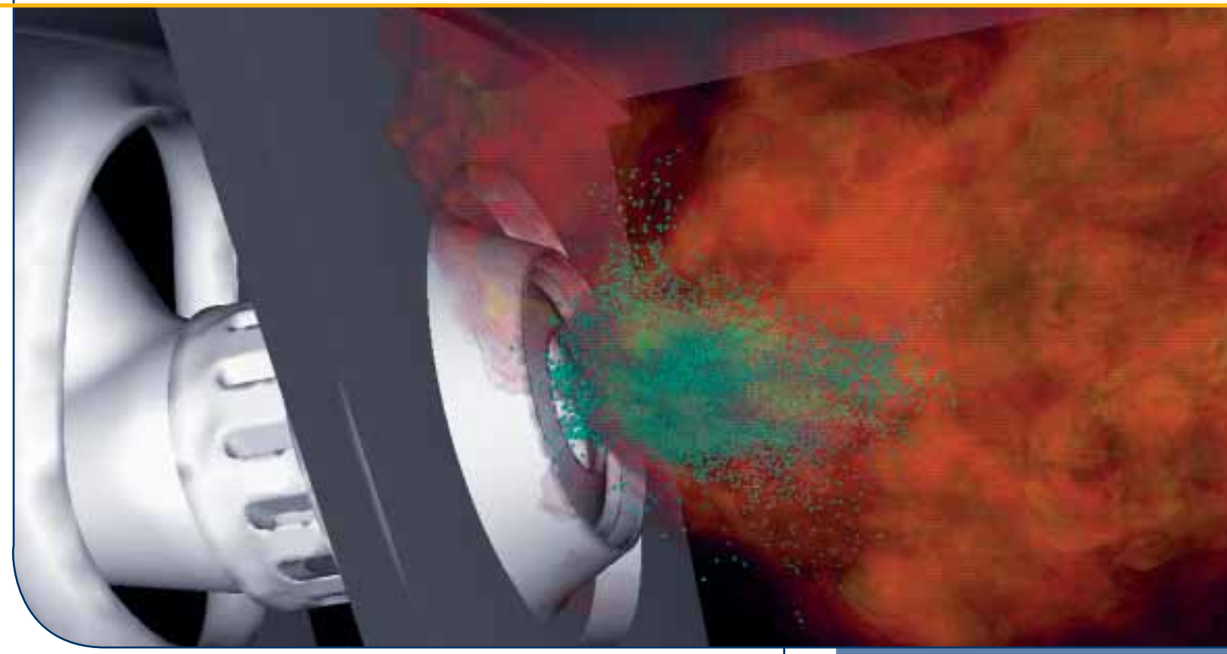
A unique partnership with aerospace giant Pratt and Whitney has helped the CITS team validate their tools. "Pratt and Whitney gave us access to their proprietary temperature profile and emission data at the exit of the combustor so we were able to compare and validate our model," says Moin. The results were so convincing, both visually and quantitatively, that the company has begun to use the model in their design process.

Once completed, full engine simulations will allow engineers to investigate component interactions and the dynamics of the entire engine system. For example, by slightly varying the simulation conditions over multiple simulations, engine performance can be optimized long before an engine prototype even exists.

But success for director Moin also comes in knowing that the multidisciplinary model of CITS has caught on at Stanford, as shown in the creation of a new Institute for Computational and Mathematical Engineering. "We've shown that it is possible to be productive across university departments, and that led to a major new institution," he says. "This will have a huge impact on training the next generation of scientists." The Institute for Computational and Mathematical Engineering at Stanford has a broad graduate curriculum with focus on scientific computing and is training a new generation of modern computational engineers.

NOT ONLY THE JET ENGINE

Although Stanford's grand challenge is the simulation of a jet engine, the engineering software being developed has a very broad range of applications. Recent studies include the prediction and control of helicopter noise, the investigation of nutrient transport and hydrodynamics in coral reefs, the analysis and modeling of the mixing characteristics of buoyant plumes and fires. In addition, a collaboration has been initiated with Los Alamos National Laboratory with the objective of investigating the mechanism of tsunami wave generation due to landslides. In this case the same software technology used to model the spray and fuel atomization in the jet engine is used to simulate the dynamics of a massive rock slide splashing into the sea.



Results from a simulation showing atomized fuel droplets superimposed on instantaneous contours of flame temperature in a realistic jet engine combustor.

THE MERRIMAC PROJECT

Despite the advances in computational power provided by today's massively parallel computers, the CITS group realized early on that a new computer architecture designed specifically for scientific applications will be necessary for its complex engineering simulations.

The computer architecture is a departure from commercially produced processors, which are not designed with scientific computing in mind.

"Most of the cost and energy of modern computing systems is going into communication, that is, moving data and instructions around," says Bill Dally, director of the Merrimac project. "When conventional architectures were first developed 40 or 50 years ago, arithmetic was expensive and communication was cheap, so nobody worried about communication. Today it is completely reversed, but we are still using architectures that were developed in another era. The whole focus of new architecture is to make the moving of instructions and data efficient, and in doing so to get the overall efficiency up by a couple orders of magnitude."

The core of Merrimac is a single-chip stream processor that is expected to have 128 gigaflops peak performance. This processor chip, along with 16 high-bandwidth DRAM chips with 2 gigabytes of memory form a single Merrimac node. The scientific team estimates that once the initial prototype is built, computers using the Merrimac architecture could be built for an estimated parts cost of less than $1,000 (in today's costs) per 128 GFLOPS node.

BRIGHTER THAN A BILLION SUNS

How big is the Universe? Why is it expanding at an accelerating rate? How do we accurately measure the rate of expansion? These are some of the large questions on the minds of researchers at the University of Chicago's Center for Astrophysical Thermonuclear Flashes. To help answer them, they're blowing up stars in supercomputers.

Started in 1997 as one of the five university centers supporting the NNSA Advanced Simulation and Computing program, the Flash Center is a world leader in the computational simulation of supernovae, or exploding stars.

These simulations are a key to answering the core question raised by the surprising 1998 discovery that the universe's rate of expansion is accelerating: What's the immense "dark energy" that's causing it to fly apart? This research also contributes to solving the terrestrial challenge of ensuring the safety and reliability of the U.S. nuclear stockpile (see sidebar this page).

"To understand why the universe is accelerating – what the properties of so-called 'dark energy' are – we need a tenfold increase in the accuracy of the distances that we derive from Type Ia supernovae," says astrophysicist Don Lamb, the Flash Center's Director. "This is going to be difficult to achieve unless we have a physical understanding of these supernovae, and this is what we're committed to achieving with first-principle computational simulations."

DIAGNOSING THE COSMIC PING

Type Ia supernovae are produced when an aging star called a white dwarf shrinks to the point at which the intense pressure at its core ignites a thermonuclear flash – a pulse of energy that heats the dying star's core to billions of degrees Fahrenheit in a fraction of a second. It's this flash that gives the Center its name.

"That energy release unbinds the star gravitationally and blows it to smithereens," says Lamb, after 30 years of studying them, his voice still expressing awe over the power of these cosmic blow-outs.

Since the flash occurs in white dwarfs that are always of the same size and mass, Type Ia supernovae all have about the same peak brightness. This uniformity makes them invaluable "cosmic yardsticks" that are used as a key way of measuring distances in the Universe.

It was astronomers' use of Type Ia supernovae to measure distances that led to the discovery of "dark energy." It is the value that Type Ia supernovae have as a means of measuring the rate of acceleration of the Universe and therefore of determining the properties of "dark energy" that makes understanding them so important.

However, the light they emit isn't exactly the same. About fifteen percent of the difference in their peak brightness cannot be calibrated away. This isn't too much for cosmologists to spot the universe's expanding acceleration, but it is too great to gauge cosmic distances with enough accuracy to understand important aspects of the expansion. For example, how much has the acceleration increased as the Universe has aged?

Lamb says that the key challenge in understanding these cosmic firecrackers is what turns a burning star into an exploding one. It's what physicists call the deflagration-detonation transition (DDT), or what a car mechanic might call a cosmic ping.

"Automobile makers are very interested in this problem. Because when your engine is pinging, that's a tiny detonation. The fuel isn't burning, it's detonating," says Lamb.

The stardust, or mix of elements, produced by Type Ia supernovae indicates that the flash is probably followed by a burning phase, one with flame-like characteristics. This phase produces fairly light atoms, such as silicon. At some point though, there's a detonation whose more intense energy melds nuclei together to form heavier elements, including nickel and iron. When and how this transition occurs has been a mystery.

In most terrestrial situations, a DDT happens when sound waves reflect off interior walls, such as inside a car's piston chamber. "But stars have no walls," says Lamb. "So how a DDT can happen in a star has been a puzzle. By carrying out large-scale, 3-D, multi-physics simulations, we have discovered a way in which a DDT can occur in a star, causing it to explode."

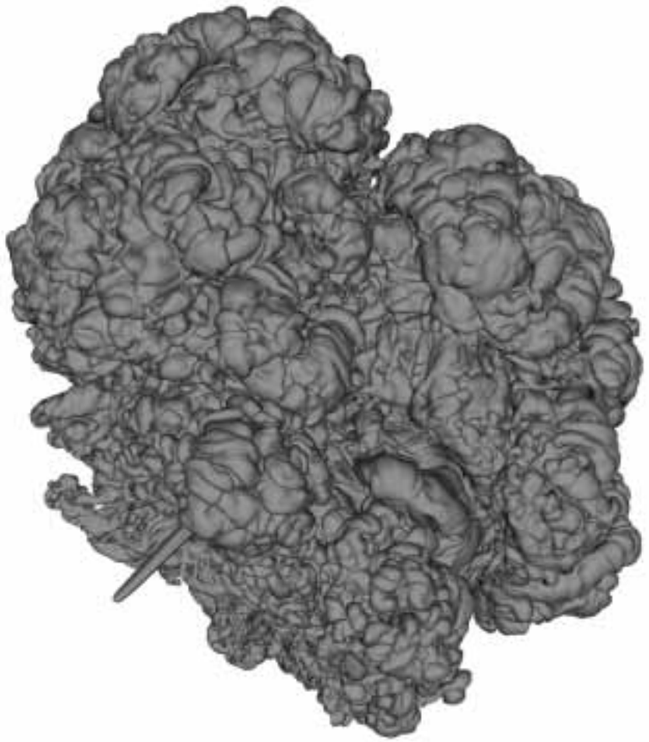


Image of the rising bubble of hot ash from the off-center ignition of a white dwarf star. The bubble comprises only a few percent of the mass of the star. But when the bubble breaks out of the star, the hot material in it spreads over the surface of the star at high speed and crashes into itself at the opposite point on the stellar surface. The converging flow compresses and heats the surface layers of the star, initiating a detonation that explodes the star. This completely unexpected result represents an entirely new and very promising model of how Type Ia supernovae explode and demonstrates the importance of large-scale, 3-D, multi-physics simulations. The simulation was carried out using the FLASH code on the ASC Frost machine at Lawrence Livermore National Laboratory.

SUPERNOVAE AND STOCKPILE STEWARDSHIP

How do you know your computer simulations accurately reflect reality? Known as validation, answering this question is particularly difficult when the whole phenomenon under study can not be explicitly studied by experiment. It is a vexing problem that faces both the Flash Center and the Stockpile Stewardship program, and is a growing area of scientific research in its own right.

"Just as in the case of nuclear weapons, we can't set up a supernova and explode it," says Don Lamb, director of the University of Chicago's Center for Astrophysical Thermonuclear Flashes.

To cut this Gordian knot, the Flash Center has developed an extensive, multi-step, hierarchical, verification and validation process that has set a new standard in the astrophysics community. The process includes comparisons with other codes, comparisons with experiments that allow the validation of sub-units of the FLASH code, and comparison with observations of Type Ia supernovae that allow the validation of the full simulations of this phenomenon.

Above all, the FLASH code is developed from first principles so that any detected deviation from real-world data can be linked back to the basic mathematics and physics used in the simulation. And importantly, the basic physics of exploding stars and nuclear weapons is very similar, from the nuclear physics, to the rapid energy transfer, the turbulence of burning, and finally detonation.

Lamb says that learning how to do validation when the whole phenomenon under examination cannot be studied explicitly by experiment is a part of the Flash Center's contribution to ASC's role in supporting the U.S. commitment to the 1992 Comprehensive Test Ban Treaty.

"If an Alliance Center can take an overarching computational problem of the same magnitude of challenge and complexity as the Stockpile Stewardship problem, and succeed – in terms of predicting the key observed features of the phenomenon being studied – then the scientific community can look at us and have more confidence that a simulation approach, rather than direct testing, is actually possible for verifying the reliability and safety of the nuclear stockpile."

THE CODE

To solve this problem, and others related to the fate of stars, the Flash Center's team of 50 physicists, astrophysicists, computer scientists, mathematicians, and others, has created one of the world's most advanced hydrodynamic simulation computer codes.

During the past eight years the FLASH code has itself exploded to more than 25 times its initial size, and now has more than half-a-million lines of executable instructions. As a community code, it is freely available for download from the Flash Center website to researchers around the world. And in the ultimate test of a code's value, it is being used by scores of scientists in the United States, Europe, and Japan. It is also being used by scientists at Los Alamos National Laboratory and Lawrence Livermore National Laboratory for doing astrophysical problems.

"The FLASH code is very capable. It can be used for things from the study of large-scale structure in the universe – and our three key problems of supernovae, x-ray bursts and novae – to fluid dynamics experiments in a lab. Wherever you have the elements of hydrodynamics, magnetic fields and gravity – which is pretty much everywhere – it can be used," says Lamb. The code includes its own visualization tool, called FLASHVIEW, developed in collaboration with Argonne National Laboratory.

The code's public nature plays an important feedback role in ensuring its high quality. Since it must always be useable, the Flash Center's code group has taken the science of code management to new levels for a university research effort.

"Maintaining the code is a big job," says Lamb. Every night, the code group runs verification tests on the FLASH code to ensure it hasn't developed any bugs or errors during the previous day's work.

Its wide use also demonstrates the code's portability, a key requirement for the ASC program. The FLASH code runs on more than 30 different computer platforms, from Linux clusters with tens to hundreds of processors, to Linux clusters and supercomputers with thousands of processors, including the ASC machines ALC at Lawrence Livermore National Laboratory and QSC at Los Alamos National Laboratory.

A new, fully modular version of the code is currently being developed. This version, called FLASH 3, will make it easy for users to write their own modules for the code.

SIMULATIONS

In 2004, the Flash team used its code to run the first-ever 3-D supercomputer simulations on the "Frost" supercomputer at Lawrence Livermore National Laboratory of a Type Ia supernova from flash through flame in an entire star. These computationally intensive simulations had an effective resolution of more than 10 billion individual elements and required 300,000 processor-hours, enough computational juice to set a single desktop processor running for 35 years.

The simulations revealed a surprising story: If ignition occurs even slightly off center in the star, a hot bubble of burned ash forms that rises rapidly toward the surface of the star. When the hot bubble breaks out of the star, it spreads over the surface of the star, crashing into itself at the opposite point on the stellar surface and initiating a detonation (see page 13). This completely unexpected result, which researchers at the Flash Center have termed "gravitationally confined detonation," represents an entirely new and very promising model of how Type Ia supernovae explode. "This result demonstrates the importance of large-scale, 3-D, multi-physics simulations," says Lamb. "The simulations revealed for the first time how a deflagration-detonation transition can happen in a star. They led us to discover an entirely new supernova mechanism that I doubt we would otherwise have guessed could happen."

The Center's ultimate goal is to model a Type Ia supernova from ignition through the flame that burns a volume comparable to the size of the Earth, the DDT, the resulting explosion, and all the way to the star's ultimate demise about 100 days later. Lamb notes that within five years ASC will have computers that will support simulations with 100 trillion individual elements, a thousand times more than presently used.

The "Connecting Quarks to the Cosmos" report from the National Research Council, April 2002, has endorsed a space mission that would use Type Ia supernovae to accurately measure the acceleration of the universe. The simulations carried out by the Flash Center can provide input on the design of instrumentation and on planning the observing strategy for such a mission. But most importantly, says Lamb, data from FLASH simulations may provide a better understanding of Type Ia supernovae that will allow for a more detailed analysis of the data from such a mission – and consequently a computational leg-up on what promises to be one of the most important physics discoveries of this century: the nature of dark energy.

"We have a code and computer resources that are second to none," says Lamb. "We're now expanding the frontier of knowledge about Type Ia supernovae. Our greatest challenge is to gain a physical understanding of how this kind of supernova explodes in order to support efforts to determine the nature of dark energy."

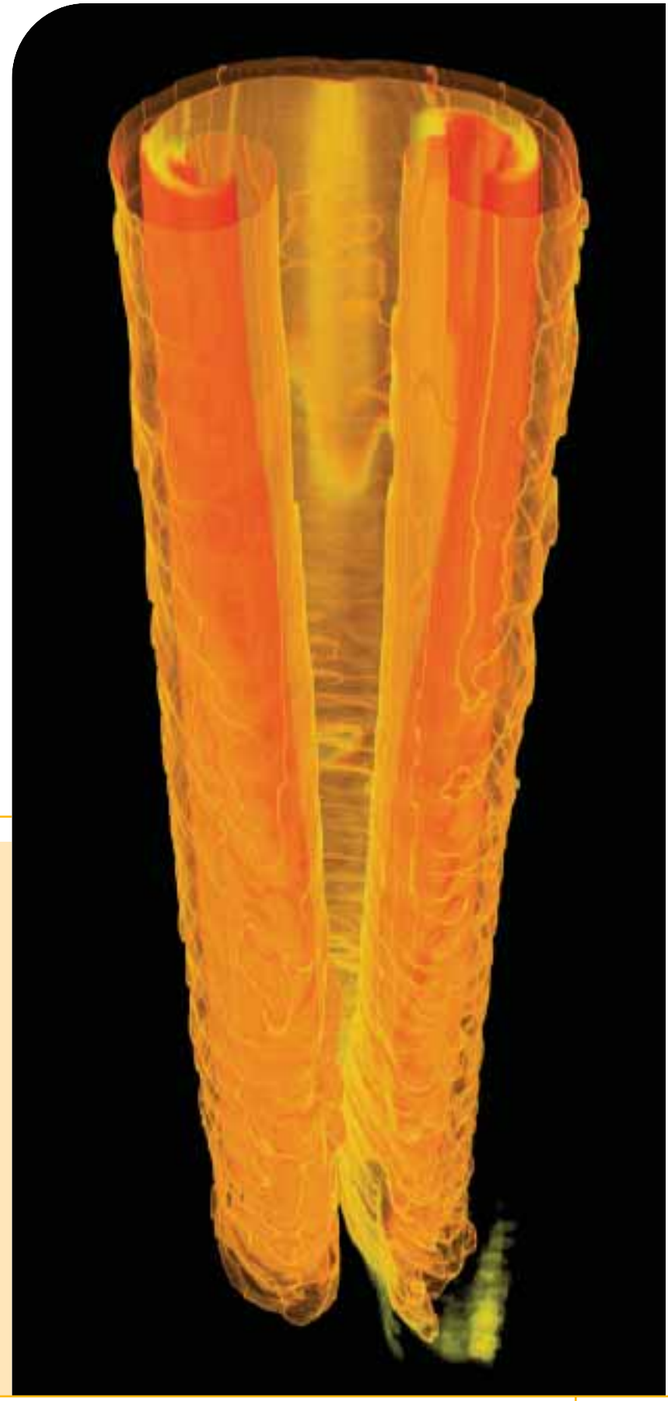


Image of the flow in a column of sulfur hexafluoride 825 microseconds after the passage of a Mach 1.2 shock wave through it. The initial conditions match those in experiments carried out at Los Alamos National Laboratory. The vortex structure is induced by the passage of the shock wave through the column. The shock also induces vertical motions because of the misalignment between pressure and density gradients characteristic of the shock wave and the material in the column. Small-scale irregularities develop because of fluid dynamic instabilities. This large-scale 3-D numerical simulation revealed the unexpected importance of 3-D effects in the experiment. It was carried out using the FLASH code on the ASC Q machine at Los Alamos National Laboratory.

VIRTUAL ROCKETRY

Building and testing solid rocket boosters (SRBs), such as the pair used to launch the Space Shuttle, has always been an expensive and potentially dangerous enterprise. Until recently, the U.S. rocket industry has relied primarily on scientific and engineering experience, together with trial and error with physical prototypes, to design its most sophisticated propulsion systems.

Now, the team at the Center for Simulation of Advanced Rockets (CSAR) at the University of Illinois at Urbana-Champaign (UIUC) is leading the way in radically changing how U.S. rockets are designed and tested. They're working to provide new design tools and put computational testing, using supercomputer simulations, ahead of rocket building. The CSAR research promises to make rocket design and testing faster, cheaper, and safer. The new material models, algorithms, and computational tools developed for CSAR's rocket simulations are also making critical contributions to the advancement of technologies necessary to ensure the safety and reliability of the U.S. nuclear stockpile.

CSAR's interdisciplinary staff of 100, including graduate students, post-doctoral researchers, faculty, and staff, covering ten departments from computer science and engineering to chemistry, are quickly approaching a final frontier in computational simulation of rockets – the ability to design and test entire rockets in silico. "We have achieved unprecedented detail in creating three-dimensional simulations of a rocket," says Michael Heath, Director of CSAR (pronounced 'Caesar', as in the Roman emperor).

PUTTING THE TEST BEFORE THE LAUNCH

SRBs – which are the focus of CSAR's work – are bullets by another name. Their basic structure is a canister, hollow in the middle, with the solid fuel and oxidizer mixture (called propellant) lining the inside of the canister, and with an igniter at the top. Once ignited, an SRB begins an unstoppable burn. In the case of the Space Shuttle's SRBs, this produces enough thrust to lift a system weighing about 4.5 million pounds 30 miles into the upper atmosphere in a heart-pounding two minutes.

But an SRB's strength is also its Achilles' heel. With this enormous release of energy, there's a razor-fine line between blast-off and blow-up. With no way to quench the burn, small faults – a developing crack in the propellant, or a frozen O-ring as in the 1986 Challenger disaster – can have catastrophic consequences. In the spring of 1999 alone, a series of three consecutive Titan IV rocket launch failures resulted in the incineration of more than $3.5 billion of rocket hardware and payloads.

Computational design and testing is a key way of avoiding these expensive mishaps. Known as ***virtual prototyping***, it's a design approach that's already a core part of the design of components of new cars and airplanes. However, applying it to something as complex as a complete SRB is unprecedented.

"Our simulations will enable rocket engineers to quantify the margin of safety inherent in a given rocket design to a much higher degree than has ever been possible before and eliminate some of the actual test firing required to prove that a given design will perform as expected," says Robert Fiedler, CSAR's Technical Program Manager.

And, says Heath, virtual prototyping of rockets is a perfect analogy for demonstrating the validity of supercomputer simulations to support the work of the Department of Energy National Nuclear Security Administration (DOE/NNSA) Advanced Simulation and Computing program, which funds CSAR.

"An SRB is a multi-component system in the same way as many of the devices of direct interest to DOE/NNSA, from nuclear weapons to energy production facilities. The various components influence each other, and that's the same sort of coupling we have in a rocket," says Heath, a computer scientist with a near three-decade career in scientific computing.

LEARNING TO FLY IN PARALLEL

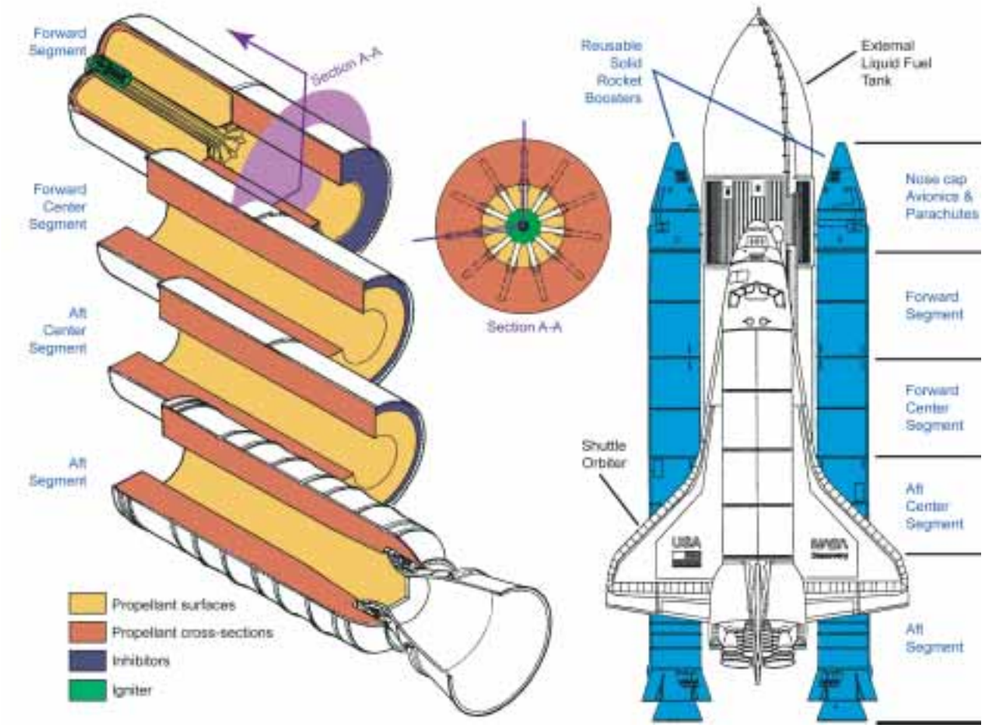
Begun in September 1997 as an outgrowth of UIUC's Computational Science and Engineering program, CSAR has by necessity taken a staged approach to a virtual lift-off. "We knew we needed to learn to walk before we could run, much less fly," says Heath.

After eight years, the program has shown that it's rapidly gaining its flight feathers. Prior to CSAR, most SRB simulations involved simple one-dimensional modeling of individual components in isolation. CSAR set the ambitious goal of full 3-D simulation, from first principles, of all the components together using massively parallel computers.

"We have developed new coupling methods for integrating the separate modules, including algorithms for transferring data between components that are twenty times more accurate than other methods recently described in the literature," says Fiedler.

A key part of this work has been the creation of new simulation tools for the individual components of an SRB. Heath says that CSAR's Rocfire software for modeling the surface combustion of an SRB's complex fuel mix of ammonium perchlorate, aluminum, and a polymeric binder is "so far out in front that it's absolutely unique." New propellant material models under development at CSAR will soon enable the simulation of Titan IV failures in unprecedented detail, and thus potentially the ability to predict and avoid such situations in the future.

Reusable Solid Rocket Motor (RSRM) is primary booster for NASA Space Transportation System (STS). Section A-A shows eleven-point slot and fin structure in forward segment of RSRM. Propellant in forward-center and aft-center segments form straight-walled cylinders, aft segment propellant tapers outward to submerged nozzle. Inhibitors between segments are used to tailor burning surface to meet thrust requirements of motor.



And, Heath notes, that CSAR's various component simulations and its overall SRB computer code, dubbed *Rocstar*, have proven themselves to have excellent parallel scalability – the ability to move from running on one single-processor desktop computer to running efficiently on massively parallel supercomputers with thousands of processors. The CSAR simulations have been run on a broad variety of computers, including CSAR's 1280-processor Turing Xserve Cluster, academic supercomputers at Illinois, Pittsburgh, and San Diego, and up to 2048 processors on the supercomputers at the three Defense Program Laboratories.

MOVING TO THE DIGITAL LAUNCH PAD

Presently, CSAR researchers are testing a variety of rockets on the virtual launch pad, from tiny guidance motors to laboratory-scale rockets, to large space-launch vehicles such as the Titan IV and the Space Shuttle's Reusable Solid Rocket Motor (RSRM). These simulations, whose validity is established by comparison with test data from actual firings, are yielding new insights into phenomena such as ignition transients, combustion instabilities, and potential failure modes.

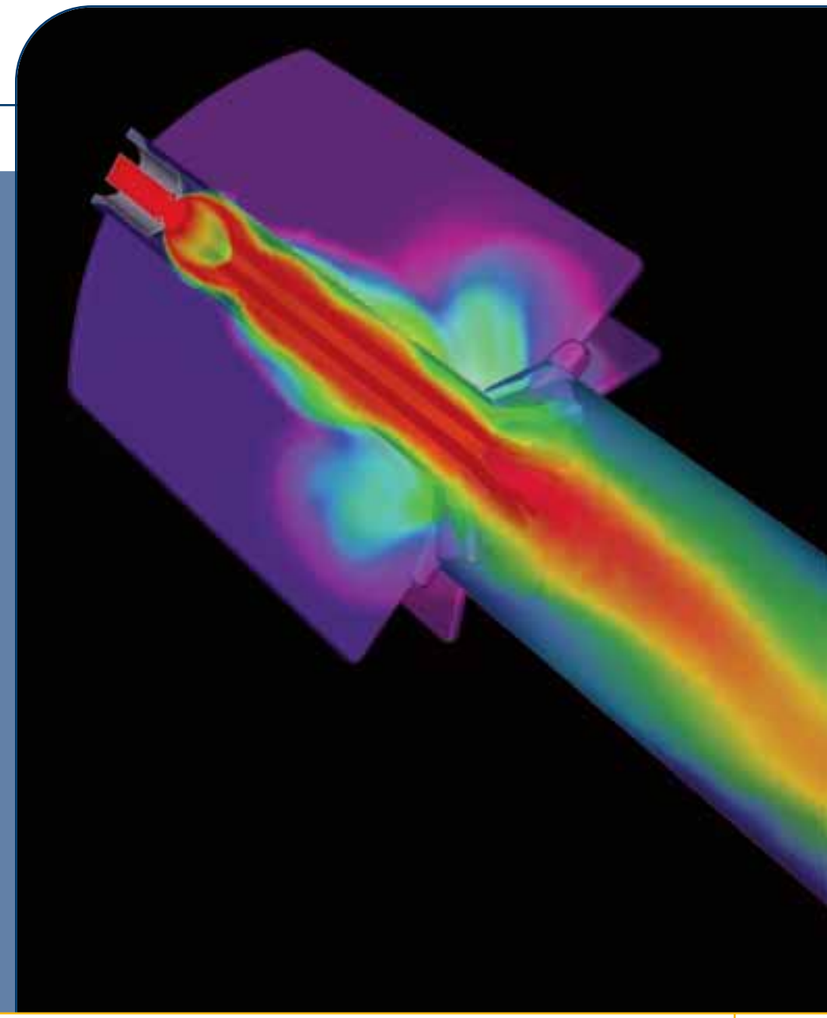
"We are at the point where we have a full 3-D simulation of a complete SRB, including the igniter, nozzle, and solid propellant – all the parts are there – and it already works well enough to match experimental data to within a margin that is often smaller than the variation in repeated experiments. But beyond comparison with experiments, one of the cardinal virtues of simulation is the ability to see inside a rocket motor, where instruments cannot go or cannot survive. Our simulations have yielded a number of new insights into previously unknown or ill-understood behavior. For example, we have discovered that flame spreading during ignition behaves very differently in different portions of the rocket, that the inhibitors that protect segments of the propellant flex far more than had been expected, and that such inhibitors induce turbulence that explains unexpectedly large oscillations in pressure. The sheer size of our simulations also makes new discoveries possible. For example, our ability to simulate many thousands of particles has illuminated the previously unexplained relationship between the amount and size distribution of aluminum particles and the resulting pressure. Our simulations have also shown that some previous attempts to explain rocket failures were fundamentally flawed."

CSAR's simulations to date have focused on ignition and behavior shortly thereafter, when many accidents initiate. To simulate a full firing all the way to burn-out, CSAR researchers face two key challenges. One is how to accommodate the complex geometrical changes taking place within the rocket as it burns. A second major hurdle is how to bridge the enormous differences of time and space scales spanned by the simulations. Whereas combustion turbulence is measured in millionths of an inch and thousandths of a second, the 125-foot long rocket burns for what is by comparison a two-minute eternity.

"You can't simulate the full rocket at the micron level, it's just too big," says Heath. "So you have to find some way to homogenize your model while maintaining reasonable accuracy. Both diverse scales and dynamically changing geometries are very much present in the DOE ASC problems as well."

As a testament to the quality of the simulations to date, the CSAR program has already attracted the attention of a broad community of rocket scientists in government and industry. Recently the CSAR group was invited to join a new U.S. Air Force modeling and simulation program that includes the major U.S. rocket manufacturers.

"These rocket scientists are very excited about our simulations because there are improvements in material and combustion modeling, spatial and temporal resolution, and component coupling that they've never contemplated. And the main reason they haven't is they've never had the computing capacity," says Heath. "But we're showing that you can do it."



Results from a 3-D simulation of the Space Shuttle solid rocket booster 52 milliseconds after the igniter is triggered. The propellant and gas domains are cut in half lengthwise to show a cross section of the interior of the head-end segment. The igniter is the gray and red object at the upper left. The rest of the visible surface represents the propellant, whose geometry includes 11 slots (4 are visible) which increase the burning surface area (and therefore the thrust) at liftoff. Further down, the geometry changes to a cylindrical bore. The colors (purple - magenta - blue - cyan) indicate the surface temperature from 350 to 500 degrees K. Also shown is the gas temperature, represented as a translucent surface (to allow geometric details to show through), whose colors (green - yellow - red) correspond to the range 300 K to 1700 K.

The hot gas from the igniter flows down the combustion chamber and heats the propellant over a period of about 125 ms, when the surface temperature at some locations reaches the ignition temperature (850 K) and burning begins.

SUPPORTING THE ASC STRATEGIC PLAN

The *Rocstar* integrated multiphysics simulation code developed at CSAR over the past few years reflects an enormous effort by a large, multidisciplinary team of researchers. It incorporates a number of new models and simulation capabilities developed at CSAR, including multiscale models of heterogeneous composite energetic materials, new approaches to turbulent multiphase fluid flow, three-dimensional propellant combustion models of unprecedented detail, conservative data transfer techniques of dramatically higher accuracy than previous methods, and a highly modular and flexible software integration framework. The resulting simulation code has reached a sufficiently high level of sophistication and detail, both in the physical models it incorporates and the coupling of those models, that it enables meaningful comparisons with physical experiments. Accordingly, CSAR has been carrying out an aggressive program to verify the code's correctness, validate its fidelity to the complex physical systems it simulates, and quantify the sensitivity of its results to uncertainties in the input models and data. These validation efforts are based on extensive test data from government laboratories and rocket motor manufacturers. To complement these comparisons with historical data, CSAR is engaged in a joint effort with the U.S. Air Force's solid propulsion program to use *Rocstar* to predict results in advance of future experiments using a laboratory test rocket motor. Such predictive capability is the ultimate test of simulation methodology and the cornerstone of the ASC strategic plan.

TAKING THE HEAT

The University of Utah's Center for the Simulation of Accidental Fires & Explosions (C-SAFE) has an overriding goal. "We aim to push the state of the art in high-performance computer simulation of meaningful, real world problems," says Chuck Wight, the Center's deputy director.

To achieve that goal, the Center develops state-of-the-art, science-based tools to simulate accidental fires and explosions. Successful simulations can provide the information necessary for scientists and policy makers to evaluate the risks and safety issues associated with preventing and controlling fires in the aerospace, chemical and petroleum industries.

The risk analysis supports the Department of Energy Stockpile Stewardship Program designed to ensure the security of the country's nuclear weapons. "The DOE is charged with providing improved predictive capability for this program through validated large-scale simulations that include multi-disciplinary contributions from the fields of physics, chemistry, and nuclear engineering," Wight explains. "We are collaborating with the DOE/NNSA national laboratories in advancing the techniques required to develop this type of software."

C-SAFE's work contributes to the future as well as the present. For example, "We train tomorrow's scientists and engineers to work in the field," Wight explains. Critical to the entire exercise is the ability to take advantage of continuing advances in computer technology. "One absolute necessity is to write code that runs on massively parallel computer architectures," Wight says. "We are also developing techniques to effectively acquire, visualize, and store large data sets."

The nature of the simulations makes it essential for the Center to use a multidisciplinary approach to its research. Take a typical target for simulation: a large fire that surrounds an explosive object. The simulation must take account of the physical and chemical changes that occur in the containment vessel as the fire ignites and spreads, the resulting mechanical stresses and rupture of the container, and the chemistry and physics of the explosive material inside the fire. To do so, the Center needs computer scientists, mechanical engineers, chemical engineers, chemists, and physicists who collaborate to develop its simulations.

LEARNING THROUGH SIMULATION AND VALIDATION

The ASC Alliance programs support the mission of the DOE/NNSA laboratories by developing new methods for improving the predictive value of large-scale multi-physics simulations. Three essential elements of this are creating models (computer algorithms) that reflect the underlying fundamental physics of the processes of interest, verifying that the models compute the desired quantities, and validating the simulation results against known behavior (e.g., laboratory experiments, field tests or accident investigations). C-SAFE scientists are engaged in all of these activities, making individual contributions to an overall simulation code that is capable of simulating many different types of complex physical and chemical processes.

In particular, C-SAFE has developed models based on molecular fundamentals for describing the complex process of forming soot in fires, how soot plays a crucial role in transferring heat energy from the fire to the container, for computing the mechanical properties of composite plastic-bonded explosives under extreme conditions of temperature and pressure, and for simulating the combustion process that liberates huge quantities of heat and gas from explosives.

The C-SAFE simulation code, which is named Uintah, is unique in its ability to simulate tightly coupled interactions between multiple materials in the simulation domain. It has been learned, for example, that heating of a container suspended over a fire is not always greatest on the bottom of the container, as intuition might suggest, and there are conditions where turbulent mixing can cause hot spots on the *top* side of the container. Such conclusions are made possible by a hierarchical system of validation, which ensures that every element of the simulation code works properly, and that the models work together to generate a reliable representation of physical reality. The Uintah code has been used to simulate many other interesting physical systems including wounding of the human torso, a study of the stress distribution within newly developing blood vessels, and a direct simulation of foam microstructures under high compression. In each case, Uintah has provided a simulation capability that was previously non-existent.

Simulation and validation experiments have also revealed the basis of interesting behavior of damaged explosives. For example, 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 container 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), then 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 container fragments can be up to ten times higher.

Photograph of a large pentane pool fire experiment. C-SAFE scientists have designed software to simulate the complex dynamics of large fires like this one, including buoyant plumes, turbulent mixing and reaction of fuel with air, formation of soot, and radiant heat transfer to explosive devices embedded in the fire. Used with the kind permission of Professor Axel Schoenbucher, University of Duisberg-Essen.

SPACE AND TIME

The C-SAFE simulations must cover a large range of size and time scales. In terms of size, researchers must be able to move seamlessly from the atomic level to the scale of several meters involved in a fire that is rapidly growing and that ultimately results in the explosion of the container. Time periods under study range from the few minutes that a fire typically takes to develop down to less than a millisecond for the generation of an explosion.

Development of any simulation involves three steps that mirror happenings in the real world. The Ignition and Fire Spread phase focuses on simulating the initial ignition of a fire or explosion, its growth into a flame, and its subsequent development into a full-blown fire. Container Dynamics involves study of the types of change,

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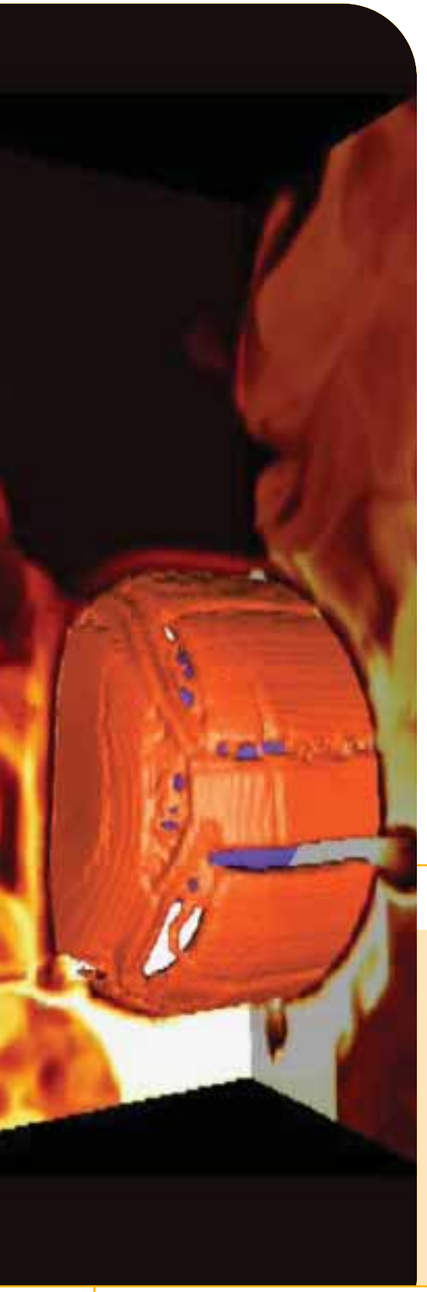

such as buckling and rupture, that a fire or explosion causes in the vessel containing the explosive. The Molecular Fundamentals team deals with changes in the high-energy material itself as a result of a developing fire – changes that can lead to an explosion.

C-SAFE has the overall task of combining those computational steps into an integrated system that permits accurate simulation of entire sequences of fires and explosions. Not surprisingly, that work demands excellent scientific teamwork. Thus, the Molecular Fundamentals team studies molecular dynamics, electronic structures, and statistical mechanics to understand high-energy transformations and the basic chemical and physical properties of all the materials involved in fires and explosions. Applications scientists develop computational models designed to bridge the length and time scales between molecular scale properties and behavior that can be simulated at the macro scale. Computational engineers write the simulation code that describes the structural properties of a fire or explosion as it develops and grows. Finally, the Computer Science team sets out to create an overall computational framework that integrates codes and data from all disciplines involved in the research.

What makes this approach feasible is the Center's development and use of a software system architecture that facilitates the integration. "Our structure allows applications scientists and computer scientists to focus on what they each do best without having to understand everything about the simulation code or software architecture," Wight says.

Image of a simulation of a steel container (orange) at the point of rupture following a period of heating by a rising column of air at 1000 Kelvins. The remaining solid explosive (blue) can be seen through the cracks inside the container. The ignition of the explosive and rupture of the container occurs in about 300 microseconds.

COMPUTING POWER

Any significant simulation initiative demands plenty of computing power. Each aspect of a simulation, from representation of a container which has dimensions no larger than a few centimeters to that of a fire that can spread across several meters, requires up to a billion specific "mesh points" relating the computer simulation to reality. The need to simulate events that can last from microseconds to many minutes adds extra demands for computer power, new algorithms, and storage capacity.

Volume rendered temperature data from the transient simulation of a 10-m diameter heptane pool fire (red indicates highest temperature, yellow lower, black lowest). This simulation is performed on a 300x300x300 uniform computational mesh for several seconds of simulated time. The simulations capture the roll-up of vortices observed in real large-scale fires.

To meet those demands, C-SAFE researchers have access to three DOE/NNSA supercomputers that can carry out more than one trillion calculations per second. The Scientific Computing and Imaging (SCI) Institute at the University of Utah also provides support for the Center's computing needs. ATK/Thiokol Propulsion, C-SAFE's industrial partner, sets up and ignites actual explosives intended to generate data needed to validate the predictions of C-SAFE's simulations.

The Center also works closely with the three DOE/NNSA Laboratories – Lawrence Livermore, Los Alamos, and Sandia – to develop the fundamental simulation science that may find application in the Stockpile Stewardship program. However, C-SAFE does not undertake any classified research. "None of the problems that we work on are of direct interest to nuclear applications," Wight says. "But the laboratories are interested in how our findings might impact their work."

ADDED APPLICATIONS

As befits a university-based program, the work of the Center has potential applications far beyond the needs of the specific problem being studied. "We set a target simulation scenario as a large hydrocarbon fire with an explosive object embedded in it," Wight says. "But as we have written the application codes and developed the integrated software architecture, we've found that it's capable of being used in many application domains. It helps research groups to spin off their technology into different areas." As a result, for example, faculty members associated with the Center have recently received two grants from the National Institutes of Health to apply the computer codes to simulating tissue damage and cell membranes. "Our overall goal is to create a highly capable code that can simulate many different kinds of chemical and physical processes," Wight comments.

The Center also offers another type of spin-off – in educational terms. "We concentrate on fires and explosives, but we also train students who will get involved in computer simulation," Wight explains. The training focuses predominantly on postdoctoral fellows and Ph.D. students, who carry out fairly fundamental research for their theses. "But we also have a few undergraduates," Wight adds. "If someone talented comes along and shows interest, we'll keep him or her involved as long as possible."

MORE INFORMATION

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