

DIRECT NUMERICAL SIMULATION OF WEAK SHOCKS IN GRANULAR MATERIAL

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The behavior of Plastic Bonded Explosives (PBXs) is not fully understood. Local phenomena, at the scale of the constituent grains, play a role in macroscopically observable mechanical response and chemical decomposition. Weak shock stress wave propagation validation calculations are discussed, and preliminary results on a representation of the fully three-dimensional granular microstructure of a particular PBX formulation, PBX-9501, are presented. The calculations include resolution of stress distributions in individual grains and frictional contact between grains, and predict the development of preferential load paths, or stress bridging, in the compaction of dense granular assemblies. A foundation for further investigation of these systems, including a massively parallel computational capability is established. Future work includes statistical analysis and data visualization

INTRODUCTION

The response of plastic-bonded explosives (PBXs) is not fully understood, particularly in the weak-shock impact range characteristic of some accident scenarios. PBXs are composed of polydisperse grains, ranging in size from less than one to a few hundred micrometers, and a matrix of polymeric binder. Low levels of applied stress sometimes cause unanticipated, violent reactions. The inhomogeneity of the deformation at the microscale (the scale of the grains) contributes to the development of local "hot spots". If a small volume of the explosive is heated sufficiently, the consequent release of chemical energy may grow unstably and lead to violent reaction. Many mechanisms for the formation of hot spots have been proposed¹. Mechanical explanations include stress concentrations resulting in localized heating due to material deformation, and frictional contact between grains.

Two-dimensional numerical simulations of both compaction and shear have been performed to gain insight into energy localization modes in both dry granular materials (without binder) and PBXs^{2,3}. These simulations modeled large deformations, complex constitutive response and frictional contact between grains. The development of preferential load paths, or "force chains", was simulated, and their presence related to the statistics of the material state at the microscale, in general agreement with experimental results. Here the objective is similar studies in three dimensions. The importance of the statistical character of the response of granular material and PBXs seems to be a general property; 3-D numerical studies of PBX response to

strong shocks also indicate the importance of fluctuations at the microscale⁴.

For simplicity, attention is focused on dry granular material. Dry granular materials have many interesting properties, as they share behavior characteristic of both fluids and solids.⁵ Dry granular materials may be considered a limiting case for PBXs, which are polymeric composites with relatively weak interstitial binder material. This simplification permits a focus on modeling intergranular contact, a defining characteristic of dry granular materials which is expected to play a role in the mechanical and chemical response of PBXs as well.

The more fluid-like regime of rapid granular flow, as may be found in grain chutes and snow avalanches, has received some attention from modelers. Grain contacts are modeled as instantaneous inelastic collisions, of varying complexity, between elastic bodies. While justifiable for rapid granular flow, these models are inadequate when grain deformation due to contact may be large.

For dense granular materials (large solid fraction, as in PBXs) relative velocities of grains are small, and grains remain in contact for substantial fractions of the total loading time. In this regime incorporation of the appropriate physics requires accurate modeling of contact, frictional sliding, and the associated deformation of the grains. Powder consolidation via shock compression is an example of this deformation regime. Numerical simulations have provided insight into the character of the microstructures generated in powder compaction. The transition from "quasi-static" compaction (grain morphology remains essentially unchanged) to

“dynamic” compaction (grain morphology is substantially altered by melting and “jetting”) has been simulated numerically.^{6,7}

The simulations described here are designed to provide insight into the nature of the deformation at the microscale in PBXs, with an eye toward energy localization and possible initiation mechanisms. As the microstructures are inherently three-dimensional, resolving grain deformation and interactions in a representative volume of the microstructure requires tremendous computational power. These calculations were performed using the parallel computing infrastructure developed at the University of Utah’s Accelerated Strategic Computing Initiative (ASCI) center, the Center for the Simulation of Accidental Fires and Explosions (C-SAFE).

COMPUTATIONAL TECHNIQUE

The Material Point Method (MPM)⁸ algorithm is used to perform simulations. This computational technique is a mix of Eulerian and Lagrangian approaches, providing a robust treatment of large deformation problems and a convenient framework for modeling contact between large numbers of contacting bodies.

The fundamental idea behind the particle-in-cell numerical technique MPM is that particles carry all the information required to advance the solution. The solution is advanced by interpolating particle information to a convenient computational grid (providing a cost savings as well as computational ease), solving the governing equations there, and interpolating changes back to the particles. With the updated particles reflecting current solution information (including

spatial position), the grid is discarded, and a new one is used in the next computational cycle. This technique may be viewed as using Lagrangian particles to advect information through an Eulerian grid. Discretization of the material is into Lagrangian particles, or material points, which naturally advect material properties and state variables through the Eulerian grid. Advantages of this method include low numerical diffusion and elimination of mesh tangling problems.

MPM provides a convenient setting for modeling frictional contact efficiently and robustly in a way which has advantages over both traditional Eulerian and Lagrangian techniques. Lagrangian finite element codes require identifying contacting surfaces, expensive search algorithms for neighboring nodes during deformation, and dependence of results on degree of interpenetration allowed.⁹ Eulerian codes require the determination of interface location and the average response of mixed cells.¹⁰ Details of the MPM contact algorithm may be found in the references.^{11,12}

VALIDATION CALCULATIONS

Because frictional contact between grains is a defining characteristic of dry granular material, numerical simulation of granular material response is a natural test of modeling capability. This was done previously for dynamic compression² and shear³ loadings, with good agreement with experimental results, both in the nature of force transmission and the statistics of the stress state. However, a direct comparison of experimental and numerical results for a specific microstructure was not made.

Stress waves in quasi two-dimensional granular media have been studied extensively by Shukla and co-

workers^{13, 14}, who used detonators to load collections of photoelastic disks. Using high-speed photography, the stress state was temporally and spatially resolved as the impulse traveled through various assemblies. Recently similar experiments have been undertaken, but using a Hopkinson bar to dynamically load Plexiglas disks¹⁵. For this case the loading results in compression at constant velocity rather than an unsteady impulse of short duration. This loading condition is better characterized, and provides a much easier boundary condition to simulate.

Collections of Plexiglas disks, a photoelastic material, are held in place by a mild steel loading frame. The dimensions of the loading frame adjust easily, allowing various configurations to be tested. One-quarter inch grooves in the sides of the frame hold the assemblies in-plane. The loading is applied via a split Hopkinson bar. The transfer of the stress wave to a loading pin of equal thickness as the disks ensures plane stress loading conditions. The input strain pulse is recorded and analyzed to give a striker velocity. Spatial and temporal measurements of the progression of the stress wave are made using a high speed camera and the technique of photoelasticity. The camera is triggered by wave propagation in the Hopkinson bar prior to reaching the disks¹⁵.

Photoelasticity generates fringes at contours of constant maximum shear stress. Because the spatial variation of the stress state is known in the simulations, it is straight-forward to calculate fringe positions. The stress tensor is diagonalized and for isotropic elastic response the out-of-plane direction is decoupled from the in-plane response. The difference in in-plane principal stresses is calculated and is

proportional to the maximum shear stress in-plane. Fringes are generated by taking the cosine of the maximum in-plane shear stress divided by a parameter (a material property) to adjust fringe density.

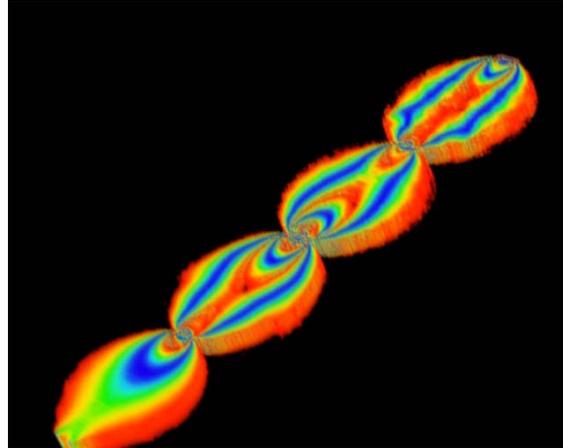


FIGURE 1. STRESS WAVE PROPAGATION THROUGH FOUR COLLINEAR DISKS.

The experimental setup was designed to allow a variety of configurations of disks to be tested, providing a general capability to examine configurations representative of granular material. Several simple configurations were examined in conjunction with validating the MPM contact algorithm. An example configuration and numerical result can be seen in Figure 1. Four collinear disks were impacted at one end (top right) and a stress wave has propagated all the way to the fourth disk. *It should be noted that the figures in this paper are in color on the CD accompanying this volume. Clarity of the presentation is greatly enhanced by viewing them in color rather than the black and white reproduction in print.* For this case and two other configurations, simulations were compared to experiments with good results¹². A more complex configuration of 20 disks, which was found

to carry load very heterogeneously, i.e. exhibit stress bridging, was also simulated¹⁵.

The flexibility of the experimental setup has been used more recently to examine configurations of disks with an interstitial material. These configurations are being used to test the ability to simulate wave propagation for simple validation configurations, but will ultimately be scaled up to elucidate more complex behavior of particulate composites such as PBXs.

NUMERICAL SIMULATIONS

Ultimately of interest is the capability to simulate PBX response, particularly PBX 9501, to weak shock stimulus characteristic of accident scenarios. It should be emphasized that these simulations, like the validation simulations discussed in the previous section, are for dry granular material. Dry granular material has received substantial attention in the scientific community recently⁵, resulting in an extensive validation data set. It provides a useful first step toward simulating polymeric composites and PBXs.

Attention is paid to the construction of the initial configurations used in the simulations. PBX 9501 is composed of a mixture of 75% coarse and 25% fine HMX, the energetic particulate material (95% by wt.), and polymeric binder (5% by wt.). The average size of the coarse crystals is approximately 150 micrometers, and the fines 5 micrometers. The typical crystal is somewhat rectangular, but with substantially rounded corners (presumably broken off during processing). However, there is also quite a bit of irregularity in crystal shapes, as some are the fusion of

several (single) crystals and some are parts of fractured crystals.

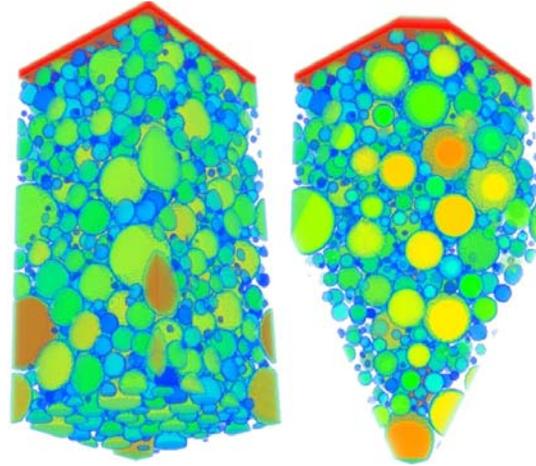


FIGURE 2. PACKED SPHERE INITIAL CONFIGURATION WITH CUT-AWAY VIEW ON THE RIGHT.

The approximation to the particulate geometry is a dense packing of spheres of various sizes. A 1mm x 1mm x 2mm box packed with 1603 spheres is used in the simulations presented below. See Figure 2. The compacting piston is shown in red. The grains are colored differently only to distinguish one from another.

Initial configurations were created using a Monte-Carlo approach to pack hard spheres in an orthorhombic box with periodic boundary conditions. The boxes were considered densely packed when the Monte-Carlo moves available became very small relative to the smallest grain diameter. The distribution of sphere diameters, d , was chosen consistent with experimental results,¹⁶ see Figure 3. However a minimum diameter was selected so that only the coarse HMX and the larger fines are represented, i.e. $50\mu\text{m} \leq d \leq 390\mu\text{m}$. Repeated packings of the same 1603 spheres, as well as larger sample sizes, resulted in packing densities

between 62 and 65%, in general agreement with previous work⁴.

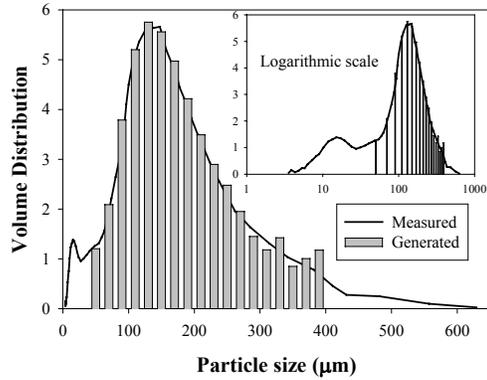


FIGURE 3. MEASURED PARTICLE SIZE DISTRIBUTION FOR PBX 9501 AND THE DISTRIBUTION USED IN THE GENERATION OF FIGURE 2.

Grain mechanical response and intergranular contact are modeled. HMX crystals are modeled as isotropic elastic-plastic materials, with elastic properties determined from Molecular Dynamics simulations¹⁷. Intergranular contact is governed by Coulomb friction. Some work has been done to indicate appropriate frictional contact parameters for various energetics.¹⁸ A coefficient of sliding friction of .5 is used in these simulations.

Stress propagation due to a 100 m/s impact was simulated. The calculation ran on 1000 processors for 11 hours on the Nirvana machine at Los Alamos National Laboratory. A computational cell size of 5 micrometers was used, resulting in ~17 million computational cells and ~10.5 million material points used in the discretization.

Results are depicted in Figure 4, where the stress tensor has been processed to generate fringes on three orthogonal

planes, at various times after impact. It should be noted that because only stress components perpendicular to the plane of view determine fringe locations, the process is inherently two-dimensional. These fringes could not be obtained experimentally, where the light transmitted through the entire three dimensional packing would be processed.

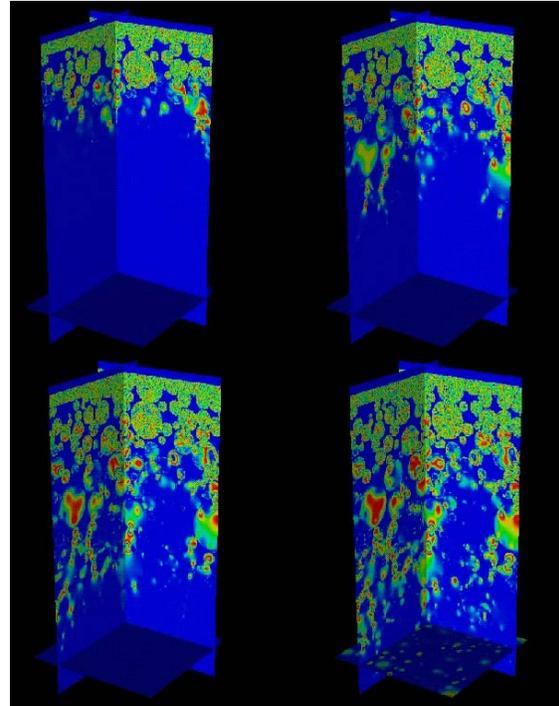


FIGURE 4. STRESS PROPAGATION THROUGH THE GRANULAR COMPACT (FIGURE 2) AT VARIOUS TIMES AFTER IMPACT.

Especially at later times, connected paths of contacting grains can be seen, resulting in “stress fingers” preceding a compaction wave in which all grains are brought into contact. The same phenomenon was previously simulated in two dimensions². The wave transit time through the granular configuration is approximately twice that for a homogeneous block with same material properties, and is indicative of the winding

path which must be traversed through the network of contact points. These results are encouraging, as the expected structure of the stress wave has been realized. However, a convergence study is still needed to assess the resolution of the stress in the individual grains and the contact mechanics.

While in two dimensions it is fairly straightforward to visualize the geometry of the stress fingers, in three dimensions this is not the case. While Figure 4 gives an idea of the connectivity of stressed grains in particular planes, the three-dimensional structure is not clear. In order to gain insight into the three-dimensional character of the stress fingers, the equivalent stress (proportional to the norm of the stress tensor) is volume rendered in Figure 5 at the end of the simulation. Stress fingers are highlighted by establishing a cutoff value of equivalent stress above which all values are plotted in red. This threshold is needed to wash out the stress concentrations at contacts. There is also a lower cutoff value, below which the stress is not plotted at all to remove the unstressed material altogether.

Although the representation in Figure 5 complements that given by the depiction of fringes, it is clearly no panacea. The structure is too dense to see into the interior. Because the norm of the stress tensor takes lower values in the interior of big grains than small ones it fails to identify all of the grains involved in the stress fingers. An example is seen midway down the right-hand side of the figure where a large grain exists. The norm of the stress tensor does not provide the desired connectivity information.

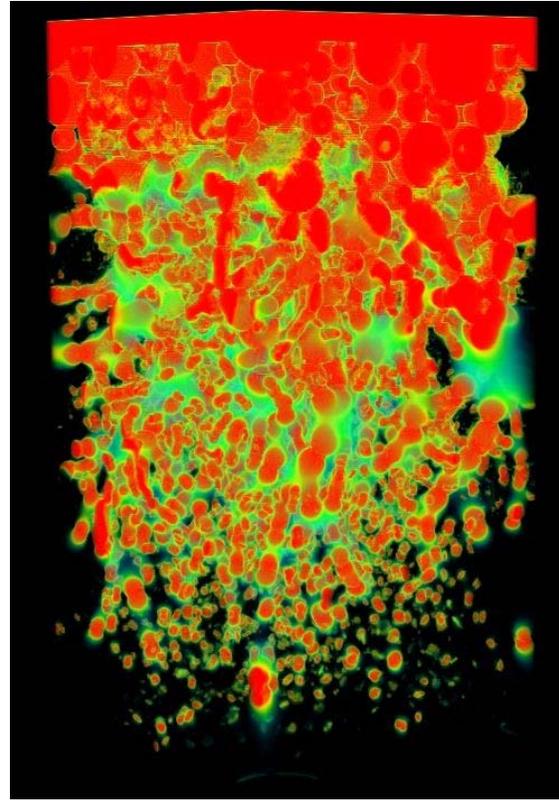


FIGURE 5. VOLUME RENDERING OF THE EQUIVALENT STRESS IN THE GRAINS AT THE END OF THE SIMULATION.

Nevertheless, further indication of the structure of the stress wave is revealed by taking slices of the data in Figure 5. The data is sliced vertically into ten slices, each 100 μm thick. Two such slices (non-adjacent) are shown in Figure 6. Although the structure of the stress wave is partially revealed by removing material, this representation still has the shortcomings associated with plotting equivalent stress. More work is needed to find an appropriate scalar representation of the stress state, and/or to reduce the data in a manner which identifies connectivity.

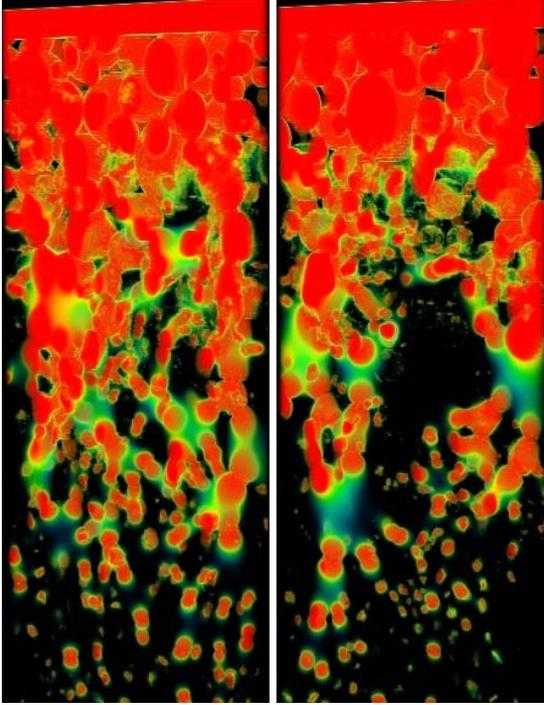


FIGURE 6. VERTICAL SLICES OF THE DATA IN FIGURE 5.

It appears, based on previous work in two-dimensions, that the computational resolution required to elicit the heterogeneous structure of the stress wave has been obtained. There is also evidence that intergranular contact is resolved for this grain size distribution. On the left in Figure 7 all the material points used in the discretization are depicted, colored by the magnitude of the equivalent stress which they carry at the end of the simulation. The figure is similar to Figure 5, except that low stress regions have not been removed. On the right in Figure 7, only the material points with near zero equivalent stress are depicted, showing the collection of grains which, at the end of the simulation, are stress free. Recall the initial configurations were created by randomly moving spheres to increase the packing density, there is no requirement that all grains touch neighbors. It is evident from the simulation that a number

of the smaller grains are floating free in the interstitial space between bigger grains, and therefore do not participate in stress transmission initially. The fact that these grains are *not* in contact is well resolved. At later times of course, as stressed grains move appreciable distances, the smaller grains will come into contact with their neighbors.

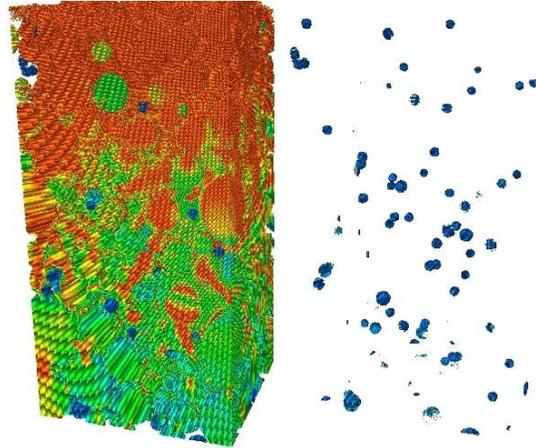


FIGURE 7. MATERIAL POINT EQUIVALENT STRESSES. ALL GRAINS ARE PLOTTED ON THE LEFT, AND ONLY STRESS-FREE GRAINS ON THE RIGHT.

Future work includes a computational resolution study to assess convergence of the results presented here. Once the quality of the solution can be assessed, data analysis can begin. Visual analysis tools are under development to extract statistics from the data sets. Determining the material state distribution at the microscale, whether it is different in three dimensions than in two, and, ultimately, how the distribution is effected by the presence of an interstitial material, are the near term goals of this study.

CONCLUSIONS

Computation on this scale is an area of research unto itself, with great promise to permit the numerical study of complex systems previously well out of reach. Simulations such as this one complement the computer science by testing the robustness of the computational infrastructure. Progress can be slow under these conditions, and is further hampered by practical issues brought to light such as data (on the order of Terabytes) storage, transfer, processing and visualization. Nevertheless, progress is encouraging and the scale of the possibilities is exciting.

It is expected that the physical behavior exhibited by the simplified systems examined here will be born out in larger simulations, more representative of PBX's. Evidence for the development of force chains in PBXs has already been found experimentally¹⁹. These features are expected to provide insight into possible hot spot mechanisms in PBXs.

While one aspect of this work is to include the relevant physics in numerical simulations at the microscale, another is interpreting the results. Toward this end there are analytical averaging techniques which can be employed to assist in validation of the results, and provide connections to engineering models. However, there is mounting evidence that standard engineering models, designed to capture average response, are inappropriate for these materials⁴. The distribution of material state parameters is very large on spatial scales below that which engineering models can resolve. Further, it is the local variations which drive aspects of the response, such as damage and initiation. Incorporating this information presents the greatest challenge.

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