Multiscale Modeling of Accidental Explosions and Detonations

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Accidental explosions are exceptionally dangerous and costly, both in lives and money. Regarding world-wide conflict with small arms and light weapons, the Small Arms Survey has recorded over 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 [45]. As the recent fertilizer plant explosion that killed 15 people in West, Texas demonstrates, accidental explosions are not 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 PEPCON disaster in 1988, where windows were shattered, doors 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 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 which occur on micrometer scales. Whether this reaction remains a deflagration (burning) or builds to a detonation depends both on the stimulus and the 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, i.e. the unintended detonation of one entity by the explosion of another, generally caused by an explosive shock wave or blast fragments.

While experimental work has been and will continue to be critical to developing our fundamental understanding of explosive initiation, deflagration and detonation, there is 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 "macro-scale", have been contributing increasingly to our understanding of these materials. Still, simulations on this scale require both massively parallel computational infrastructure and selective sampling of mesoscale response, i.e. advanced computational tools and modeling. The computational framework Uintah [1] has been developed for exactly this purpose.

Motivation

In 2005 a truck carrying 16,000 kg of seismic boosters, driving through Spanish Fork Canyon, Utah took a corner too quickly and over-turned. The semi-truck caught fire and within three minutes detonated creating a crater in the road approximately 24 m wide and 10 m deep (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 size of the crater and the lack of any unexploded boosters suggests 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 is 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 in order to provide predictive simulations.

Since 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 size of the crater (Figure 1) is characteristic of a detonation. The mechanism of a DDT in solids is still unknown but various mechanisms have been proposed. One 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 is reminiscent of a porous material rather than a monolithic solid. We suspect that the convective burning mechanism is 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 will 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 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 during the slow deflagration and very rapid detonation regimes. As deflagration is occurring 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 macro-scale due to averaging, necessitating the use of statistically based, sub-grid scale models. Mesoscale modeling has the potential to provide statistics needed for sub-grid models that live on the discrete elements of the simulation domain. Mesoscale simulations are computationally expensive, requiring sophisticated material models capable of capturing 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, and will be discussed later.
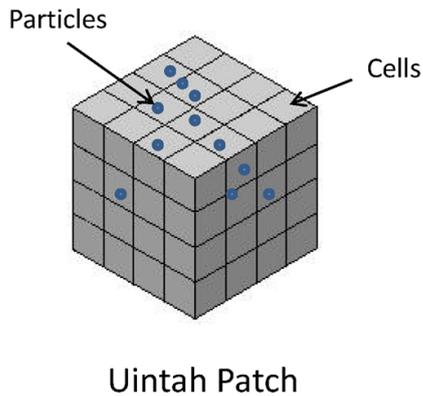
Figure 2: *Uintah Mesh with Particles.*

Uintah Computational Framework

The open source (MIT License) Uintah software originated in the University of Utah DOE Center for the Simulation of Accidental Fires and Explosions (C-SAFE) [22], 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 [10]. Uintah is a computational framework that integrates multiple simulation components, analyzes the data dependencies and communication patterns between them and efficiently executes the resulting multi-physics simulation. Uintah presently contains four main simulation components or algorithms: 1) the finite volume mulit-material CFD formulation (ICE) [23, 24, 25, 26], 2) the Material Point Method (MPM) [44] for structural mechanics, 3) the combined fluid-structure interaction (FSI) algorithm MPMICE [21, 17, 18] and 4) the ARCHES turbulent reacting Large Eddy CFD component [42, 40]. Uintah exhibits good scalability characteristics [27, 12], runs on both NSF and DOE parallel computers (Stampede, Kraken, Titan, Lonestar, Vesta, etc.) and is used by many NNSA, DOD, DOE and NSF projects.

The main Uintah component used in this research is the MPMICE in which the multi-material CFD formulation (ICE) is used to model fluids and the Material Point Method (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 does not have to worry about parallelism and communications between patches as this is all au-

tomatically 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 fluid-structure interactions at different length- and times-scales. These embedded models live inside a framework that hides the parallelization of the method, allowing simple science or engineering models to scale to hundreds of thousands of processors.

Fluid-Structure Interactions

Our methodology for solving fluid-structure-interactions 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 [25, 24, 23, 26] 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 [44] is used that is capable of simulating complex behaviors including material damage, stress and strain, and elastic and plastic responses.

The algorithm has its foundation in a "multi-material" 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 does not exist. In addition to the physical state (i.e., mass, momentum, 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 [24, 25].

To solve the discretized multi-material equations we use a cell-centered formulation of the ICE method of Harlow [20], further developed by Kashiwa and others at Los Alamos National Laboratory [24, 26]. 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 multi-material equations also include exchange terms for mass, momentum and heat. Inter-material 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 rela-

tive material velocities or temperatures, respectively, computed in a point-wise implicit manner to ensure conservation.

This formulation makes no explicit distinction between the fluid and solid materials in the model equations. Fluid-solid interfaces are not 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 [44] is an extension to solid mechanics of FLIP [13], which is a particle-in-cell method for fluid flow simulations. Development of the MPM has continued, both studying and improving the MPM algorithm [4, 47, 43], as well as extending the technique by generalizing particle shapes [5, 39]. 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 [5], large deformations [34] and fracture [7], to name a few.

Lagrangian particles or material points are used to discretize the volume of a material, each particle carries state information (e.g. 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 (velocity, mass etc) are defined on a mesh, 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 the particles moved by mapping velocities back to particles.

The combination of MPM and the multi-material CFD algorithm to form our fluid-structure interactions algorithm (MPMICE) involves a complex 14 step algorithm described in [17, 18, 21]. What makes this methodology unique is: 1) that the exchange of mass, momentum and energy between the solid reactant and product gases occurs in the governing equations, and 2) that boundary conditions are not applied to surfaces that are tracked. Clearly, surface tracking in these types of simulations would be difficult.

Deflagration and Detonation Models

Our reaction models convert mass from the energetic materials (e.g., 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, deflagration-to-detonation transition (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 [38].

The numerical model for deflagration is based on a two-step global kinetics model described by Ward, Son and Brewster (WSB) [48]. As originally formulated, this model predicts the steady combustion rate of the energetics as a function of pressure of the product gas and the temperature of the solid material. We extended the 1-D WSB model to 3-D and validated the parameters against the experimental strand burner measurements of Atwood et al. for the correct temperature and pressure dependence of the burn rate [3, 49]. 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++ [41] 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 object 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 a ~ 0.15 m radius, hockey-puck shaped explosive is impacted at increasing speeds. A sharp speed threshold was observed in impact under about 75 m/s 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 occurred while "1" indicates a high explosive violent reaction event was seen.

The general approach for simulating the DDT process relies on the idea that high pressure forces hot gases through the voids (pores, cracks, etc.) in an
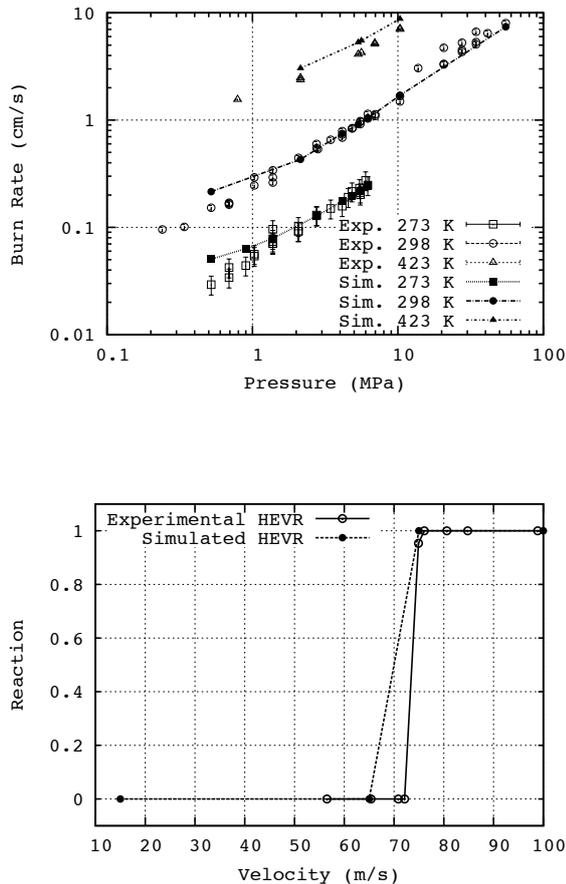
Figure 3: *DDT reaction model results compared with experimental results. The top plot shows the burn rate at three initial solid temperatures verse pressure where simulated data is compared against data from Atwood et al. for the explosive PBX9501 [3]. The bottom image shows comparison of threshold for reaction against velocity for weak impacts [46]. Plots used with permission from [38].*

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 are able to model deflagration-to-detonation transitions in solid materials.

Our DDT model agreed well with experimental data for the pressure and temperature dependence of the burn rate and detonation velocities, including convective deflagration propagation (Figure 3). Con-

vective deflagration, is the process of burning within the cracks of the energetic solid, rapidly increasing the reaction rates and pressure. Without convective deflagration, DDT would not occur in an unconfined explosive, because deflagration would only occur on the surface of the solid. We are able to model convective deflagration by using a crack model which describes the crack development as a function of pressure [9, 8]. With this model we are able to represent the damage of a material, 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, or 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 very 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 256K 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 task's data dependencies. An example of a high level Uintah taskgraph for the MPM is shown in Figure 4.

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 [36, 1]. In the second phase the data structures were greatly improved and fast mesh refinement algorithms were developed to scale to 100K cores [28, 11, 32, 27, 29]. In this phase tasks were executed in a dynamic or even out-of-order way. Finally, in the third and current phase we are moving to a hybrid MPI-Pthread model in which there is 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
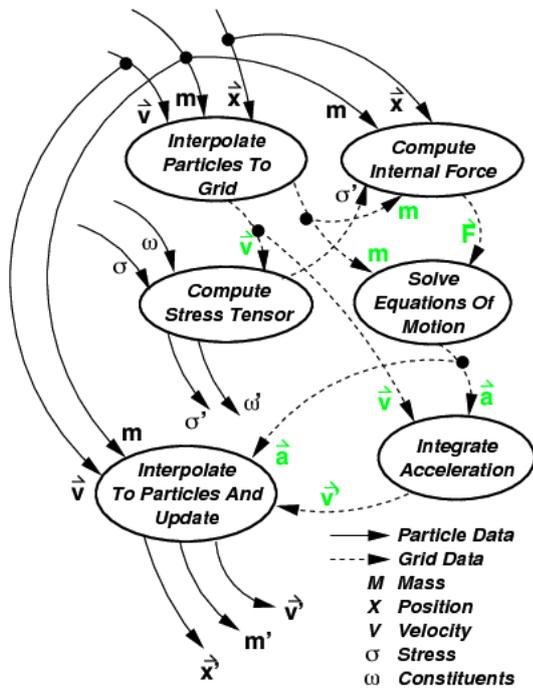
Figure 4: *An example of a Uintah Task Graph for the Material Point Method.*

Figure 5: *Strong and weak scaling of a MPMICE problem with a steel container traveling at Mach-2 through ideal gas [30]. Adaptive mesh refinement was used.*

when available. This approach reduces the total global memory usage per node by up to 90% on the Jaguar XT5 system [31]. Using a recently designed de-centralized multi-threaded 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 [30].

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 [30]. The performance was tested with four problem sizes with each problem containing approximately eight times as many cells as the previous problem. The number 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 macro-scale simulations up to 256K cores on the then Jaguar XK6, now Titan, architecture at DOEs Oak Ridge Laboratory [30].

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 macro-scale. 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, i.e. the explosive grains. There are many possible hot spot mechanisms [16, 2, 33] and it is 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 macro-scale simulations to resolve hot spot distributions and predict ignition in areas of interest. These simulations bridge the gap between molecular and macro-scale 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 (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 seen in Figure 6(c). These hot-spots may either dissipate their energy to colder surrounding material, or may coalesce and cause a sustained reaction, depending on their size, intensity and number density [6, 35].
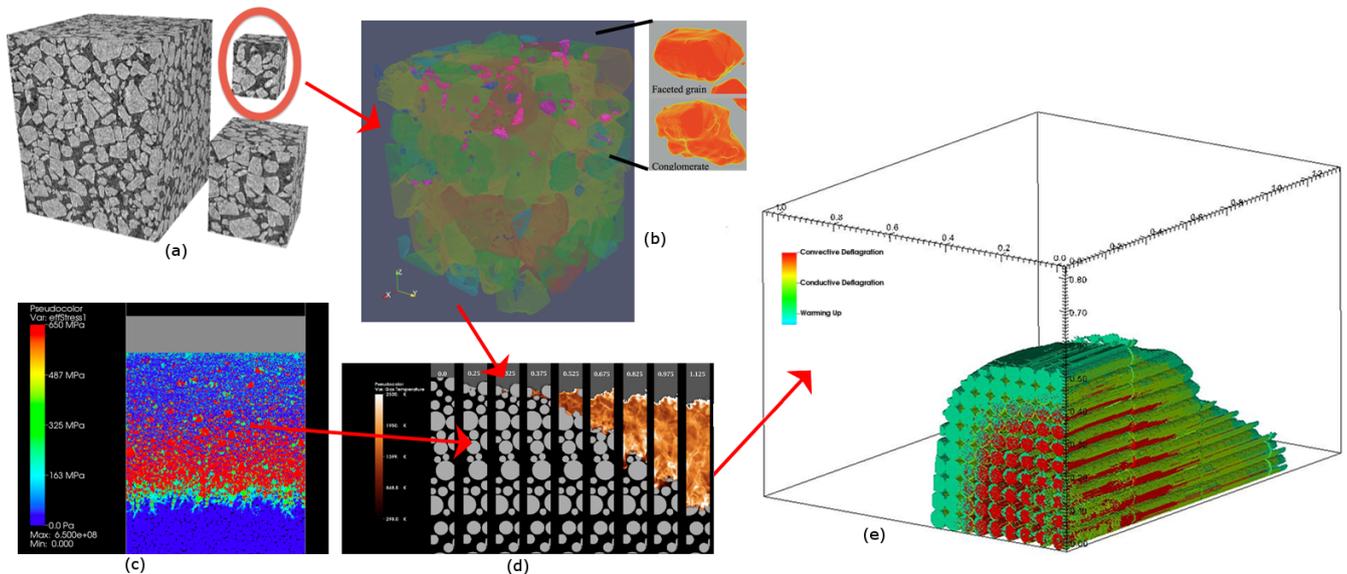
Figure 6: *A schematic of how mesoscale simulations can be used to inform macro-scale simulations. Images (a) and (b) show how real microstructures can be included in shock studies and hot-spot distributions can be quantified. At the same time, idealized microstructures can be used to study many different initial setups and the resulting reactions shown by images (c) and (d). 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 average stress rate. These can then be formulated as sub-grid scale models that are used in macro-scale simulations, such as those damage and cracking materials we already use. Image (e) shows the deflagration on the macro-scale 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.*

Initially our studies utilized idealized geometries of the explosive grains that were impacted by a piston at varying speeds and compared against experimental results [37]. These studies were designed to validate our material model which includes the elastic and plastic response as well as temperature varrying 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% [37]. With this agreement, we sought to study hot-spot distributions to find what critical densities could cause a sustained reaction.

The WSB reaction model was used to determine if the hot-spots could sustain a reaction [48]. The simple temperature threshold used in the original formulation [49] was not correct 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 (Figure 6(d)). 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 is 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 6(a). Analysis of this mesostructure gave grain size distributions in good agreement with formulation measurements [6]. Fractured bits, as well as conglomerates (as seen in Figure 6(b)), 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

6(b). It was found that different mock materials had substantially different grain and simulated hot spot morphologies.

We are 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 3-D simulations of the real microstructures in order to either validate or refute the utility of the ideal simulations. The knowledge learned from these simulations will then be used to develop sub-grid scale models that are applicable on the millimeter length scale to validate our current work on the truck sized explosions (Figure 6(e)).

Macro-scale 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 GPa for the explosive PBX9501. What is interesting about this pressure is that under adiabatic conditions the deflagration of PBX9501 will produce pressures around 2 GPa, far below what is required for detonation. To investigate the possible mechanism we ran small scale (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 pressures needed for detonation [19] (Figure 7). 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 [15]. 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 (Figure 8). These results are an important step towards simulating explosions at the semi-truck scale and show the utility of sub-grid scale statistical models for material damage and crack propagation in macro-scale simulation.

The ultimate goal of our research is to assess the safety of transporting arrays of explosives. Specifically we are interested in the 2005 transportation
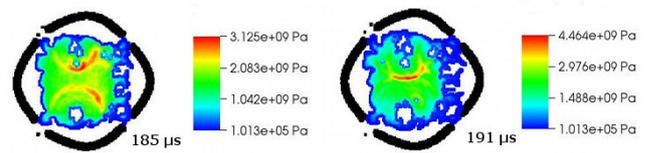
Figure 7: *A simulation of a square explosive device heated on one side. As the material decomposes, the pressure increases, deforming the steel case (shown in black) until it ruptures. Pockets of hot combustion gas cause stress waves to propagate out from those points. These waves can collide forming a high pressure region that initiates a detonation.*

accident described in the motivation section, since a detonation should not have occurred. Our macroscale simulations involve homogeneous solid materials to represent the PBX9501 grains and binder. With validation from mesoscale simulations and experimental data we have 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 ~ 20 cylindrical boosters, 5.7 cm in diameter ranging from 33 to 74 cm in length. Our simulations are being used to investigate if inertial confinement, how the explosives were packed in the semi-truck, was a significant contributor to the DDT. Determining the level of confinement needed for deflagration to detonation transitions 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 un-reacted boosters creating "pores" or regions where the product gases were trapped. Pressure or stress waves propagated outward from the "pores" and collied forming regions of high pressure, sufficient for a DDT.

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 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. The research is ongoing and we are looking at how the
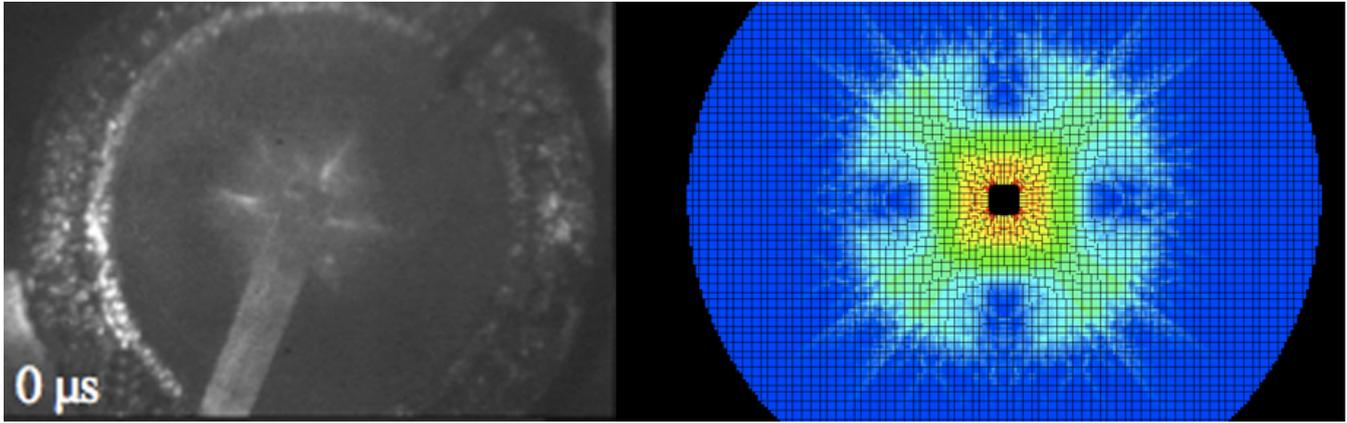
Figure 8: *Comparison of an experiment with a simulation. A one inch hockey-puck shaped disk is heated to just under the ignition point of the material, approximately 200° C, and then ignited via a wire in the center. In the experiment shown on the left, cracks can be seen to form as the reaction stresses the material, and convective burning spreads through the cracks, which is seen as regions of high illumination [15]. The simulation at the same physical time shows considerably more cracking, but the general structures appear to be similar. The sub-grid scale cracking/damage model we use, as well as the convective burning model result in similar reaction characteristics. Plots used with permission from [15].*
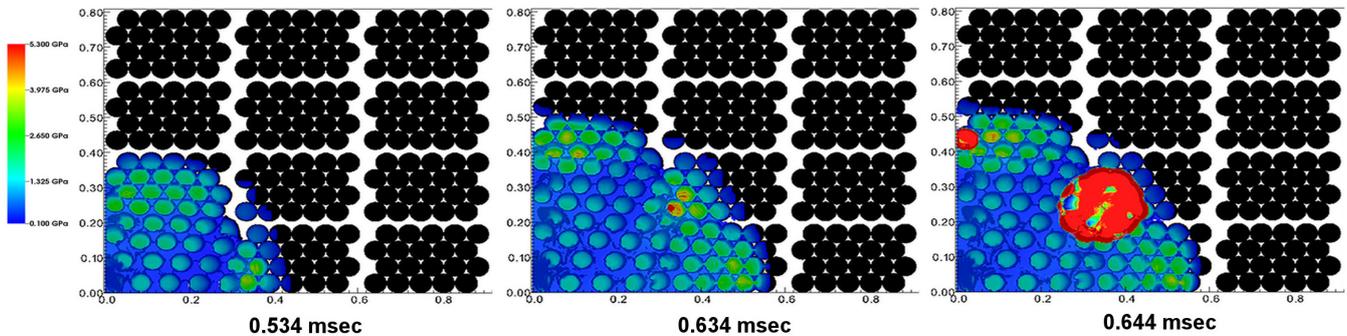
Figure 9: *Pressure profile of a Deflagration-to-Detonation Transition in an array of tightly packed explosive cylinders confined by symmetric boundaries on all sides. Realistic booster geometries were used. Thermally activated deflagration occurred in lower left corner. This simulation suggests inertial confinement can be reached with 6 cases of tightly packaged explosives as seen by detonation (in red) occurring before the pressure wave hits a symmetric boundary.*

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

Future Work

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 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 DDT. Considerations will be made for a variety of "what-if" local packing geometries (e.g., 3-D 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 structural integrity of the load.

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. Though a great deal of our focus is on the deflagration to detonation transition, the Uintah computational framework has the capability of one day modeling all aspects of

explosives and similar substances.

Acknowledgments

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