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MULTISCALE MODELING OF ACCIDENTAL EXPLOSIONS AND DETONATIONS

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The Uintah Computational Framework is the first software to enable effectively simulating the development of detonation in semi-truck-scale transportation accidents.

Accidental explosions are exceptionally dangerous and costly, both in lives and money. Regarding worldwide conflict with small arms and light weapons, the Small Arms Survey has recorded more than 297 accidental explosions in munitions depots across the world that have resulted in thousands of deaths and billions of dollars in damage in the past decade alone.[1] As the recent fertilizer plant explosion that killed 15 people in the town of West, Texas demonstrates, accidental explosions aren't limited to military operations. Transportation accidents also pose risks, as illustrated by the occasional train derailment/explosion in the nightly news, or the semi-truck explosion detailed in the following section. Unlike other industrial accident scenarios, explosions can easily affect the general public, a dramatic example being the Pacific Engineering and Production Company of Nevada (PEPCON) plant disaster in 1988, where windows were shattered, doors were blown off their hinges, and flying glass and debris caused injuries up to 10 miles away.

While the relative rarity of accidental explosions speaks well of our understanding of the safety hazards to date, their violence rightly gives us pause. A better understanding of these materials is clearly still needed, but a significant barrier is the complexity of these materials and the various length-scales involved. In typical military applications, explosives are known to be ignited by the coalescence of hot spots that occur on micrometer scales. Whether this reaction remains a deflagration (burning) or builds to a detonation depends both on the stimulus and boundary conditions or level of confinement. Boundary conditions are typically on the scale of engineered parts, approximately meters. Additional dangers are present at the scale of trucks and factories. The interaction of various entities, such as barrels of fertilizer or crates of detonators, admits the possibility of a sympathetic detonation—that is, the unintended detonation of one entity by the explosion of another, generally caused by an explosive shock wave or blast fragments.

Although experimental work has been and will continue to be critical to developing our fundamental understanding of explosive initiation, deflagration, and detonation, there's no practical way to comprehensively assess safety on the scale of trucks and factories experimentally. The scenarios are too diverse and the costs too great. Numerical simulation provides a complementary tool that, with the steadily increasing computational power of the past decades, makes simulations at this scale begin to look plausible. Simulations at both the micrometer scale (the *mesoscale*) and at the scale of engineered parts (the *macroscale*), have contributed increasingly to our understanding of these materials. Still, simulations on this scale require both a massively parallel computational infrastructure and selective sampling of mesoscale response, such as advanced computational tools and modeling. With this in mind, we developed the computational framework Uintah (see www.uintah.utah.edu) for exactly this purpose.

Motivation

In 2005, a truck carrying 16,000 kilograms of seismic boosters, driving through Spanish Fork Canyon, Utah took a corner too quickly and overturned. The semi-truck caught fire and within three minutes detonated, creating a crater in the road approximately 24 meters wide and 10 meters deep (see Figure 1). The detonation hurled hot metal shards as far as one-quarter mile away, which started grass fires in the surrounding hills. Fortunately, the driver was coherent enough to relay to nearby drivers that the truck was carrying mining explosives, and to evacuate the area immediately. Only minor injuries were sustained, but if this had occurred in a densely populated region, the death toll could have been substantial. What has scientists and engineers puzzled is the extent of the damage. The crater's

size and the lack of any unexploded boosters suggest that a mode of combustion called *detonation* occurred. The safety characteristics of a single device suggest detonation should never occur in transportation accidents; instead, a mild, relatively slow mode of combustion, called *deflagration*, should have occurred. In confined deflagrations, only a small percentage of the explosive is consumed before it's ejected away from the ignition site. We hypothesize that it was inertial confinement or the way the explosives were loaded inside the trailer that caused the deflagration reaction to transition into a detonation. This accident, along with several other petascale simulation efforts, has driven the development of the Uintah Computational Framework. The complex physics of this accident requires modeling at multiple spatial and temporal scales to provide predictive simulations.

Because the reaction rates and subsequent energy release rates of deflagration and detonation differ by roughly five orders of magnitude, a Deflagration-to-Detonation Transition (DDT) leads to extremely violent events. The mechanism of a DDT in solids is still unknown, but various mechanisms have been proposed. One such mechanism involves the advection of hot combustion gases through cracks in the explosive, a process called *convective deflagration*. Convective deflagration occurs when the pressure outside a damaged combustible forces hot gases into the explosive, increasing the burning surface area, damaging the material in several different directions simultaneously, and accelerating the reaction. In this particular accident, 8,400 explosive boosters were arranged in a way that's reminiscent of a porous material rather than a monolithic solid. We suspect that the convective burning mechanism was partially responsible for DDT. Using large-scale simulations, we intend to investigate why DDT occurred and determine if inertial confinement contributed to the detonation. If inertial confinement was the cause, we'll use our simulation capabilities to suggest alternative, safe packing configurations.

Figure 1. A 24-meter-wide crater produced from an unexpected Deflagration-to-Detonation Transition (DDT) of 16,000 kilograms of high explosives, carried by a truck through Spanish Fork Canyon, Utah.

Challenges in Modeling Explosives

The deflagration-to-detonation transition of high explosive materials is a multistep process with fluid-structure interactions (FSIs) during the slow deflagration and rapid detonation regimes. As deflagration is occurring, a cold solid reactant is heated to the point of ignition to form hot gas, which can flow through pores or cracks in the damaged material. The greatest difficulty of a DDT simulation is accurately modeling stress-induced material damage so that it statistically captures cracking and the formation of pores in the explosive, which allows convective burning in the cracks.

Cracking, porosity, and convective burning are difficult to capture at the macroscale, due to averaging, necessitating the use of statistically based, subgrid scale models. Mesoscale modeling has the potential to provide the statistics needed for subgrid models that live on the discrete elements of the simulation domain. Mesoscale simulations are computationally expensive, requiring sophisticated material models capable of capturing the material fracture, elastic yield, plastic flow, melting, and heating due to the energy conversion from these forms of mechanical work. Finally, detailed reaction modeling of explosives at the mesoscale involves many reaction species and the complex interplay of the reacting species further complicates the problem. The development of simple reaction models that capture the complex behaviors at this scale are needed, which we'll discuss later.

Uintah Computational Framework

The open source (MIT license) Uintah software originated in the University of Utah Department of

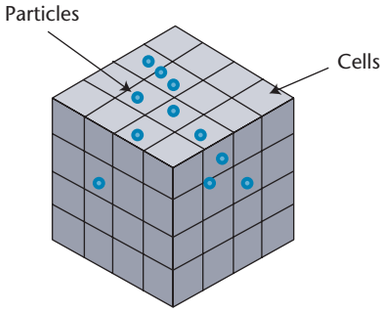

Figure 2. The Uintah patch—a Uintah mesh with particles. The Implicit, Continuous-fluid Eulerian (ICE) algorithm uses a hexahedral block of cells and the Material Point Method (MPM) particles reside within that block.

Energy (DOE) Center for the Simulation of Accidental Fires and Explosions (C-SAFE),[2] and has been in use for a number of years. The present status of Uintah, including applications, documentation, and releases, is described in a recent report.[3] Uintah is a computational framework that integrates multiple simulation components, analyzes the data dependencies and communication patterns between them, and efficiently executes the resulting multiphysics simulation. Uintah presently contains four main simulation components or algorithms:

- the finite volume mulitmaterial computational flow dynamics (CFD) formulation (the Implicit, Continuous-fluid Eulerian algorithm, or ICE),[4,5]
- the Material Point Method (MPM)[6] for structural mechanics,
- the combined FSI algorithm MPMICE,[7] and
- the ARCHES turbulent-reacting Large Eddy CFD component.[8]

Uintah exhibits good scalability characteristics,[9] runs on both National Science Foundation (NSF) and DOE parallel computers (Stampede, Kraken, Titan, Lonestar, and Vesta), and is used by many National Nuclear Security Association (NNSA), Department of Defense (DOD), DOE, and NSF projects.

The main Uintah component used in this research is the MPMICE, in which the multimaterial CFD formulation (ICE) is used to model fluids, and the MPM code is used to model the solid explosive. The ICE algorithm uses a hexahedral block of cells and the MPM particles reside within that block as shown in Figure 2.

A unique feature of Uintah is that the application developer is only asked to write code to solve equations on a hexahedral patch of the computational domain, and doesn't have to worry about parallelism and communications between patches, because this is all automatically resolved by the framework. The Uintah computation framework has a wide range of material models, reaction models, and equations of state that allow simulations of exothermic FSIs at different length- and timescales. These embedded models live inside a framework that hides the method's parallelization, allowing simple science or engineering models to scale to hundreds of thousands of processors.

Fluid-Structure Interactions

Our methodology for solving FSIs uses a strong coupling between the fluid and solid phases, with a full Navier-Stokes representation of the fluids and transient, nonlinear response of the solids, including exothermic solid-to-gas reactions. The Eulerian-based ICE method[4,5] is used to represent materials on a hexahedral grid. It allows simulation of complex gas flows with heat and momentum coupling inside a compressible flow paradigm. For solid mechanics, a Lagrangian-based MPM[6] is used that's capable of simulating complex behaviors, including material damage, stress and strain, and elastic and plastic responses.

The algorithm has its foundation in a "multimaterial" CFD approach in which each material (either fluid or solid) is defined at the continuum level over the entire computational domain, including regions where a material doesn't exist. In addition to the physical state (that is, mass, momentum, and energy) at each discrete point, the volume fraction of each material is tracked with the constraint that the volume fractions of all materials must sum to unity in any grid cell.[4]

To solve the discretized multimaterial equations, we use a cell-centered formulation of the ICE method of Harlow, further developed by Kashiwa and others at the Los Alamos National Laboratory.[4,5] The use of a cell-centered, finite volume solution technique is convenient in that a single control volume is used for all materials, simplifying the conservation of mass, momentum, and energy, and the exchange of these quantities between the materials. The method is fully compressible, an important consideration in simulations involving explosions of any type, particularly detonations. In addition to the source terms present in any CFD formulation, the multimaterial equations also include exchange terms for mass, momentum, and heat. Intermaterial mass exchange is based on the reaction models, such as those described in the next section. Momentum and heat exchange is typically modeled as a drag law based on relative material velocities or temperatures, respectively, computed in a point-wise implicit manner to ensure conservation.

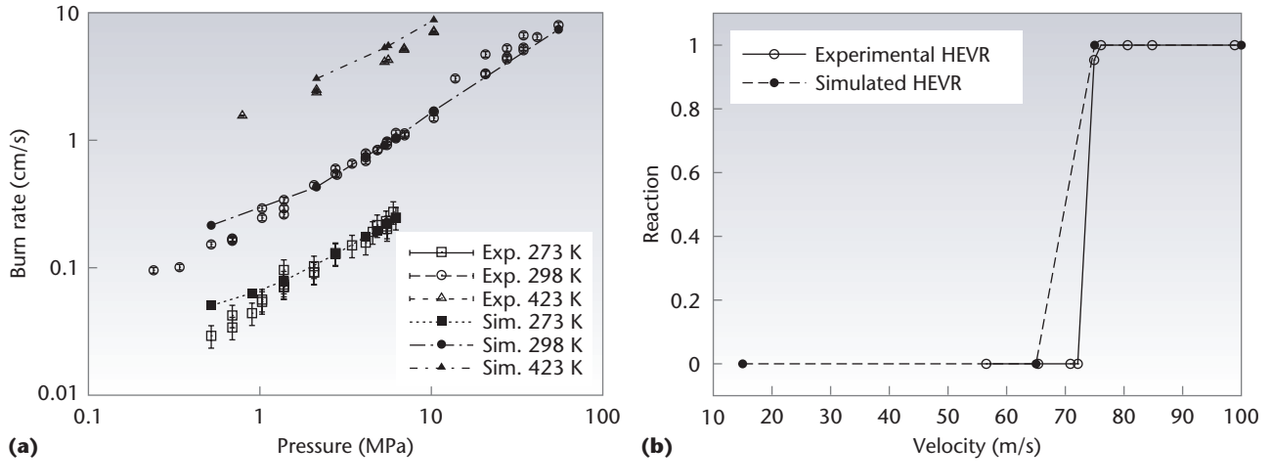

Figure 3. DDT reaction model results compared with experimental results. (a) The burn rate at three initial solid temperatures versus pressure where simulated data is compared against data from A.I. Atwood and her colleagues for the plastic-bonded explosive PBX9501.[18] (b) Comparison of the threshold for reaction against velocity for weak impacts.[20] Plots used with permission from Joseph Peterson and Charles Wight.[16] (HEVR = high explosive violent reaction.)

This formulation makes no explicit distinction between the fluid and solid materials in the model equations. FSIs aren't tracked, nor are boundary conditions passed through them. To maintain the integrity of the fluid-solid interface and provide a mechanism to track the deformation history of the solid(s), we employ the Lagrangian particle technique MPM. The MPM is used to evolve the equations of motion for solid materials, in part on account of advantages in interfacing with the ICE method. The MPM[6] is an extension to solid mechanics of the Fluid-Implicit-Particle (FLIP) method,[10] which is a particle-in-cell method for fluid-flow simulations. Development of the MPM has continued, both studying and improving the MPM algorithm,[11,12] as well as extending the technique by generalizing particle shapes.[13] The MPM has become a powerful technique for computational solid mechanics in its own right, and has found favor in applications involving complex geometries,[14] contact mechanics,[13] large deformations, and fracture,[15] to name a few.

Lagrangian particles or material points are used to discretize a material's volume, and each particle carries state information (such as mass, volume, velocity, and stress) about the portion of the material that it represents. Our implementation uses a Cartesian grid as a computational scratchpad for computing spatial gradients—the same grid used by the ICE component. In MPM, particles with properties (such as velocity or mass) are defined on a mesh, and particle properties are then mapped onto the mesh points. Forces, accelerations, and velocities are then calculated on the mesh points. The mesh-point motion is calculated, but only particles are moved by mapping velocities back to particles.

The combination of MPM and the multimaterial CFD algorithm to form our FSIs algorithm (MPMICE) involves a complex 14-step algorithm described elsewhere.[7] What makes this methodology unique is that the exchange of mass, momentum, and energy between the solid reactant and product gases occurs in the governing equations, and also that boundary conditions aren't applied to tracked surfaces. Clearly, surface tracking in these types of simulations would be difficult.

Deflagration and Detonation Models

Our reaction models convert mass from the energetic materials (for example, the plastic-bonded explosive PBX9501) to product gases, with the appropriate release of heat and exchange of momentum. Uintah now includes models validated against various detonation, deflagration, DDT, and shock-to-detonation transition (SDT) experiments. These models give us the capability to simulate steady and unsteady thermally activated deflagration and pressure-induced detonation of high explosives, including the DDT.[16]

The numerical model for deflagration is based on a two-step global kinetics model described by M.J. Ward, S.F. Son, and M.Q. Brewster (called WSB).[17] As originally formulated, this model predicts the steady combustion rate of the energetics as a function of the product gas's pressure and the solid material's temperature. We extended the 1D WSB model to 3D, and validated the parameters against the experimental strand burner measurements of A.I. Atwood and her colleagues for the correct temperature and pressure dependence of the burn rate.[18,19] Figure 3 shows a validation of our burn model over a range of temperatures and pressures.

A simple shock-to-detonation model known as JWL++[21] is used to simulate detonation formed when a

shock wave, initiated by a mechanical insult, passes through the explosive. The model captures the SDT as a function of pressure in the solid-gas mixture, allowing for the advantageous use of simple equations of state. These equations of state model pressure at high-compression levels, while neglecting the calculation of complicated material processes. Shock-based ignition can occur when an explosive is dropped or perhaps impacted by a forklift or other moving objects, and has the potential to lead to an accidental explosion. We validated our SDT model with a standard test developed at Los Alamos National Laboratory, in which an approximate 0.15-meter radius, hockey puck-shaped explosive is impacted at increasing speeds. A sharp speed threshold was observed in impact under about 75 meters per second (m/s), which caused cracking and other material damage but no reaction, while anything higher caused an explosion. Figure 3 compares experimental and simulated results for the test, where "0" indicates cracking and material damage, while "1" indicates a highly explosive, violent reaction.

The general approach for simulating the DDT process relies on the idea that high pressure forces hot gases through the voids (pores, cracks, and so on) in an explosive, which increases the reaction rate. Relating this to the normal factors cited for causing DDT, such as hot-spot nucleation and growth, shear and heating of a solid near hot-cavity gases, and frictional heating, leads to the startling conclusion that all of these phenomena can be related to the simple process of hot products of reaction flowing through the solid explosive. By merging the WSB deflagration model with the JWL++ detonation model inside a fluid-structure algorithm with a few experimentally derived thresholds, we're able to model the DDT in solid materials.

Our DDT model agreed well with experimental data for the pressure and temperature dependence of the burn rate and detonation velocities (see Figure 3), including *convective deflagration* propagation. Convective deflagration is the process of burning within the cracks of the energetic solid, rapidly increasing the reaction rates and pressure. Without convective deflagration, DDT wouldn't occur in an unconfined explosive, because deflagration would only occur on the solid's surface. We're able to model convective deflagration by using a crack model that describes the crack development as a function of pressure.[22] With this model, we're able to represent a material's damage, dependent on the surface pressure and the propagation of the reaction through a damaged explosive.

Scaling

Modeling explosions from mesoscale up to a full semi-truck requires a linearly scalable framework—in other words, the time to solution decreases with the number of processing units. Though mesoscale simulations are small in physical size, they can be computationally expensive, when the explosive grains and binders are fully resolved. At the other end of the scale, simulating an entire semi-truck with high spatial resolution is also expensive, and requires the largest computing platforms. The Uintah Computational Framework has been shown to linearly scale from 16 cores to 256,000 cores, running the MPMICE component. This scalability has relied heavily upon the asynchronous task-graph approach that allows components to be written as a series of tasks, where each task is a major step in the MPMICE algorithm. Each task has required inputs from the data warehouse and writes outputs to the data warehouse. The actual execution of the tasks is managed by a runtime system that maps the tasks onto processors after an analysis of the task's data dependencies. Figure 4 shows an example of a high-level Uintah task graph for the MPM.

The scalability of Uintah has proceeded in three distinct phases. In Phase 1 (1998–2005), Uintah overlapped communications with computation and executed the task graph in a static manner using standard data structures and one message-passing process per core (see www.uintah.utah.edu).[23] In the second phase, the data structures were greatly improved and fast mesh-refinement algorithms were developed to scale to 100,000 cores.[9,24,25] In this phase, tasks were executed in a dynamic or even out-of-order way. Finally, in the third and current phase, we're moving to a hybrid MPI-Pthread model, in which there's only one MPI process per node and individual task threads are bound to available CPU cores. Individual tasks are sent to available CPU cores and GPUs when available. This approach reduces the total global memory usage per node by up to 90 percent on the Jaguar XT5 system.[26] Using a recently designed decentralized multithreaded scheduler and lock-free data warehouse, the overhead of using this hybrid approach has been significantly reduced, and both

single-node performance and overall scalability of Uintah are further improved.[27]

The scalability of the MPMICE component used for modeling explosives with adaptive mesh refinement has been tested in both the weak and strong sense on the Jaguar XK6 system.[27] The performance was tested with four problem sizes, with each problem containing approximately eight times as many cells as the previous problem. The numbers of particles representing the solid material created in the four runs were 7.1 million, 56.6 million, 452.9 million, and 3.62 billion respectively. The grid contained three levels of mesh refinement, with each level being a factor of four more refined than the coarser level. Figure 5 shows good weak and strong scaling, for macroscale simulations up to 256,000 cores on the then Jaguar XK6 (now Titan) architecture at DOEs Oak Ridge Laboratory.[27]

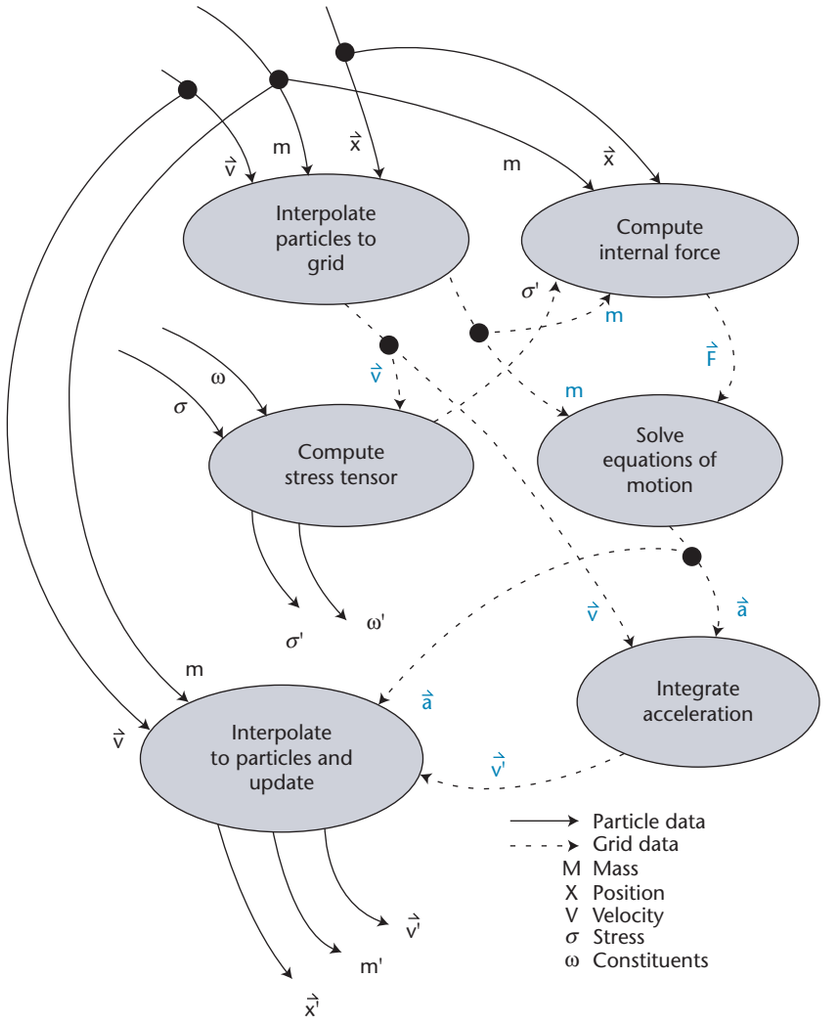

Figure 4. An example of a Uintah task graph for the MPM.

Mesoscale Explosions

When the relevant physics occurs on scales smaller than the computational resolution, additional information is needed. For accidental explosions, the vast majority of the simulation scenario needs only to resolve the macroscale. However, ignition occurs on the mesoscale, by the coalescence of hot spots. Hot spots are energy-localizing mechanisms that occur on the scale of explosive heterogeneity—that is, the explosive grains. There are many possible hot-spot mechanisms,[28] and it's clear that the dominant mechanisms vary with the scenario considered. Here, we use mesoscale simulations to gain insight into the ignition process. Our long-term goal is to judiciously place mesoscale simulations directly in macroscale simulations, to resolve hot-spot distributions and predict ignition in areas of interest. These simulations bridge the gap between molecular and macroscale modeling.

At the micrometer-length scale, interactions between explosive grains and the plastic binder that hold them together, or other explosive grains, are explicitly resolved (see Figure 6). When the binder and grains are fully resolved, we can investigate the different mechanisms. When a sufficient force is applied to the explosive and binder, there will be plastic deformation or work that generates hot spots, as Figure 6c shows. These hot spots could either dissipate their energy to colder surrounding material, or coalesce and cause a sustained reaction, depending on their size, intensity, and number density.

Initially, our studies utilized idealized geometries of the explosive grains that were impacted by a piston at varying speeds and compared against experimental results.[29] These studies were designed to validate our material model, which includes the elastic and plastic response as well as temperature-varying thermal parameters. We compared the velocity and stress traces at the impact surface, for all of the impact speeds, and found good comparison within 10 percent.[29] With this agreement, we sought to study hot-spot distributions to find

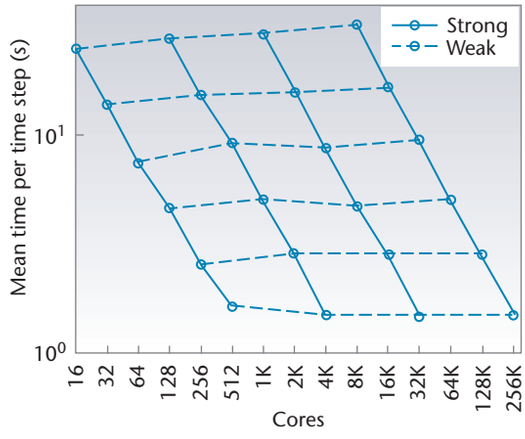

Figure 5. Strong and weak scaling of an MPMICE problem with a steel container traveling at Mach-2 through ideal gas.[27] We used adaptive mesh refinement.

what critical densities could cause a sustained reaction.

The WSB reaction model was used to determine if the hot spots could sustain a reaction.[17] The simple temperature threshold used in the original formulation[19] was incorrect at the time- and length-scales of the mesoscale simulation, necessitating the use of an Arrhenius-based adiabatic induction time model. The model is able to capture the time to rapid reaction based on the local temperature in the material. We applied this model to impacts of approximately 100 and 700 m/s. An insufficient number of hot spots were formed in the low-velocity impact, and the reaction was ultimately quenched. At the high-velocity impact, the material temperature rises immediately, and a sustained reaction is formed as one pore is collapsed (see Figure 6d). The reaction then propagated through the bed. These results are qualitatively in agreement with experiments. Further investigation is needed to see if the model is able to capture hot-spot criticality for the initiation of rapid reaction that was seen to be somewhere in the range of 400–500 m/s for the scenario studied.

It's unlikely that idealized mesoscale geometries will result in the same hot-spot distributions and the same ignition behavior as real explosives. X-ray microtomography has been used to determine mesoscale morphology for a mock explosive, as seen in Figure 6a. Analysis of this mesostructure gave grain-sized distributions in good agreement with formulation measurements. Fractured bits, as well as conglomerates (see Figure 6b) created during formulation, were also identified. Using these same morphological tools, hot-spot size and shape distributions were quantified. An example calculation, with hot spots depicted in magenta, may be seen in Figure 6b. It was found that different mock materials had substantially different grain and simulated hot-spot morphologies.

We're in the process of studying the critical-impact velocity that our model predicts, and the associated hot-spot distributions from our idealized simulations. Looking further, we plan to use full 3D simulations of the real microstructures to either validate or refute the utility of the ideal simulations. The knowledge learned from these simulations will then be used to develop subgrid scale models that are applicable on the millimeter-length scale to validate our current work on truck-sized explosions (see Figure 6e).

Macroscale Explosions

The exact mechanism of DDT is still being investigated, but numerical analysis has shown that this transition takes place when the local pressure exceeds a threshold of 5.3 gigapascals (GPa) for the explosive PBX9501. What's interesting about this pressure is that under adiabatic conditions, the deflagration of PBX9501 will produce pressures around 2 GPa—far below what's required for detonation. To investigate the possible mechanism, we ran small-scale (a few millimeters) simulations of confined PBX9501. In these simulations the explosive was enclosed in a steel shell and heated externally. We discovered that the collision of two pressure waves yielded the pressures needed for detonation (see Figure 7).[30] By analyzing the interference of the waves over a range of device sizes and applied heat fluxes, a trend was discovered. Depending upon the applied heat flux, the convective deflagration traversed the explosives at different rates, producing pressure waves. Depending upon the heating rate, the origins of the pressure waves and the resulting interference pattern varied.

In a separate series of simulations, we looked at the crack propagation and the resultant flame-propagation velocities, and qualitatively compared them with experiments.[31] In these tests, a hot wire ignited a disk of explosives in the center and high-speed photography captured the crack and flame-propagation velocities and patterns (see Figure 8). These results are an important step towards simulating explosions at the semi-truck scale, and show the utility of subgrid-scale statistical models for material damage and crack propagation in macroscale simulations.

The ultimate goal of our research is to assess the safety of transporting arrays of explosives. Specifically, we're interested in the 2005 transportation accident described in the motivation section, since a detonation should not have occurred. Our macroscale simulations involve homogeneous solid materials to

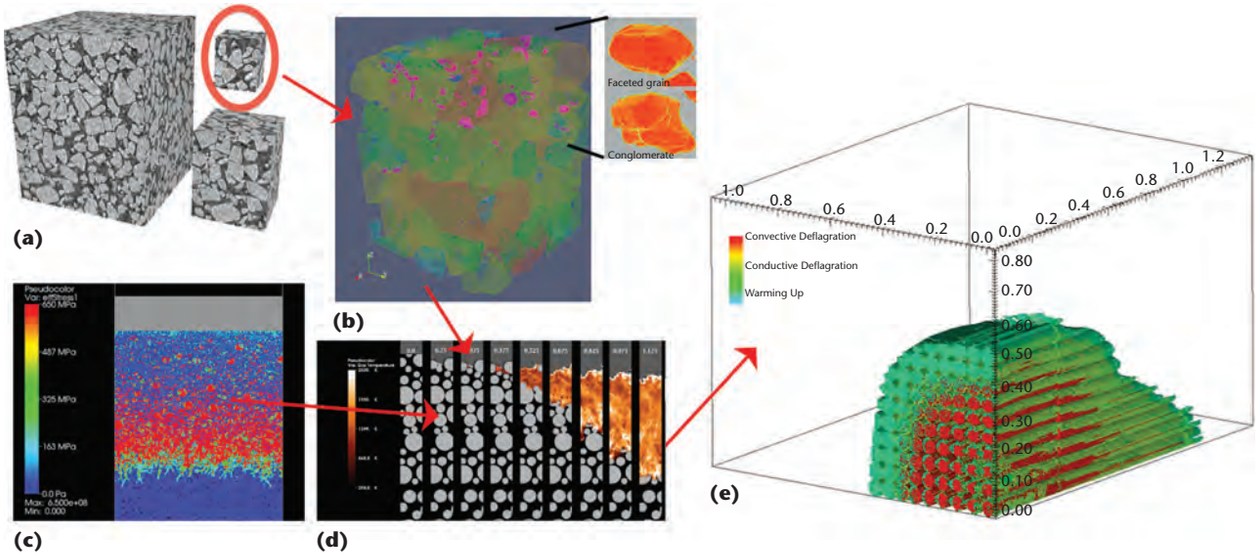

Figure 6. A schematic of how mesoscale simulations can be used to inform macroscale simulations. (a, b) Real microstructures can be included in shock studies and hot-spot distributions can be quantified. At the same time, idealized microstructures can be used to study many different initial setups and (c, d) the resulting reactions. Real microstructure simulations can be used to validate the idealized microstructures when possible, which will provide some certainty of the validity of the idealized simulations. From the many-varied simulation setups for the idealized simulations, statistics can be extracted regarding hot-spot distributions, average reaction rates, and time to reaction as a function of some metric such as the average stress rate. These can then be formulated as subgrid scale models that are used in macroscale simulations, such as those damage and cracking materials we already use. (e) The deflagration on the macroscale of explosive cylinders using the reaction models validated on the mesoscale. In this simulation, deflagration and convective burning can propagate as far as 0.5 m or more prior to detonation. (MPa = megapascal.)

represent the PBX9501 grains and binder. With validation from mesoscale simulations and experimental data, we developed reaction models for deflagration and detonation that are helping us understand the underlying mechanism of DDT. To keep the computational costs reasonable, the reaction models rely on a global kinetics model, with the understanding that reactants go to products at a known energy release.

In the 2005 accident, explosive cylinders were packaged in boxes containing approximately 20 cylindrical boosters, 5.7 cm in diameter, ranging from 33–74 cm in length. Our simulations are being used to investigate if inertial confinement was a significant contributor to the DDT, considering how the explosives were packed in the semi-truck. Determining the level of confinement needed for DDT is computationally expensive, requiring machines like Titan. Through our simulation, we hope to understand how pressures can reach the necessary threshold and produce an extremely violent detonation reaction. We hypothesize that the individual boosters reacted and the pressure forces deformed the nearby unreacted boosters, creating "pores" or regions where the product gases were trapped. Pressure or stress waves propagated outward from the "pores" and collided, forming regions of high pressure, sufficient for a DDT.

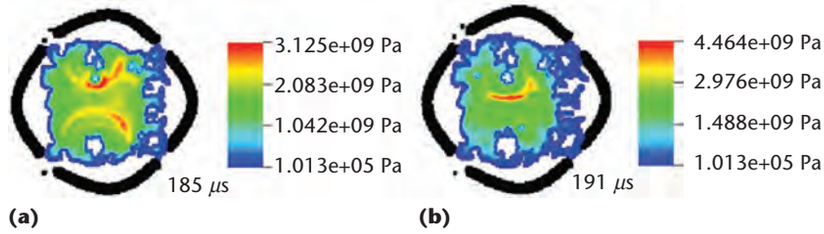

Figure 7. A simulation of a square explosive device heated on one side. As the material decomposes, the pressure increases, deforming the steel case (shown in black) until it ruptures. Pockets of hot combustion gas cause stress waves to propagate out from those points. These waves can collide, forming a high-pressure region that initiates a detonation. (Pa = pascal; μs= microseconds.)

Figure 9 shows results from our initial effort. In the simulation, we used realistic booster geometries ignited by hot gas (in the lower left corner of each graph), with burning propagating outward. These preliminary results suggest that inertial confinement can lead to a DDT. These results are preliminary, and we used artificial wall boundaries in the x, y, and z directions. This research is ongoing, and we're looking

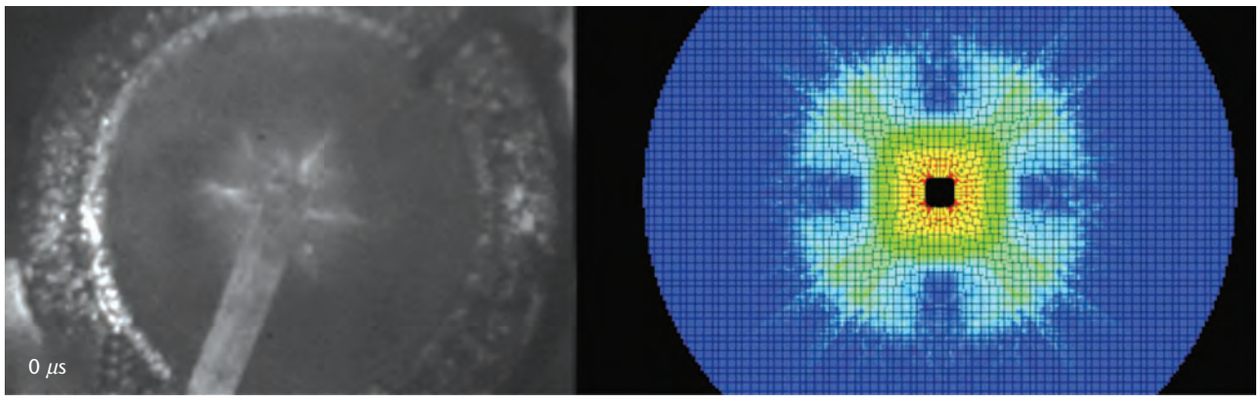

Figure 8. Comparison of an experiment with a simulation. A one-inch hockey puck-shaped disk is heated to just under the ignition point of the material, approximately 200° C, and then ignited via a wire in the center. In the experiment shown on the left, cracks can be seen to form as the reaction stresses the material, and convective burning spreads through the cracks, which is seen as regions of high illumination.[31] The simulation at the same physical time shows considerably more cracking, but the general structures appear to be similar. The subgrid scale cracking/damage model we use, as well as the convective burning model, result in similar reaction characteristics. The plots shown are used with permission.[31]

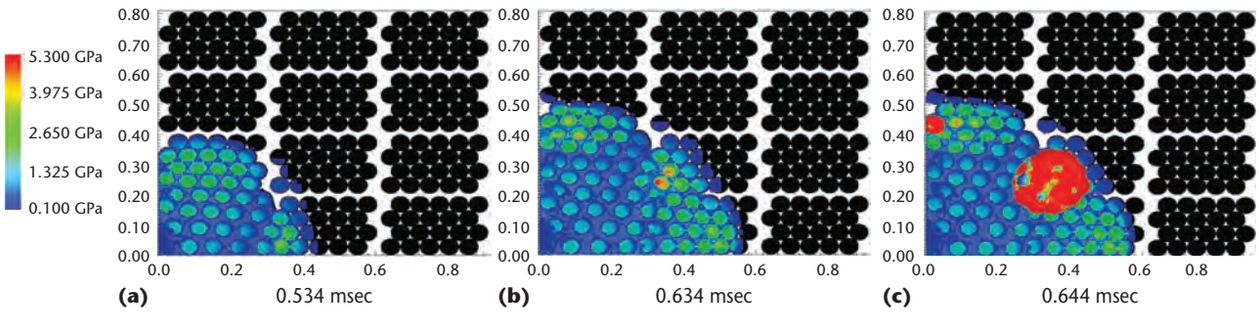

Figure 9. Pressure profile of a DDT in an array of tightly packed explosive cylinders confined by symmetric boundaries on all sides: (a) at 0.534 milliseconds (msec), (b) at 0.634 msec, and (c) at 0.644 msec. Realistic booster geometries were used. Thermally activated deflagration occurred in the lower left corner. This simulation suggests inertial confinement can be reached with six cases of tightly packaged explosives, as seen by detonation (in red) occurring before the pressure wave hits a symmetric boundary.

at how the explosive boosters interact without wall boundaries. These simulations are being run on Oak Ridge's Titan machine.

With a strong understanding of the inertial confinement needed for DDT to occur in an array of explosives, considerations will be made on the proper packing configuration needed to prevent large transportation accidents. The main goal is to reduce the possibility of the pressure building to the detonation threshold, diminishing the risk of a detonation transition.

Our approach to preventing a DDT in truck-size shipments of explosives is to simulate the effect of packing arrangements that can avoid inertial confinement and rapid pressurization that causes the DDT. Considerations will be made for a variety of "what-if" local packing geometries (for example, a 3D checkerboard with alternating empty containers) as well as more global arrangements (large open areas in the center of the load) to maximize the mitigation effect on explosion violence without compromising the load's structural integrity.

The capability of modeling explosive devices on a wide range of temporal and spatial scales will give great insight into the many chemical and physical processes involved with explosives. Although a great deal of our focus is on the DDT, the Uintah Computational Framework has the capability of one day modeling all aspects of explosives and similar substances.

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References

1. S.A. Survey, *Unplanned Explosions at Munitions Sites*, tech. report, Small Arms Survey, Mar. 2013.
2. T.C. Henderson et al., "Simulating Accidental Fires and Explosions," *Computing in Science & Eng.*, vol. 2, no. 2, 2000, pp. 64–76.
3. M. Berzins, *Status of Release of the Uintah Computational Framework*, tech. report UUSCI-2012-001, *Scientific Computing and Imaging (SCI) Inst.*, Univ. Utah, 2012.
4. B.A. Kashiwa, *A Multifield Model and Method for Fluid-Structure Interaction Dynamics*, tech. report LA-UR-01-1136, Los Alamos Nat'l Laboratory, 2001.
5. B.A. Kashiwa et al., *A Cell-Centered ICE Method for Multiphase Flow Simulations*, tech. report LA-UR-93-3922, Los Alamos Nat'l Laboratory, 1994.
6. D. Sulsky, S. Zhou, and H.L. Schreyer, "Application of a Particle-in-Cell Method to Solid Mechanics," *Computer Physics Comm.*, vol. 87, nos. 1–2, 1995, pp. 236–252.
7. J.E. Guilkey, T.B. Harman, and B. Banerjee, "An Eulerian-Lagrangian Approach for Simulating Explosions of Energetic Devices," *Computers and Structures*, vol. 85, nos. 11–14, 2007, pp. 660–674.
8. J. Spinti et al., "Heat Transfer to Objects in Pool Fires," *Transport Phenomena in Fires*, WIT Press, 2008.
9. J. Luitjens and M. Berzins, "Improving the Performance of Uintah: A Large-Scale Adaptive Meshing Computational Framework," *Proc. 24th IEEE Int'l Parallel and Distributed Processing Symp.*, IEEE, 2010; http://ieeexplore.ieee.org/xpl/abstractKeywords.jsp?reload=true&arnumber=5470437.
10. J.U. Brackbill and H.M. Ruppel, "FLIP: A Method for Adaptively Zoned, Particle-in-Cell Calculations of Fluid Flows in Two Dimensions," *J. Computational Physics*, vol. 65, no. 2, 1986, pp. 314–343.
11. S.G. Bardenhagen, "Energy Conservation Error in the Material Point Method for Solid Mechanics," *J. Computational Physics*, vol. 180, no. 1, 2002, pp. 383–403.
12. M. Steffen, R. M. Kirby, and M. Berzins, "Decoupling and Balancing of Space and Time Errors in the Material Point Method (MPM)," *Int'l J. for Numerical Methods in Eng.*, vol. 82, no. 10, 2010, pp. 1207–1243.
13. S.G. Bardenhagen, J.U. Brackbill, and D. Sulsky, "Numerical Study of Stress Distribution in Sheared Granular Material in Two Dimensions, *Physical Review E*, vol. 62, 2000, pp. 3882–3890.
14. A.D. Brydon et al., "Simulation of the Densification of Real Open-Celled Foam Microstructures," *J. Mechanics and Physics of Solids*, vol. 53, no. 12, 2005, pp. 2638–2660.
15. S.G. Bardenhagen, J.A. Nairn, and H. Lu, "Simulation of Dynamic Fracture with the Material Point Method Using a Mixed J-Integral and Cohesive Law Approach," *Int'l J. Fracture*, vol. 170, no. 1, 2011, pp. 49–66.
16. J.R. Peterson and C.A. Wight, "An Eulerian-Lagrangian Computational Model for Deflagration and Detonation of High Explosives," *J. Combustion and Flame*, vol. 159, no. 7, 2012, pp. 2491–2499.
17. M.J. Ward, S.F. Son, and M.Q. Brewster, "Steady Deflagration of HMX with Simple Kinetics: A Gas Phase Chain Reaction Model," *Combustion and Flame*, vol. 114, nos. 3–4, 1998, pp. 556–568.
18. A.I. Atwood et al., "Burning Rate of Solid Propellant Ingredients, Part 1: Pressure and Initial Temperature Effects," *J. Propulsion and Power*, vol. 15, no. 6, 1999, pp. 740–747.
19. C.A. Wight and E.G. Eddings, "Science-Based Simulation Tools for Hazard Assessment and Mitigation," *Advancements in Energetic Materials and Chemical Propulsion*, vol. 114, no. 5, 2008, pp. 921–937.
20. C.M. Tarver and S.K. Chidester, "On the Violence of High Explosive Reactions," *J. Pressure Vessel Technology*, vol. 127, no. 1, 2005, pp. 39–48.
21. P.C. Souers et al., "JWL++: A Simple Reactive Flow Code Package for Detonation," *Propellants, Explosives, Pyrotechnics*, vol. 25, no. 2, 2000, pp. 54–58.
22. H.L. Berghout et al., "Combustion of Damaged PBX9501 Explosive," *Thermochimica Acta*, vol. 384, nos. 1–2, 2002, pp. 261–277.
23. S.G. Parker, J. Guilkey, and T. Harman, "A Component-Based Parallel Infrastructure for the Simulation of Fluid Structure Interaction," *Eng. with Computers*, vol. 22, nos. 3–4, 2006, pp. 277–292.
24. J. Luitjens and M. Berzins, "Scalable Parallel Regridding Algorithms for Block-Structured Adaptive Mesh Refinement," *J. Concurrency and Computation: Practice and Experience*, vol. 23, no. 13, 2011, pp. 1522–1537.
25. M. Berzins et al., "Uintah: A Scalable Framework for Hazard Analysis," *Proc. Teragrid 2010*, ACM, 2010; doi:10.1145/1838574.1838577.
26. Q. Meng, M. Berzins, and J. Schmidt, "Using Hybrid Parallelism to Improve Memory Use in the Uintah Framework," *Proc. Teragrid 2011*, ACM, 2011 doi:10.1145/2016741.2016767.

27. Q. Meng and M. Berzins, *Scalable Large-Scale Fluid-Structure Interaction Solvers in the Uintah Framework via Hybrid Task-based Parallelism Algorithms*, tech. report UUSCI-2012-004, SCI Inst., Univ. of Utah, 2012.
28. R.W. Armstrong, S.G. Bardenhagen, and W.L. Elban, "Deformation-Induced Hot Spot Consequences of AP and RDX Crystal Hardness Measurements," *J. Energetic Materials and Chemical Propulsion*, vol. 11, no. 5, 2012, pp. 413–425.
29. J.R. Peterson et al., "Multiscale Modeling of High Explosives for Transportation Accidents," *Proc. 2012 XSEDE Conf.*, ACM, 2012; http://doi.acm.org/10.1145/2335755.2335828.
30. M. Hall et al., "The Influence of an Applied Heat Flux on the Violence of Reaction of an Explosive Device," *Proc. 2013 XSEDE Conf.*, ACM, to be published, 2013.
31. P.M. Dickson et al., "Thermal Cook-Off Response of Confined PBX 9501," *The Royal Society A*, vol. 460, no. 2052, 2004, pp. 3447–3455.

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