SIMULATING ACCIDENTAL FIRES AND EXPLOSIONS

The Utah C-SAFE project is a highly multidisciplinary effort to build an integrated, large-scale high-performance simulation framework to simulate accidental fires and explosions involving hydrocarbons, structures, containers, and high-energy materials.

The Center for the Simulation of Accidental Fires and Explosions at the University of Utah focuses on providing state-of-the-art, science-based tools for the numerical simulation of accidental fires and explosions, especially in the context of handling and storing highly flammable materials. C-SAFE will provide a scalable, high-performance problem-solving environment (PSE) in which fundamental chemistry and engineering physics are fully coupled with nonlinear solvers, optimization, computational steering, visualization, and experimental data verification. The availability of simulations using this system will help to better evaluate the risks and safety issues associated with fires and explosions. As this article discusses, we will validate and document our five-year product, termed Uintah 5.0, for practical application to accidents involving both hydrocarbon and energetic materials.

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The challenge

The ultimate C-SAFE goal is to simulate fires involving a diverse range of accident scenarios, including multiple high-energy devices, complex building–surroundings geometries, and many fuel sources (see www.csafe.utah.edu). During the first five years, however, we will focus on the computation of a specific, well-defined scenario: rapid heating of a container with conventional explosives in a pool fire. Such a simulation could be characteristic of the coupled response of explosive materials subject to heating from accidental fires. The simulation should be able to predict the coupled fire-structure response through a realistic representation of the relevant physical processes. These processes include fundamental gas- and condensed-phase chemistry, structural mechanics, turbulent reacting flows, convective and radiative heat transfer, and mass transfer in a time-accurate, full-physics simulation of accidental fires. This simulation will be expansive enough to include the physical and chemical changes in containment vessels and structures, the mechanical stress and rupture of the container, and the chemistry and physics of organic, metallic, and energetic material inside the vessel.

Each of these issues provides challenging research and simulation problems in its own right. Coupling these processes in a unified computational framework provides an additional level of

sophistication that requires close interaction and integration among researchers and software engineers in all aspects of the project. We will focus heavily on coupling the micro- and meso-scale contributions to the macroscopic application to provide full-physics simulation across the breadth of supporting mechanistic disciplines and to efficiently utilize ASCI program supercomputers.

As we'll show, two elements are essential for C-SAFE to achieve its goals:

- A working organizational structure that requires and facilitates interactions among different research and simulation development tasks in different disciplines. These interactions focus on integration of research and code development into a unified PSE.
- A rigorous experimental validation program that functions at all levels of code development and integration.

Validation issues and problem specification

Validation is an ongoing process in all discipline areas and at all levels of code development. This involves testing individual submodels as they are developed and validating code on model problems as complexity increases. In addition, we are investigating issues of large-scale fire–explosion scenarios to help guide our research efforts in model and code development. Figure 1 shows a specific experimental setup that our validation team is exploring for taking data to validate simulation results and guide simulation development.

This photograph illustrates the explosion of a cylindrical steel container filled with explosive material. Propane served as the fuel to allow for as much visual information as possible both before and during the explosion. We used six propane burners, aimed at the container so as to provide a uniform heat flux to the container's bottom. An aluminum shield served as a windscreen. We took real-time video of the tests from several camera angles and took high-speed video (2,000 frames/second) at a single camera angle. A fast-response pressure transducer measured the pressure in the void space between the explosive material and the container wall. We used 23 thermocouples to measure temperature at the explosive–container interface, as well as on the container's exterior.

For these tests, we used the explosive formulation PBX9501, which is a pressed material supplied by the Los Alamos National Laboratory in

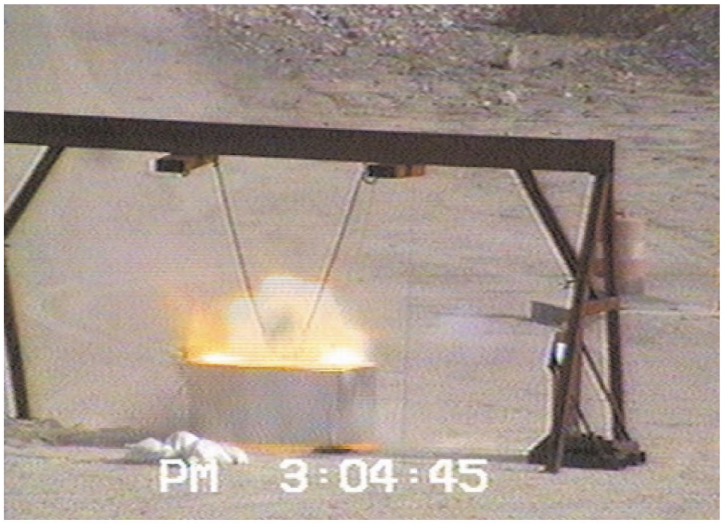

Figure 1. A field test illustrating the explosion of contained energetic material caused by heating from a propane fire.

4 × 4–inch cylindrical pellets. PBX9501 is an HMX-based formulation with an estane binder. HMX (1,3,5,7-octanitrotetrazocene) is the most powerful high explosive that is currently used in military weapon systems. We loaded three of these pellets into a 12-inch-long, 4-inch nominal-diameter schedule 40 steel pipe; some of the binder material sealed the interface between each of the three pellets. Two steel end caps were machined and threaded onto the ends of the pipe. We machined a 1-inch hollow bore down the center of the pellets to allow for gas generation and provide access for running the internal thermocouple wires.

Aspects of this field experiment important to our simulation development include characterization of the flame, heat transfer to the container, evolution of temperature and pressure within the container, descriptive features of the explosion, and the nature of the container's rupture.

Simulation development roadmap

C-SAFE is organized, in part, to mirror the physical processes that a large-scale simulation of energetic materials in fires must account for. Figure 2 illustrates this structure with a simulation development roadmap, consisting of three distinct, sequential steps that parallel the events in the physical problem: ignition and fire-spread, container dynamics, and high-energy (HE) transformations. A fire or explosion initiates with an ignition event (which is assumed to occur and which is not computed in detail). The fire spread computations define the extinction of an ignition event

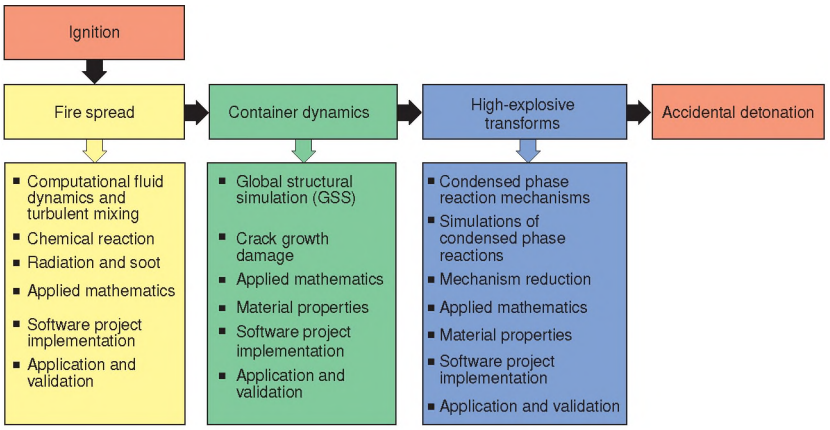

Figure 2. The C-SAFE roadmap.

or its growth into a large fire. The fire results in thermal loading to a container containing HE material. The fire's impact on the container results in thermal, chemical, and structural changes to the container and its HE contents, perhaps resulting in explosion and rupture of the container.

Our container dynamics group is responsible for the simulation tools necessary to describe the thermal and structural changes to the container and its contents. The HE transformations group focuses on discovering reaction mechanisms and developing reaction models that can be incorporated in the structural simulation. The overall mission is to integrate these computational steps into a coupled fire and explosion system. To fulfill this mission, we are drawing on three core disciplines: molecular fundamentals, computational engineering, and computer science. The plan and algorithmic structure to couple these different physical processes together is the responsibility of each roadmap step. The overall integration of these different algorithms into a single computational format is the responsibility of a group of software engineers representing each step. We'll now look at the activities of the three teams.

Fire-spread

The fire-spread team is concerned with modeling the propagation of an ignition event over a pool of liquid hydrocarbon fuel (see Figure 3).

During the first two years, the fire-spread team has focused on four major areas: computational fluid dynamics; chemical reaction and turbulent mixing; chemical kinetics for the fire, including the soot; and radiative heat transfer.

The propagation of a fire or explosion around the HE container depends on the availability of fuel and oxidizer and the rate of the ensuing reaction. The mixing between the fuel and oxidizer depends on the fluid mechanics of the vapor phase. Generally, the fluid flows are highly turbulent, leading to large variations in the length and time scales over which mixing occurs. Interactions with 3D geometries representing containers or surrounding structures add to the difficulty in predicting such flows. The chemical reactions involve several thousand elementary steps and hundreds of major and minor species and intermediates. These reactions are highly exothermic, and the resulting energy transfer occurs through both convection and radiation.

Radiation is the dominant mode of heat transfer at high temperatures and depends strongly on the gas mixture's absorptive, emissive, and scattering properties. The presence of soot in the gas mixture therefore strongly affects radiation. The large heat generation from these reactions leads to rapid changes in the properties of both solid and gaseous materials. When these events affect the container rupture, fragments of the container, which are ejected further, interact with the gas phase. In addition, all these processes are highly coupled. For example, chemical reaction depends on the level of mixing. However, chemical reaction affects the temperature through the amount of heat generated, and this changes the density and thus the level of mixing through fluid flow.

By focusing on the four major areas we've discussed, the fire-spread team is addressing the complex problem of fire simulation:

- *Computational fluid dynamics*. We have used large-eddy simulations in which large, energy-carrying length and time scales are resolved and the smaller scales are modeled. Also, because the governing equations are highly nonlinear and tightly coupled, robust and efficient solvers must be implemented. A significant part of the CFD effort has gone into identifying, implementing, and benchmarking such solution strategies.
- *Chemical reaction and turbulent mixing*. We use subgrid-scale models to describe the physical and chemical processes that occur at length and time scales that cannot be resolved on the computational mesh. In particular, we have worked on systematically separating the effect of the coupled processes of mixing and reaction in these subgrid-scale models.
- *Chemical kinetics*. We are developing the

chemical-kinetic sets required for the mixing and reaction models in two ways. First, the fire-spread team has been building up all necessary tools for first-principles calculations of reaction rates. Second, they have been collecting and refining the chemical-kinetic mechanisms developed by leading researchers from around the world.

- *Radiative heat transfer*. We are developing two radiation models: discrete ordinates and Monte Carlo methods.

Container dynamics

The container dynamics team is addressing the mechanical and thermal response of structures in the fires, including phase transformations and their corresponding energetics. We have devoted our first two years' effort primarily to global structural simulation and material response. Together with the fire spread team, we have selected a one-mesh–integrated-solution approach based on the material point method (MPM). The team has formulated a framework to treat the solid-to-gas chemical conversion, created and evaluated an initial MPM code, and integrated it into the PSE. The material response efforts have focused on determining material properties through molecular-dynamics simulations, explicit treatment of cracks through a dynamic-fracture approach, and micromechanics modeling to bridge the information obtained from the molecular simulations and the continuum level.

In a Lagrangian finite-element approach, the convenient treatment of many of the issues just mentioned is problematic. To deal with the large deformations that structures will experience on high loading (such as explosions) and considering tightly coupling the structural aspects of the simulation to the fire, we selected the MPM. We were significantly influenced by the work at Los Alamos National Laboratory simulating multimaterial flows and fluid–structure interaction,[1] and by recent MPM developments and extensions.[2,3]

The MPM is a type of particle-in-cell method for simulating problems involving large deformations of history-dependent materials. For problems that involve large deformations, the constitutive equations are history dependent, so that material points must be followed. Traditional Lagrangian formulations (such as finite-element methods) exhibit difficulties with large deformations that can lead to mesh lockup and entanglement. The MPM avoids this difficulty by describing the complete material state vector

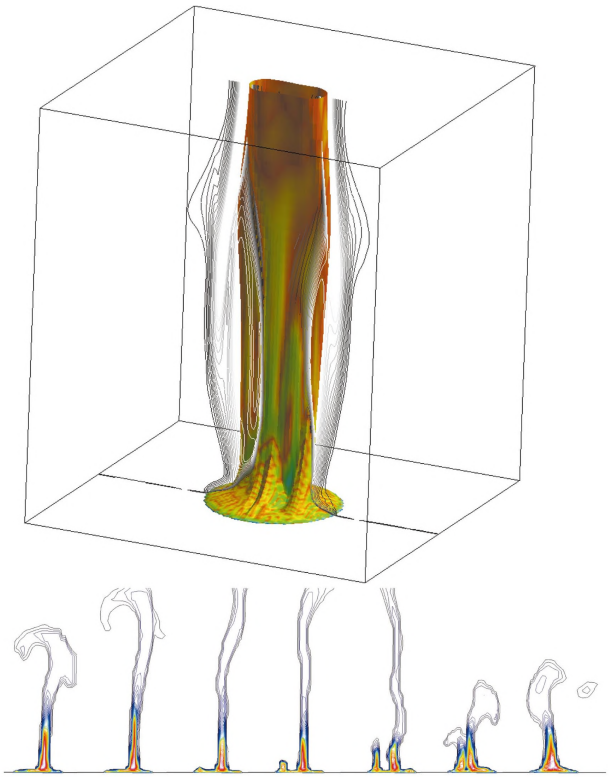

Figure 3. A large-eddy simulation of a 20-m-diameter hydrocarbon pool fire showing 3D mean temperature surfaces (top) and a time sequence of 2D slices through the middle of the pool (bottom).

on discrete mass points distributed throughout the computational domain so as to accurately represent the material state.

The original particle-in-cell approach involved representing fluid by Lagrangian mass points on a fixed or adaptive grid.[4] The approach successfully tracked interfaces in highly distorting flows but exhibited high levels of numerical dissipation, because only the mass distribution was treated in the material-point frame. This approach's dissipative properties have been significantly improved by increasing the information carried by the particles to the complete state vector.[5] In this extension, the grid no longer contains the essential information of the flow, but is used as a computational *scratch pad* to assist in the updating of particle information. There are thus no direct particle–particle interactions. All effects of material interactions take place through the grid. This *full-particle-in-cell* approach was subsequently adapted to treat suspension flows that included elastic particles.[6] With the extension of the method to include history-dependent materials (for example, plasticity), this technique has come to be known as the material-point method.[7]

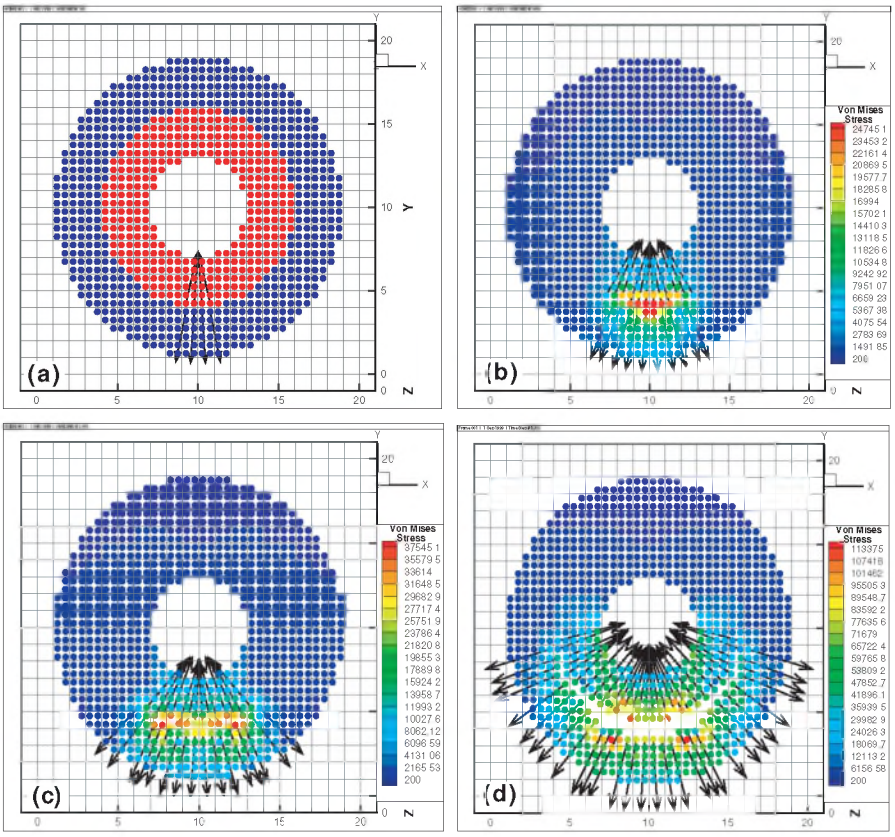

Figure 4. Simulation of a pressurized spot at the interfacial surface of a propellant-filled container. As this simulated pressure increases, the two initially bonded materials separate and the pressurized surface propagates along the interface. Color map in frames b–d indicate Von Mises stress; arrows represent applied forces (simulated pressure).

Figure 4 displays simulation results of a pressurized debond at the interface of concentric cylinders. The object represents a simplified 2D slice of a rocket motor (case in blue, propellant in red). Initially, the two materials are perfectly bonded, and forces are applied to material points near the bottom of the interface, normal to the surfaces of each material. This pressurization is intended to be a simplified representation of the propellant undergoing phase change from solid to gas because of high temperatures. These applied forces, represented by the black arrows, grow in time, and eventually the normal component of the traction at the interface exceeds nominal bond strength between the two materials. When this happens, the debond propagates along the interface, as seen in the figure sequence.

Improvements to this simulation currently underway include more accurate constitutive modeling of the propellant to include damage and possible viscoelastic response, and incorporation of rigorous fracture mechanics in the propellant and case. 3D simulations of similar configurations with plastic response and a continuum damage model have been run on 1,024 processors on Blue Mountain at LANL.

Recently, C-SAFE researchers have incorporated fracture and the generation of new surface into the MPM. The incorporation of crack growth requires a methodology to impose discontinuous displacement and velocity fields on the underlying mesh. This is accomplished by a special surface description in the MPM that incorporates a different particle → grid interpolation scheme if a particle is identified to be in a surface cell. In addition, high-stress gradients near crack tips necessitate adaptive mesh and particle refinement to achieve sufficient resolution for accurate simulations. Particle-refinement algorithms are also required in nondamaged materials to ensure that numerical artifacts due to large deformations (leaving no particles in a cell) are avoided.

In our simulations, we base the treatment of crack growth on dynamic fracture analysis and the energy release rate for crack propagation. The criterion for crack growth is when the energy release rate, given by Equations 1 and 2, exceeds the material toughness, G_c:

$$G_I + \lim_{\delta\alpha \to 0} \frac{1}{2\delta\alpha} \int_0^{\delta\alpha} \sigma_{\theta\theta}(\delta\alpha - r, 0)\overline{\mu}_\theta(r, \pi)dr \quad (1)$$

$$G_{II} + \lim_{\delta\alpha \to 0} \frac{1}{2\delta\alpha} \int_0^{\delta\alpha} \sigma_{r\theta}(\delta\alpha - r, 0)\overline{\mu}_r(r, \pi)dr \quad (2)$$

Here $\delta\alpha$ is the crack opening length, σ is the stress, u is the displacement, and G_I and G_{II} are the energy release rates for mode 1 (normal) and mode 2 (shear) loading. The total energy release rate is simply the sum of these two contributions.

The essential element to correctly predict crack growth in this approach is an accurate value of the energy release rate. Simulations performed in C-SAFE demonstrated the MPM's ability to capture this behavior from MPM simulations for the energy release rate in a double cantilever beam. Figure 5 shows the MPM results on a coarse mesh, using a lumped-mass matrix formulation. In this case, the MPM results underpredict the exact solution (given by the straight line). When we used mesh adaptivity and a full-mass matrix, we obtained the exact result. We achieved this result using a dynamic analysis. We incorporated damping into the constitutive model, which let the solution relax to the static result. Figure 5 shows results in each case for two different values of the damping coefficient μ.

We used a hierarchical tree-structured MPM cell description to achieve adaptivity in this simulation. Refinement was based on the gradient of internal-energy density (kinetic-energy density + strain-energy density).

High-energy transformations

Our high-energy transformations team performs microscale analysis of the relevant physical and chemical processes. They are focusing initially on the HMX energetic material and are directing their efforts at coupling molecular dynamics, electronic structure, and statistical mechanics in an integrated fashion to dynamically obtain properties for all materials (condensed phases, vaporized phases, and structures) in the fire and explosion. Initial work has focused on quantum chemistry calculations for dimethylnitramine (DMNA) (because it is a reasonable but simpler chemical model for HMX; quantum chemistry calculations of HMX in both the gas and condensed phases, embedded cluster computations for crystalline materials, classical molecular-dynamics calculations of DMNA, HMX, and polymer binders; and investigation of reduced kinetic mechanisms. The team has also been adapting their kinetics codes to simulate transient combustion kinetics and developing new methods for evaluating existing thermal-analysis data.

We have used conventional quantum chemistry codes (Gaussian) to compute different possible reaction mechanisms in DMNA and HMX using the B3LYP level of density-functional theory (DFT). For DMNA, which is a model system of HMX, the N-N bond energy has been determined. Scission of the N-N bond is believed to be the initial step in decomposition of most nitramines, including DMNA and HMX. For DMNA, the computed value of 45.8 kcal/mol compares favorably with the experimental value of 43.5 kcal/mol. This provides a high level of confidence for the theoretical DFT methods that will be used in future calculations. At the same level of theory, the N-N bond dissociation energy of HMX is predicted to be 35.9 kcal/mol (including the effect of zero-point vibrational energy). The gas phase has no barrier to dissociation, suggesting that N-N bond scission in condensed HMX is highly reversible.

The HMX molecule forms an eight-sided ring with two possible conformations (boat or chair, as shown in Figure 6a and 6b). We investigated the C-N bond dissociation of the ring as another possible reaction mechanism of HMX in a condensed phase. For gas-phase calculations of this mechanism, we find that a stable 10-sided ring intermediate is formed, as Figure 6c shows. This intermediate is only 11.4 kcal/mol higher in energy than that of the ground-state energy, and can present itself as an energetically possible mechanism in a condensed-phase environment.

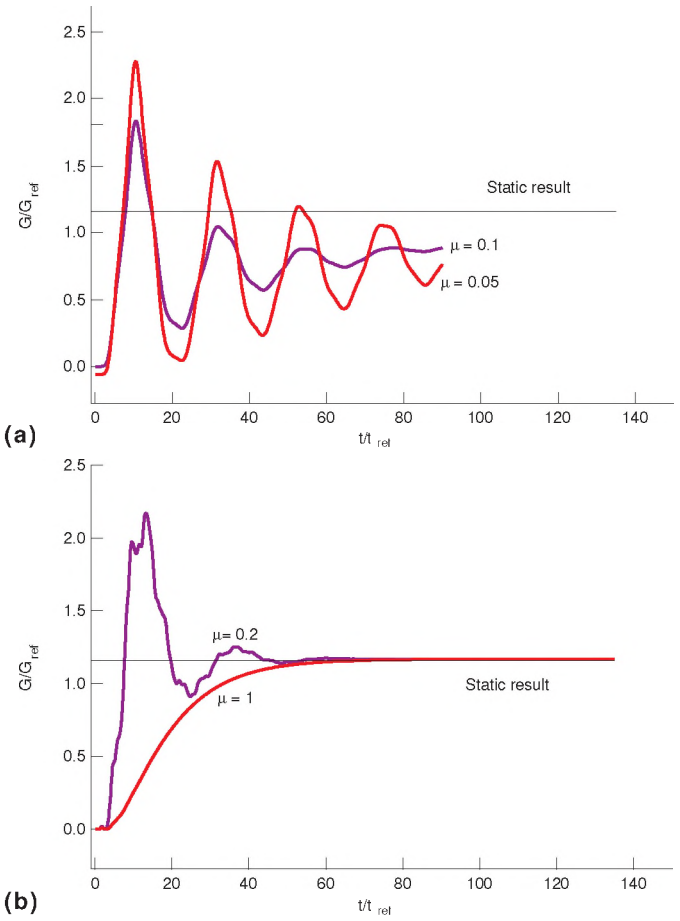

Figure 5. Energy release rate results for static-fracture analysis: (a) fixed-grid, lumped mass matrix (straight line is exact result); (b) adaptive-grid, full-mass matrix.

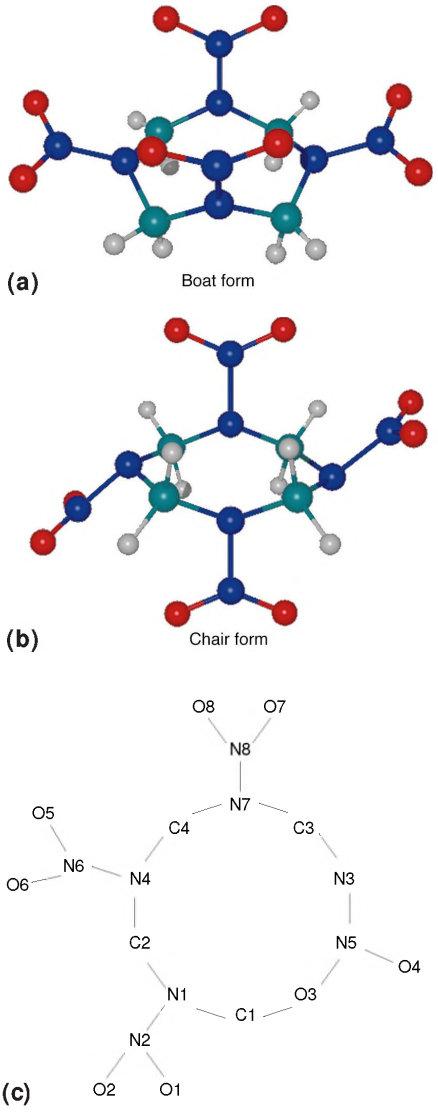

Figure 6. The HMX molecule: (a) boat form, (b) chair form, and (c) stable 10-sided ring intermediate form.

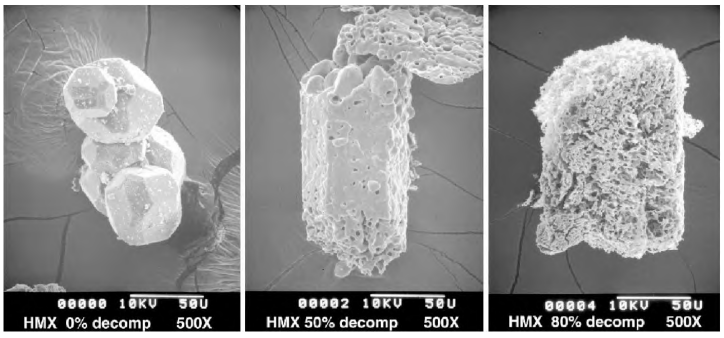

Figure 7. Micrographs of partially decomposed HMX crystals: unreacted HMX (left), after 50% decomposition (center), and after 80% decomposition (right).

The transition state structure between this intermediate and the ground-state structure yields an energy barrier of 48.4 kcal/mol, which is only 11.6 kcal/mol higher in energy than the N-NO_2 bond dissociation energy.

For HMX, we found that the known acceleration of the reaction to a maximum rate at approximately 40% conversion is not due to a decrease in activation energy, as might be expected for a mechanism involving chemical autocatalysis. Rather, the activation energy is constant with the extent of reaction, and the acceleration can be attributed to the reaction model. In essence, the acceleration is caused by the increase in surface area of HMX crystals as they are consumed. We have obtained experimental evidence for this in the form of scanning electron micrographs of partially decomposed HMX crystals (see Figure 7). These micrographs show that the HMX crystals maintain a nearly constant size during thermal degradation below the melting point. However, they develop a high degree of porosity that makes them resemble sponges.

This kinetic analysis inspired the development of a new global model of nucleation kinetics. In this model, the thermal decomposition of each HMX is activated by being located at the surface of a crystal or near a spatial defect in the crystal. Although this model is still under development, it shows great promise for providing one connection between the microscopic molecular-dynamics simulations and the macroscopic world of laboratory experiments and combustion environments. This type of process will let us bring together models connecting vast time and length scales for synthesis, validation, and eventual use in the large-scale fire simulation that is C-SAFE's ultimate goal.

Computer science and applied math

The computational efforts described in these three major steps discussed so far are integrated through a strong program emphasis in computer science and applied math. The computer science team has concentrated efforts in four primary areas: the PSE, visualization, performance, and scientific data management. Because the length scales we will attempt to resolve in a simulation will vary over at least five orders of magnitude, the applied math group has focuses on AMR and robust numerical solvers. (The relevant physics varies over a much wider range of scales—from molecular scales to macroscopic scales of meters or more. So, the development of subgrid bridging models from the micromacro range is required to achieve practical range of length scales even on massively parallel machines.)

The PSE

As one of its major goals, C-SAFE will develop a computational framework within which the disparate aspects of the system can come together in an efficient and scalable way. In addition, we are seeking to exploit special opportunities to achieve scalability within the distinct steps (such as the high-energy transformation group's molecular-dynamics calculations). The C-SAFE architecture is fairly unique in that it will be implemented directly in the PSE. Modules such as resource management, parallel services, and performance analysis will be services provided by Uintah. Other modules, notably all of the simulation modules, will be components in the Uintah PSE and will be connected into active simulation scripts using a visual-programming paradigm.

The Uintah PSE is building on the Common Component Architecture, which is being defined by the CCA Forum. The CCA Forum is a group of researchers from national labs and academic institutions who are defining a standard for high-performance computing using components.[8] Under this model, Uintah components will interoperate with other CCA-compliant components.

The features we deem most essential in the Uintah framework are scalability, integratibility, steerability, portability, and validity. To achieve them, the Uintah PSE is derived from the SCIRun system[9] and employs a blend of object-oriented (C++), imperative (C and Fortran), scripted (Tcl), and visual (the Uintah dataflow interface) languages to build this interactive environment. Figure 8 shows a screenshot of the Uintah GUI. The basic Uintah system provides an optimized dataflow-programming environment, a sophisticated data model library, resource management, and development features. Uintah modules implement components for computation, modeling, and visualization.

As we plan to use more than one of the DOE laboratory supercomputer architectures, we are designing a communication infrastructure that is largely independent of the number of nodes in the shared-memory partition. This is important because the SGI Origin 2000 clusters will contain 128 nodes per shared-memory cluster and the IBM system will contain a cluster of approximately four nodes per shared-memory partition. Creating such a flexible communication infrastructure while affording maximal scalability is challenging.

Visualization

The major areas of development for visualization are

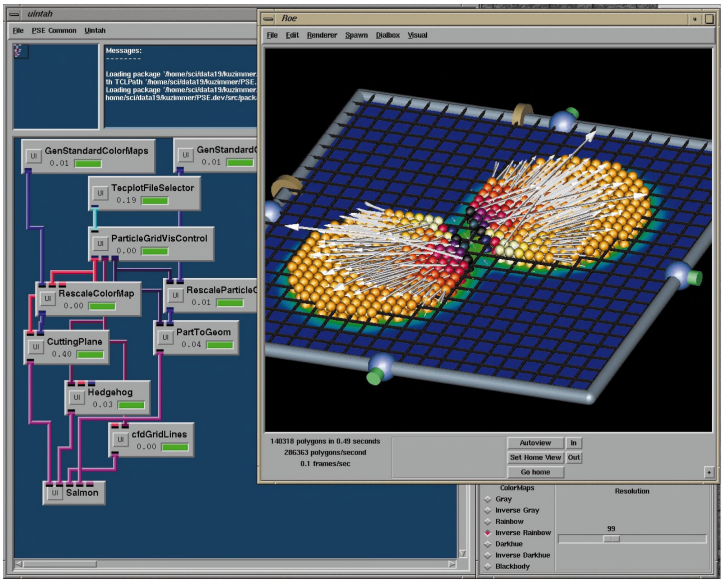

Figure 8. The Uintah PSE graphical user interface.

- creation of a new parallel method for performing isosurface extraction for very large datasets using ray tracing.
- development of new grid-specific visualization tools for the container dynamics and fire-spread steps.
- development of new algorithms and tools for multipipe rendering of large-scale surface and volume visualization.

Interactive visualization of isosurfaces in large data sets is a difficult problem. The most common technique for generating an isosurface is to create an explicit polygonal representation of the surface and then render it with attached graphics hardware accelerators. Rather than generate geometry representing the isosurface and rendering it with a z-buffer, we have created a parallel method that uses ray tracing. For each pixel we trace a ray through a volume and do an analytic isosurface intersection computation. Although this method has high intrinsic computational cost, its simplicity and scalability make it ideal for large data sets.

As an example of the success of the real-time ray tracer, we experimented with various parameters using the Visible Woman CT dataset from the National Library of Medicine, which consists of a $512 \times 512 \times 1{,}736$ volume of 16-bit data. Our technique renders a particular isosurface at approximately 10 to 15 frames per second. That is equivalent to 5 Gvoxels per second (500M cells × 10 frames per second). Ray tracing lets us directly render nontraditional primitives such as spheres. Figure 9 shows a visualization of a stress simulation in which a sphere

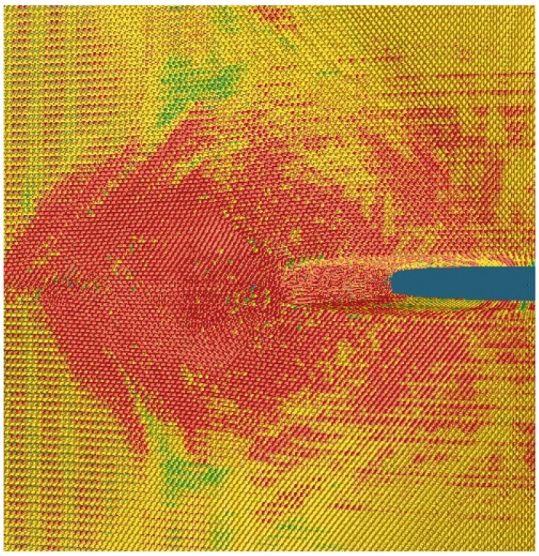

Figure 9. A simulation of crack propagation visualized using 35M spheres. This image at 512 × 512 pixels runs approximately 15 frames per second on 60 CPUs.

represents each of the 35 million nodes.

The visualization group has interacted closely with the container-dynamics team to develop a Uintah PSE visualization tool for MPM particle and mesh visualizations (see Figure 8). MPM uses both gridless (particles) and grid-based computational data structures. Our tool allows visualization of both types of data structures by exploiting spatial coherence displayed all in the same space, as well as temporal coherence provided by differing time steps.

Performance analysis

Existing performance-monitoring tools provide relatively poor support for tuning highly parallel programs on modern computing platforms. In particular, they do not provide information about crucial communication issues, and in the case of shared-memory machines, they do not provide information about the locality of memory reference. Existing tools also provide an extremely clumsy user interface, which makes them hard to use. More importantly, they collect huge amounts of data but provide no support to help the user understand the aggregate meaning of the data and to reason about the consequences of algorithmic design decisions. Furthermore, the PSE tools and the performance-tuning tools heretofore have been separate environments, so large parallel codes utilize a small fraction of the large terascale machines' peak performance. Also, most applications programmers do not thoroughly understand the host machine's architecture or what those details might mean in terms of structuring codes for optimal performance.

The C-SAFE performance-analysis effort is creating a performance tool suite that will be tightly integrated into the Uintah PSE and that uses the visualization tools to view performance data used to analyze the programs once they are optimized. The tool development is based on a detailed understanding of the underlying architecture and its effect on the program's performance.

Applied math

The major areas of work here are AMR, time integration, the solution of very-large-scale linear and nonlinear systems, and sensitivity analysis.

Our work on AMR focuses on structured AMR (SAMR) because these methods allow regular array access patterns and require no indirect addressing, and thus better utilize available cache and memory bandwidth. In addition, the mesh operations needed for parallel implementation are greatly simplified. Finally, AMR methods are inherently dynamic algorithms. Migration of patches among processors is necessary to achieve a load-balanced computation. Therefore, we will need mechanisms to estimate local computational loads, share these estimates among processors, rebalance the load, and remap the data.

In the first two years, C-SAFE has been building on top of the SAMRAI (Structured Adaptive Mesh Refinement) code developed at LLNL. SAMRAI provides more comprehensive high-level support for SAMR algorithms. For example, SAMRAI offers packages that implement strategies for subcycling in time that are needed for explicit time integration on SAMR grids. Automatic regridding in time is based on Richardson extrapolation and in space on detection of gradients in the solution. User-supplied criteria can also drive these processes. SAMRAI explicitly supports cell-centered, vertex-centered, and staggered data.

For a general-purpose solver library, we have chosen PETSc, developed at Argonne National Laboratory. This suite of high-level codes solves large-scale linear and nonlinear equations. To validate the solver strategies in PETSc, we tested the code on a model problem that is representative of problems to be addressed later in C-SAFE simulations. Specifying a temperature gradient across the cavity induces a thermally driven flow in a 2D cavity. We tested a multigrid solver that was almost 40 times faster than the single-grid solver that is in use; these problems are representative of pool fire scenarios. Finally, we have worked extensively to formulate solver strategies that will guide development of the core nonlinear solver in the Uintah PSE. Effective solvers for problems discretized on block-structured adaptive grids take advan-

tage of the grid's hierarchical nature. These solvers employ multilevel algorithms, which treat local problems defined on regions with uniform mesh size. The level solver's quality thus determines the multilevel solver's effectiveness. Because a refinement level is the arbitrary union of rectangular patches, we explored these issues by studying problems defined on individual patches.

Software engineering

Because software engineering is a major aspect of the project, we plan to have a software engineer in each of the simulation development roadmap steps (fire-spread, container dynamics, and high-energy transformations), as well as in the computer science task. Each software engineer has two major duties: oversee software development within the step or task and help migrate step modules into the common Uintah PSE. An advisory committee established to manage software development will have responsibility for the overall definition of the Uintah software architecture, module creation, and migration, and the adoption and monitoring of software development and implementation standards. We participate in the ASCI TriLab Data Models and Formats group, which has been developing a comprehensive underlying mathematics for scientific data description, and we have been developing tools to help scientists organize and keep track of large-scale simulations involving large numbers of configuration parameters and datasets used as input to various software versions of the task codes, possibly on heterogeneous architectures with concomitant visualizations.

See the "Unique features" sidebar for our discussion of the steps we will take on this project in coming years.

Beyond the five years of the current program, our long-term vision is to be able to handle large-scale accident scenarios, involving, for example, fires in industrial buildings, effects of explosions and shock waves on surrounding structures, and combustion initiated by impact.

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Unique features

The C-SAFE program has four unique features that we have further amplified during our project's first phase:

- A one-mesh–integrated-solution approach to integrating the fire with the container and its high-energy contents.
- The inclusion of first-principles molecular dynamics calculations to compute the fundamental chemistry of the high-energy materials and other reactants under specific conditions of the problem.
- Computational steering and system utilization analysis in conjunction with an advanced problem-solving environment.
- Integration of experimental testing with actual high-energy materials from the program's beginning.

One mesh–integrated solution

Owing to its combined Eulerian-Lagrangian treatment of mass, MPM can combine with a Eulerian hydrocode to provide explicit coupling and treatment of fluid–solid interactions. We can do this by using the Eulerian CFD mesh as the scratch pad mesh for evaluating particle transport processes in the MPM calculations.[1] This combined Eulerian-Lagrangian description lets us treat a number of key physical processes that are problematic in conventional applications of finite-volume or finite-element techniques individually. Besides the treatment of large deformations, these include phase transition, chemical transformations, multiple materials, interdiffusion, and interface splitting. The tight coupling results from the use of a general multimaterial formulation (see Figure A) of the governing equations where individual materials can be described either in the Eulerian or material-point framework.

In addition to the equations in Figure A, any number of individual scalar equations can be associated with each material. For example, a gas-phase material can contain several individual chemical-species reaction-diffusion-convection equations. Appropriate equations of state and constitutive relations for material response must be supplied for each material.

Mass

$$\frac{\partial \rho_m}{\partial t} + \nabla \rho_m \vec{U}_m = \overbrace{\rho_o \dot{\alpha}_m}^{(a)} \quad \text{(A)}$$

(a) Net source of m mass due to phase change

Momentum

$$\frac{\partial \rho_m \vec{U}_m}{\partial t} + \nabla \rho_m \vec{U}_m \vec{U}_m = \overbrace{\rho_o \vec{U}_m \dot{\alpha}_m}^{(a)} - \overbrace{\theta_m \nabla p}^{(b)} + \overbrace{\rho_m \vec{g}}^{(c)} + \underbrace{\nabla(\alpha_m \tau_o)}_{(d)} + \underbrace{\sum_l \theta_m \theta_l K_{m,l}(\vec{U}_l - \vec{U}_m)}_{(e)} \quad \text{(B)}$$

(a) Net source of m momentum due to mass conversion
(b) Equilibration pressure
(c) Gravitational body force
(d) Average material stress
(e) Momentum exchange among the different materials

Energy

$$\frac{\partial \rho_m e_m}{\partial t} + \nabla \rho_m e_o \vec{U}_m = \overbrace{\rho_o e_o \dot{\alpha}_m}^{(a)} + \overbrace{\frac{p_m v_m}{c_m^2} \dot{p}}^{(b)} + \overbrace{\frac{\alpha_m \tau_o : \varepsilon_o}{2}}^{(c)} - \underbrace{\nabla \alpha_m q_o}_{(d)} + \underbrace{\sum_l \theta_m \theta_l R_{m,l}(T_l - T_m)}_{(e)} \quad \text{(C)}$$

(a) Net source of m energy due to mass conversion
(b) Average multiphase work
(c) Average viscous dissipation
(d) Thermal transport by conduction
(e) Energy exchange among the different materials

Figure A. Conservation equations of mass, momentum, and energy for an individual material, m, *in a multimaterial environment.*

The general multimaterial-continuum solution involves a number of grid-based operations: using cell-centered, faced-centered, and vertex information (depending on the details of chosen solution algorithm). During the finite-volume solution process of the multimaterial equations, we treat advection, diffusion, and most of the source terms sequentially and individually material-by-material. Coupling occurs directly

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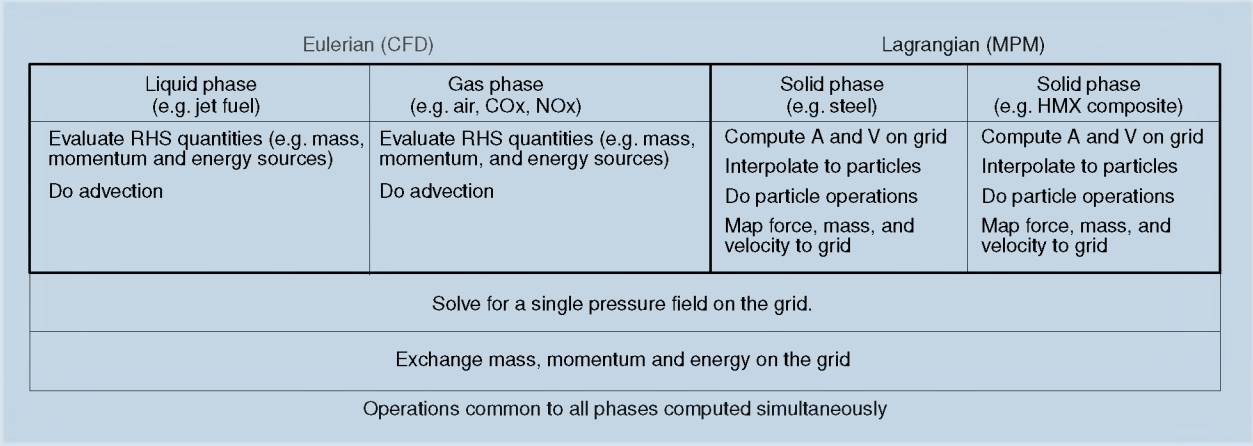

Figure B. A graphical layout of combined Eulerian-MPM solution. Columns represent operations performed independently for each material. Simultaneous operations include mass, momentum, energy transport, and the pressure solution.

though energy and momentum exchange (the terms e in Equations B and C, which are modeled here through exchange coefficients) and the overall pressure solution.

To couple the MPM techniques within a finite-volume multimaterial simulation, the MPM simulation involves both particle- and grid-based operations. The state vector of the material particle descriptions can advance in parallel with that of the Eulerian-based calculations. The fluid–structure simulation becomes tightly coupled through mass, momentum, and energy exchange, along with a single-pressure solution that occurs in a common reference frame. In particular, during the MPM solution, information is interpolated between the material points and the mesh. As Figure B shows, at the point in the computation where the material points' force, mass, and velocity exist on the grid, the operations common to all phases (that is, the pressure solution and mass, momentum, and energy exchange) are computed simultaneously.

Preliminary validation of the approach has appeared elsewhere.[1] The initial studies included a solid object falling under the action of gravity in an initially quiescent flow field and the breaking of an interface between two fluids of different density. Here we provide examples that illustrate the solid-fluid coupling in applications relevant to the effects of fires and explosions on structures.

Figure C shows an example of a three-material, tightly coupled, fluid-structure interaction problem. The initial condition consists of a deformable box (described by material points) filled with a reactive solid (described by material points). This "container" is an elastoplastic material that resides in a gas-filled domain (Eulerian description). The initial temperature is a constant value of 300 K throughout the domain. The boundary temperature at the base of the container is set to a constant value of 400 K. The reactive material undergoes a temperature-dependent reaction described by a progress variable that evolves according to temperature as $d\phi/dt = k\, exp^{(-Ea/RT)}\, \phi^{0.8}(1-\phi)$ with the products of reaction going to the gas-phase Eulerian description. As the sequence in Figure C shows, the conversion of reactive solid to gas results in a pressurization of the container, leading to its deformation and ultimate rupture. The figure clearly illustrates the effect of this rapid deformation and escaping gases on the ambient gas-phase field.

First-principles molecular-dynamics calculations

As we've described in the main text, the high-energy

mal-decomposition reactions in energetic materials (explosives and propellants). When all goes according to plan, all of this is accomplished on a milligram scale, without exploding or propelling anything about the laboratory. He received his PhD in chemistry from the California Institute of Technology. Contact him at the Univ. of Utah, Chemistry Dept., 315 S. 1400 East, Rm. DOCK, Salt Lake City, UT 84112-0850.

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transformation team is primarily responsible for generating reliable subgrid-scale descriptions for the chemical-reaction rates and mechanisms for decomposition and combustion of energetic materials. The primary parallel-code development effort is a scalable first-principles molecular-dynamics code based on a local orbitals method. It will let us treat several thousand HMX molecules for bridging to macroscale models.

Computational steering and system utilization analysis

The computer science and applied math teams will develop the Uintah PSE and explore MPI parallelism for Uintah. Another major goal is the incorporation of a SAMRAI-based version of MPM within Uintah. Scaling issues and visualization methods for the Uintah computation are being developed. Performance tools that perform data gathering in the kernel so as to minimize overhead are under development, as is a visualization tool for performance data. Large-scale simulation management tools are being applied to problems in C-SAFE. The applied math team is providing methods for AMR, time integration, solution of very large-scale linear and nonlinear systems, the associated development of preconditioners and multigrid-multilevel techniques, sensitivity analysis, and stiff solvers.

Validation

We are conducting the validation effort at four levels of complexity, starting with fundamental rates and properties, progressing through single-step, coupled-steps, and finally a fully integrated multistep experiment.

The fundamental rates and properties needed in the submodels for each task are primarily the responsibility of individual investigators, drawing extensively on the literature and parallel efforts at the national laboratories. The validation team, in conjunction with the computer science team, is exploring Web-accessible methods for comparing both submodels and validation data with other groups around the world working on similar problems. We are conducting pilot efforts with setting up the simpler submodels with short runtimes from different research groups on a common server. As the sophistication level of the models to be compared increases, the comparison will need to run on remote servers, with issues of runtime, access, and security needing to be resolved.

The single-step experiments are designed to answer key questions, which initially include

- determining the chemical structure of young soots, using the specialized skills on solid-state nuclear magnetic resonance (NMR) at the University of Utah to evaluate alternative hypotheses in the literature on the gas-solid conversion,
- studying the development of porosity in the composite explosive due to reactions that take place at the interface between explosive and binder components, and
- defining surrogate fuels to represent JP8 and other jet fuels by mixtures of fuels for which the chemical kinetics are known. The surrogate mixtures must be able to reproduce all important physical and chemical parameters of the jet fuels, including the vapor pressure curves and the sooting behavior.

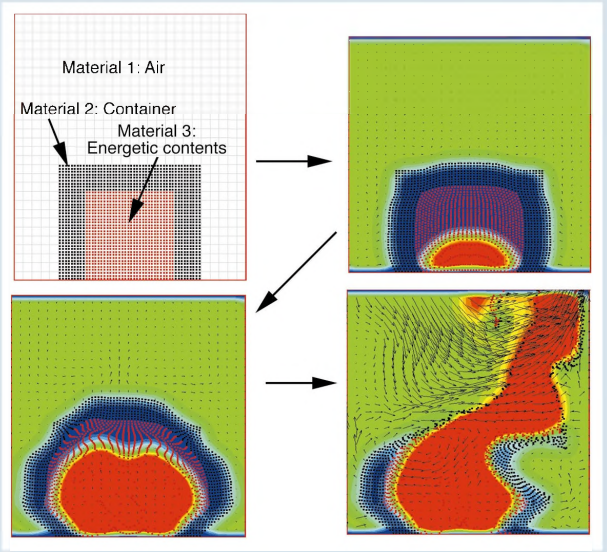

Figure C. A sequence from a simulation of an exploding container. The container and its contents have a Lagrangian material-point description. The Eulerian frame describes the surrounding air and products of reaction.

Coupled-step experiments that are important for validating the integrated model include those addressing the processes occurring at the interface of the container and the fire to address issues of the impact of soot deposition on the thermal-radiation boundary conditions. The coupled experiments will involve a container, excluding high explosives, placed in a small-scale (about 1m diameter) pool fire. These experiments will also provide soots of different maturity for the NMR studies of soot structure and test the adequacy of the representation of aviation fuels (JP4 and JP8) with surrogate fuels.

Finally, we will use the integrated experiments at Thiokol to test uncertain initial conditions, such as the bonding of the explosive to the container, as well as to provide phenomenological observations on the container rupture and a first-order testing of the calculated time to explosion. (The Thiokol Propulsion Group is working with us on the testing of high-explosive materials engulfed in a pool fire.)

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