Multiscale Modeling of High Explosives for Transportation Accidents

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ABSTRACT

The development of a reaction model to simulate the accidental detonation of a large array of seismic boosters in a semi-truck subject to fire is considered. To test this model large scale simulations of explosions and detonations were performed by leveraging the massively parallel capabilities of the Uintah Computational Framework and the XSEDE computational resources. Computed stress profiles in bulk-scale explosive materials were validated using compaction simulations of hundred micron scale particles and found to compare favorably with experimental data. A validation study of reaction models for deflagration and detonation showed that computational grid cell sizes up to 10 mm could be used without loss of fidelity. The Uintah Computational Framework shows linear scaling up to 180K cores which combined with coarse resolution and validated models will now enable simulations of semi-truck scale transportation accidents for the first time.

Keywords

Deflagration, detonation, parallel multi-scale modeling, granular compaction

1. INTRODUCTION

Analyzing risks involved with transporting and storing solid phase propellants, explosives and pyrotechnics involves understanding reactive behaviors of the materials used in the device. In such analyses, the ability to model the underlying physics of rapid reaction scenarios over large spatial and temporal scales is paramount. Motivation for this work is the 2005 incident in Utah's Spanish Fork Canyon, where a truck containing seismic booster explosives overturned, caught fire and unexpectedly detonated with violence attributed to "sympathetic" reaction of multiple explosive devices reacting in tandem [11]. A number of milestones towards predictive solution on the length scales of interest have been achieved. The scale of the problem is sufficiently large that utilizing supercomputing resources is essential to capture the physical behavior of the array of explosives. The Uintah Computational Framework [15] provides the means to both model and compute the simulation scenario on supercomputers [28, 26]. Both modeling techniques and computing resources are sufficiently mature to address tens-of-meter-scale simulations of explosions.

An energetic material model capable of accurately predicting the physics of a reaction over time scales from microseconds to minutes is desirable. Previous research in the field of granular compaction of the explosive octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) beds has led to the development of several bulk-scale analytical models that are able to predict the qualitative behavior of compaction and the resulting reaction [4, 16]. These modeling efforts have examined the behavior of materials with varying porosity, particularly noting that large differences between bulk averaged quantities of interest and micro-scale heterogeneities. This is especially relevant for temperature, which drives the decomposition of solid reactants leading to deflagration-to-detonation transition (DDT) in granular, porous, and/or damaged explosives, or shock-to-detonation transition (SDT) in solid and plastic bonded explosives (PBX). In DDT and SDT the transient energetic extremes are attributed to frictional heating, plastic flow, crystal fracture [1] and grain/binder de-bonding [35], which create hot-spots that act as nucleation sites for reaction. When enough hot-spots are formed, a self-sustaining combustion occurs that can cause a DDT or SDT. These events are extremely dangerous and damaging. A number of works in this field have highlighted the need for mesoscale simulations (micrometer scale) for the validation of bulk scale models [29, 7, 17, 3]. A conclusion from these studies is that mesoscale simulations are useful not only for validation, but also in inspirirng physically based bulk models. Mesoscale simulations of compaction have been used to validate the burning behavior of a model [32] for bulk

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reactions over the range of deflagration and detonation phenomena.

Validation is necessary as the predictability of many bulk-scale models is subject to large uncertainty associated with the applied boundary conditions, limiting the applicability of the model to conditions used for calibration. In many cases these models are limited by the range over which the reaction equations have been calibrated. This brings into question whether the model can accurately capture the physics outside this calibration range. Thus as models are extended beyond their calibration regions, careful consideration must be taken in analyzing the physical results on that temporal and spatial scale, to understand the effect on the primary metric of interest. In addition, the levels of uncertainty in the model must be addressed at a given scale in order to have confident analysis of results and observations.

Section 2 describes, very generally, the approach taken in simulating these multi-scale problems. Sections 3-5 describe modeling advancements that enable large-scale simulation of the energetic arrays found in the Spanish Fork accident. Section 6 concludes with a discussion of the current outlook of large scale accident simulations along with recommendations for further study.

2. SIMULATION METHODOLOGY

All simulations made use of a fluid-structure interaction algorithm, based on the combination of the particle-based Material Point Method (MPM) and the cell-based Implicit Continuous Eulerian (ICE) compressible multi-material CFD, known as MPMICE [21, 19]. The ICE algorithm, originally formulated by Kashiwa et al. at LANL [24, 22, 23], is capable of simulating flow scenarios with any number of materials in the compressible or incompressible regime while conserving mass, momentum and energy. ICE is necessary for solving the complex flow behavior of combustion gas interactions in surface flames, convective flames and high-density detonation product gas expansion. MPM is a Lagrangian method based on the particle-in-cell method from LANL, first described by Sulsky, et al. [37, 5, 6]. MPM excels in modeling of solid material mechanics, including large deformations [5], complex geometries [12], fracture [25], material contact [6] and even biological constructs [20]. MPMICE leverages the strengths of both methods to solve high deformation rate fluid-structure interactions (the flow field, deformation of the solid, etc.) [18]. The use of MPMICE allows simulations of flow, deformation and fluid-solid interactions at micro- to deka-meter length scales.

Simulations were performed in one, two or three dimensions. Adaptive mesh refinement was used when parts of the domain where relatively dormant to reduce computational cost. A recently developed decentralized scheduling model including on-node threading and intra-node message-passing-interface (MPI) communications was used to achieve appropriate utilization of XSEDE resources [28, 27]. Typical three dimensional problems utilized between 512 and 49,152 cores for the validation and production simulations. The largest influence on solution accuracy, aside from the particular material models used, was the grid resolution for ICE and number of particles for MPM. All validation simulations for both micro-scale compaction and bulk-scale compaction were examined for convergence. An extension of the various models to coarser resolutions was performed with a relative error bound between 5% and 10% compared with converged resolution. The limits for which the models can perform under this error bound were identified for the metric of interest (detonation velocity, burn rate, etc.) in the particular simulation.

3. MESOSCALE COMPACTION SIMULATIONS

A number of shock impact experiments on granular explosive beds have been reported [33]. The experiments consisted of a column of explosive granules packed to different extents of porosity. These granular beds are then impacted at several hundred meters per second and investigated with stress and velocity gauges at the top and bottom of the column. Experiments provided validation data for bulk scale reaction and sub-grid-scale model; reactions did not occur in every case. A modeling approach inspired by a number of other studies of mesoscale compaction of porous beds was adopted [29, 7, 17]. Simulations of randomly generated sphere packings of experimentally determined HMX distributions [14, 7] were run with a model including a Steinberg-Cochran-Guinan [36, 13] viscoelastic response of the explosive material. Melting temperature and specific heat models for HMX were taken from Menikoff and Sewell [31]. Simulation cell sizes were 5 μm with 9 particles per cell making them computationally intensive, requiring thousands of processors even in two dimensions. The model was validated against experimentally determined stress and velocity profiles for non-reactive cases. A typical example of these granular compaction simulations, excluding reaction, can be seen in Figure 1 demonstrating both the behaviors of the temperature and the stress. Features such as the compaction wave, plastic yield, work heating and frictional heating can all be seen along with a few hot-spots. The model was found to have similar behavior to previously validated non-reactive models [33, 30].

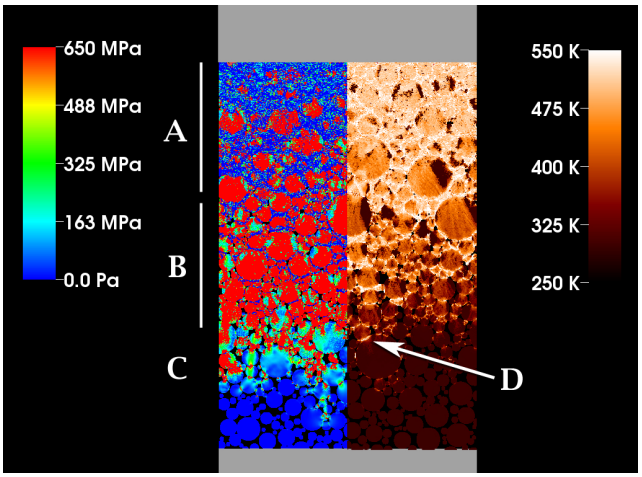

Figure 1: Stress and temperature distributions in a granular bed after being impacted from the top at 288 m/s. A plastic flow zone (A), a compaction zone (B), stress fingers (C), and friction and plastic flow induced hot-spots (D) can be seen.

A comparison of temperatures for a non-reactive case for particles and fluids is shown in Figure 2. The left image depicts the particle temperature while the right image shows

fluid temperatures. The Uintah implementation of the reaction model uses the cell centered temperatures in the determination of the burn rate while the particle temperatures are used for for determining the solid's mechanical behavior. High temperatures of gas in void spaces can enhance reaction rates and must be represented accurately to ensure the correct burn rate. These comparisons underscore the need for accurately modeling both gas and solid phases and their interactions, as gas temperatures in void spaces can be seen to be near the ignition temperature in a number of places.

Of particular interest in the granular compaction of HMX is the initiation of sustained reaction. This is important for this study as the heterogeneous nature of the bed allows for transient energy extremes, as seen in hot-spots. The decomposition of HMX was modeled using the Ward, Son, Brewster (WSB) model [39] with a decomposition temperature threshold of 450 K. While validation of the reaction model against experimental data continues, the utility of being able to model mesoscale phenomena in heterogeneous condensed explosives becomes ever more apparent. Some studies have been performed on the effects of frictional heating, melting, discretization strategies and geometries [7, 35, 29, 31, 38, 17], but relatively little work has been performed with respect to surface area, porosity and gas permeability. Bulk-scale models may be developed based on the simulations of these effects since currently some may not be probed or validated experimentally; hence our development of mesoscale models. Congruent to the development of mesoscale models is the progression of the bulk-scale material models towards correct behavior in both compaction for porous explosives and damage in solid explosive. Results from these mesoscale simulations are utilized as a validation source for bulk-scale models.

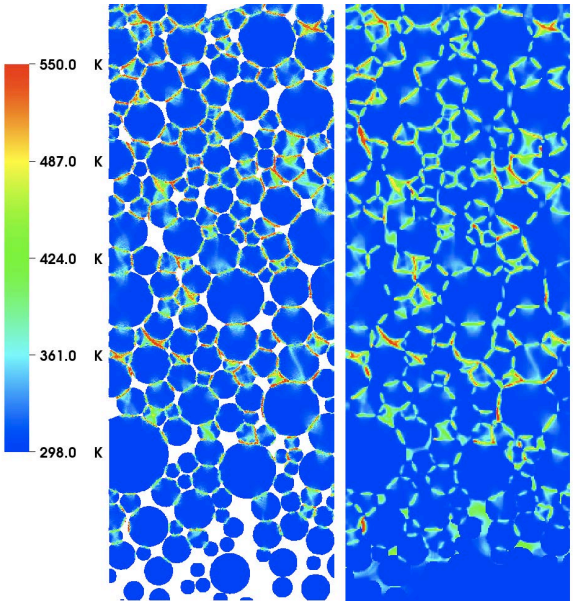

Figure 2: Temperature distribution in a granular compaction after 5 microseconds. The left image shows particle temperature and the right images shows gas temperature. The same color scale is used for both plots.

4. BULK-SCALE COMPACTION SIMULATIONS

When simulating the transportation of explosives it is important to model accurately bulk-scale compaction, since the surface area, gas confinement and damage from both mechanical and thermal insult are directly affected by porosity. For this study a new compaction model was implemented to represent a heterogeneous compaction of energetic materials. This model uses previously implemented isotropic damage model for full density explosive, ViscoScram [9], merged with an accurate representation of bulk compaction, P-α [40]. The P-α model allows a quantitative extent of porosity that is used to determine whether convective burning can occur in a material. Similarly, ViscoScram has a variable that represents the extent of cracking in the explosive material. By using these quantities, a relationship presented by Belyaev et al. [8], and a fit by Berghout et al. [10] for a PBX of interest, the WSB burn model [39] allows burning inside materials. This allows pressurization and continued damage of HMX, which can cause self-accelerated sub-sonic reactions that may undergo DDT or SDT.

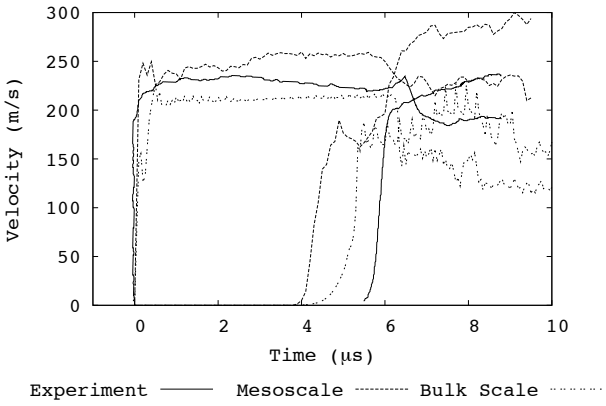

Figure 3: A comparison of bulk scale and mesoscale simulations of experimental Shot 912 [33] where the HMX bed is impacted at 288 m/s. Lines on the left are from experimental velocity gauges at the top of the bed, and those on the right are from gauges on the bottom of the bed.

To validate the compaction behavior of the P-α modified ViscoScram, a homogenized version of the simulation presented in Section 3 was run. The results have been compared to the mesoscale simulations presented in the previous section and the experimental data. Velocity profile comparisons can be seen in Figure 3. Agreement to within 10% can be seen for the velocities at the top and bottom of the specimen for Shot 912 [33]. Stress profile comparisons can be seen in Figure 4. The P-α modified ViscoScram model has larger error in stress than in velocity. Figure 5 demonstrates the utility of mesoscale simulations in that temperatures on the timescale of microseconds are difficult or impossible to obtain experimentally. The temperature computed by the bulk-scale model is larger than the average temperature for the mesoscale simulation, however it is within one standard

deviation of the averaged mesoscale temperature. By incorporating this bulk-scale compaction model, the deflagration to detonation phenomenon can be more accurately represented in porous or damaged materials. What then remains is extension of simulations to a length scale of tens-of-meters.

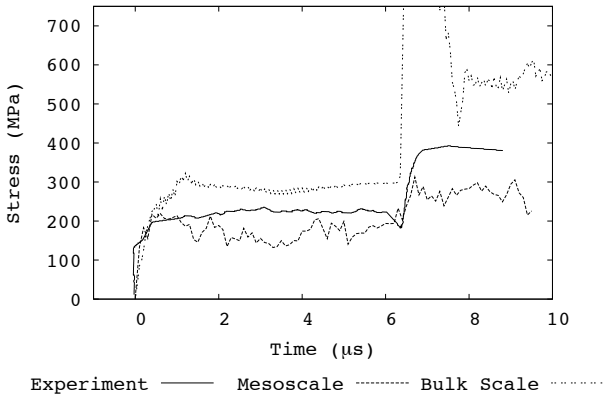

Figure 4: A comparison of bulk scale and mesoscale simulations of experimental Shot 2477 [33] where the HMX bed is impacted at 288 m/s. Lines are from experimental stress gauges at the top of the bed.

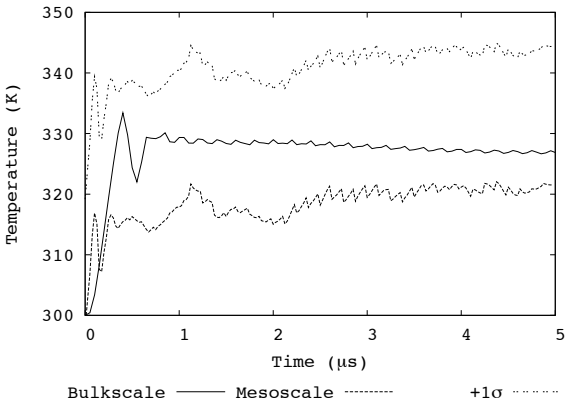

Figure 5: A comparison of temperatures computed by the mesoscale simulation and the bulk scale simulation measured at the top of the granular column. The mesoscale temperature was averaged laterally across the simulation domain and a standard deviation computed. The line marked "+1σ" has the standard deviation of the temperature added to the average for the mesoscale simulation.

5. COARSE RESOLUTION MODELS

Despite the availability of petascale machines such as NSF's Kraken, considerations must be made when weighing the accuracy of solution against the time, power and expense of the simulation. The complexity of the modeling approach and the grid cell size must be selected to maximize the accuracy while minimizing computational cost. It is desirable to extend the models to the largest cell size possible while maintaining a target level of error. The model used by Uintah to simulate multiple reaction phenomena, such as deflagration and detonation, is DDT1 [32]. Both deflagration and detonation are subject to grid cell size dependence but are barely seen to have particle density dependence [32]. The more resolution dependent model will limit the extension to coarser grid cell sizes and dictate computational costs. To extend the deflagration and detonation models used in DDT1 to regions outside the range in which they are calibrated, a metric of interest must be identified, and a convergence study performed.

Work has begun in extending the WSB model [39, 41] and the JWL++ [34] model used in the previous validation study [32] beyond their calibration ranges. In the WSB model, the metric of interest is the burn rate which often has the largest effect in the moderate strain rate region of material deformation. In the case of detonation the metric of interest is the affect of the transient pressure wave and subsequent release wave on materials close to the blast wave. These materials are accelerated and become dangerous projectiles, which is why they are of interest.

Coarsening the grid cell size will potentially allow for larger scale simulations with similar accuracies as mesoscale simulations. The burn rate is determined both experimentally and computationally by a strand burner test [2]. Experimentally a stick of explosive is confined and lit at one end. Pressurization occurs due to confinement that causes the burn rate to increase. The burn rate is measured by the time of arrival at a number of measurement gauges placed in the explosive. This allows the burn rate to be determined as a function of pressure. In many cases the initial temperature of the bulk explosive was changed to investigate the temperature dependence of the burn rate [2].

Computationally the same data can be collected by enclosing a stick of explosive in symmetric boundaries, allowing for the pressure to rise as burning occurs. These simulations were run in one dimension for simplicity and speed. Here the pressure in the gas cells were averaged, giving the simulated pressure, and the mass burned was measured. These computational experiments were used to determine the grid cell size dependence of the burn rate computed by the WSB model. The results in Figure 6 show minimal grid dependence on the burn rate for the resolutions studied. The initial bulk temperature of the HMX was 373 K. It was also observed that the burn rate was slightly overestimated at higher initial bulk temperatures and slightly underestimated at room temperature (298 K). However, at most the error was no larger than 10% of the experimental burn rate. The region of interest is dependent upon the specific explosive and our focus was on the validation of the WSB reaction model for HMX. For this simulation it is important to look at elevated pressure and temperatures, for this is where convective burning and transitions to detonations occur. The same simulation was run at initial bulk temperatures of 298 K and 423 K, which produce similar grid dependence results.

When looking at the cell size effects on detonation, the

main metric of interest is the effect of the expansion wave on other objects in the domain. For instance, if a detonation wave accelerates a piece of steel, it is desirable to know, to high accuracy, the velocity of the steel. Similarly, once the explosive material is consumed, the blast wave is largely supported by expansion of gases without the reaction to sustain the peak. This expansion wave begins at the sonic plane. The sonic plane is the point at which material behind the lead pressure wave no longer affects the detonation front. The release wave, seen in Figure 7 at the end of the plateau as the pressure begins to drop, is the main factor in the velocity of the steel plate. The release wave can effect objects on the length scale of a few millimeters while the reaction peak has a much smaller effect on the velocity of an object. Simulations were performed at various grid cell sizes showing the effect of cell size on the velocity

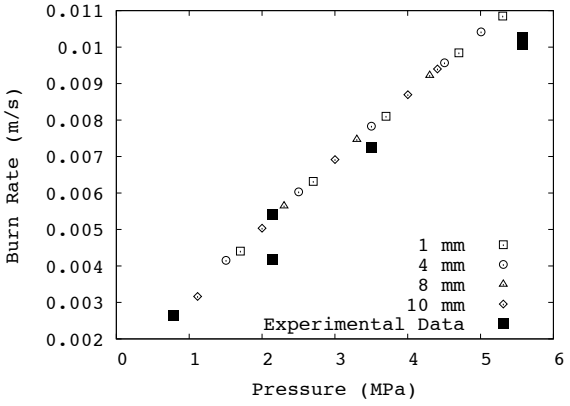

Figure 6: Resolution dependence of burn rate of WSB model at a bulk temperature of 373 K. Simulated data was compared against data from Atwood et al. for the explosive HMX [2].

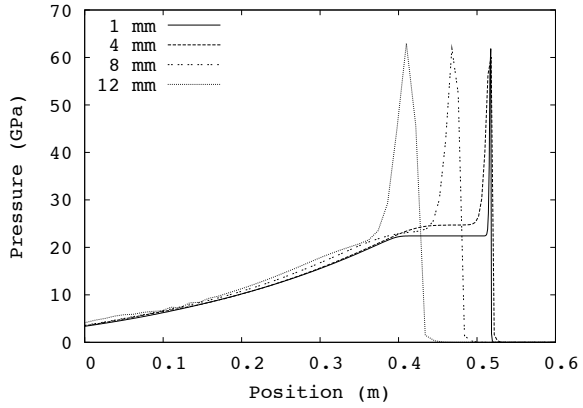

Figure 7: Pressure profiles for detonation simulations at various cell sizes.

of the steel. In these simulations a small piece of explosive was collied with a one dimensional stick of explosive causing detonation to occur. At the end of the explosive rod is a steel plate. As the detonation consumes the explosive, the pressure wave accelerates the steel plate. The velocity of the steel plate was computed and compared against a converged resolution simulation, determining the error in the velocity. With increased cell size the pressure spike due to reaction encroaches on the sonic plane affecting the amount of energy that is transferred to the steel. With increasing the grid cell size, the rate parameters for the JWL++ model had to be reduced to keep the detonation velocity constant at 8800 m/s.

Within the studied cell sizes, the differences in velocity of the steel was less than 8%. At larger grid cell sizes the reaction constant is seen to decrease more rapidly, and the velocity difference changes considerably, likely due to the reaction peak falling inside the expansion region. This changes the sonic plane and hence the amount of material that can affect the reaction front, effectively increasing the reaction rate. The shift in the reaction peak is demonstrated in Figure 7. Note the reaction peak migrates back with increased cell size, encroaching slightly on the release wave at cell sizes larger than about 10 mm. Therefore, a cell size larger than 10 mm will effect the sonic plane. A consequence of the shift due to larger cell size is that the reaction wave will reach a position slightly later in time than the more finely resolved simulations, but by no more than 10 microseconds behind the converged wave. However, this is partially offset by the fact that the interpolated pressure of the shock is felt at an earlier time because of the coarser mesh resolution. With little error associated with larger resolutions in both the burn rate and detonation propagation the capability to move up to 10 mm grid cell size while keeping the same accuracy now seems feasible.

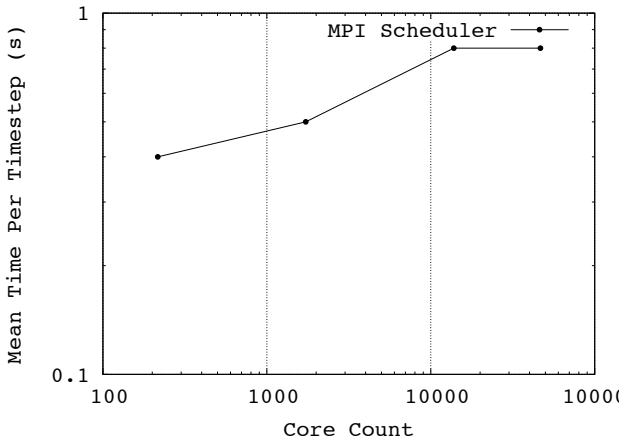

Figure 8: Weak scaling of the Uintah framework.

In addition to a grid cell size study, a scaling study was performed showing the capability of the Uintah framework to model high particle density MPMICE simulations characteristic of those seen in the trucking accident on a large number of cores. The study simulated detonation of HMX at various domain sizes ranging from 10^3 mm^3 to 360^3 mm^3 at 1 mm grid cell size. Simulations were run with 1000 grid cells/patch and 1 patch/core. The results can be seen in

Figure 8. These results can be improved upon with recent advancements made in improving memory use for the Uintah framework, allowing for linear scalablility up to 180K cores. [28, 27]. Increased zoning, along with the relaxation of the time stepsize due to the larger cell size will allow simulations of semi-truck sized explosions.

6. CONCLUSIONS

For many different reasons the safe transportation of explosives is essential. Models designed to analyze potential accident scenarios must accurately capture the relevant physics over a wide range of spatial and temporal ranges. Utilizing mesoscale results in validating bulk-scale models has proven to be useful for improving predictive capability. Furthermore, a physical quantity that is difficult to measure experimentally may be analyzed by mesoscale simulations and used to inspire bulk-scale models. A bulk-scale model for the compaction of a porous explosive, and damage evolution of fully densified material has been validated with mesoscale results. Good agreement has been shown between the simulated and experimental stress profiles for both mesoscale and bulk scale simulations. Good agreement has also been seen between temperatures in mesoscale and bulk-scale simulations, highlighting the utility of the mesoscale modeling.

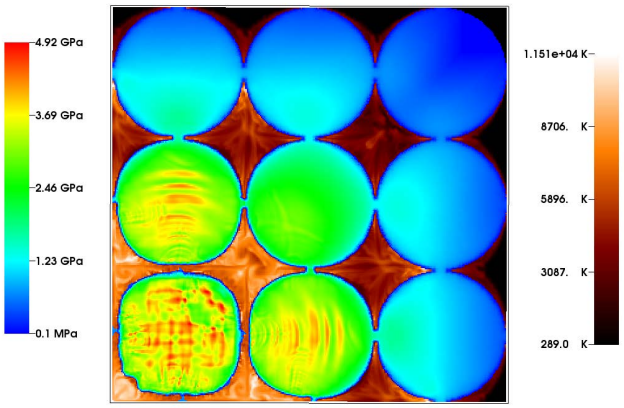

Figure 9: Demonstration of combustion in an array of explosives. The left colormap shows the pressure inside the explosive cylinders, while the right colormap shows the temperature of the product gas. The array was ignited in the lower left corner.

Using validated bulk-scale models, our studies have shown that extension of these models to larger cell sizes can capture, without significant loss of fidelity, the metric of interest. Both detonation and deflagration reactions were found to extend reasonably well to larger cell sizes. The detonation model was found to be the limiting factor with maximum cell sizes on the order of 10 mm, due to the reaction peak encroaching on the sonic plane effecting blast wave pressure and imparted kinetic energy.

Complex geometries such as those seen in the 2005 truck accident are of high interest for their potential of being a "sympathetic" explosion. For example, the 2005 accident involved 18,500 small explosive cylinders packaged in an array similar to that seen in Figure 9. The preliminary modeling efforts of this explosive array show deflagration to detonation transition in agreement with the violence of the truck explosion. This simulation will provide the benchmark needed to validate a bulk-scale array. We have shown that the current Uintah code can move to much coarser grid cell sizes, allowing accurate modeling of arrays orders of magnitude larger. The coarsened resolution, combined with Uintah's linear scalability up 180K cores [27] will allow for full-scale simulations of transportation accidents on the length scale of tens of meters.

7. ACKNOWLEDGMENTS

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