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MESOSCALE SIMULATIONS OF POWDER COMPACTION

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Abstract. Mesoscale 3D simulations of metal and ceramic powder compaction in shock waves have been performed with an Eulerian hydrocode GEODYN. The approach was validated by simulating shock compaction of porous well-characterized ductile metal using Steinberg material model. Results of the simulations with handbook values for parameters of solid 2024 aluminum have good agreement with experimental compaction curves and wave profiles. Brittle ceramic materials are not so well studied as metals, so material model for ceramic (tungsten carbide) has been fitted to shock compression experiments of non-porous samples and further calibrated to match experimental compaction curves. Direct simulations of gas gun experiments with ceramic powder have been performed and showed good agreement with experimental data. Numerical shock wave profile has same character and thickness as measured with VISAR. Numerical results show reshock states above the single-shock Hugoniot line also observed in experiments. We found that to receive good quantitative agreement with experiment it is essential to perform 3D simulations.

Keywords: Powder compaction, granular flow, mesoscale simulations.
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INTRODUCTION

Development of predictive modeling capabilities for the response of granular materials to dynamic loading remains a modern day scientific frontier. In part, this is because the behavior of granular material is far more complicated, and consequently far less understood, than that of their nonporous counterparts. The purpose of mesoscale simulations presented in this paper is not only to understand qualitative characteristics of a heterogeneous medium, but also provide quantitative information for building advanced continuum models. To tackle this task, we do not need to consider processes with "scales overlap", where the hydrodynamic flow length scale is comparable to particle size. Such phenomena can be solved with direct particle representation in the problem setup. On the other hand, problems with scales separation can be further classified into initial-condition driven flows (convergent, shear, divergent) and waves. For the former, the representative volume element (RVE) studies, when the element is deformed with a fixed strain rate:

$$\frac{\partial v_i}{\partial x_j} = \dot{\varepsilon}_x \delta_{1i}\delta_{1j} + \dot{\varepsilon}_y \delta_{2i}\delta_{2j} + \dot{\varepsilon}_z \delta_{3i}\delta_{3j}$$

Mesoscale computations of strain-stress response for different eigenvalues $\dot{\varepsilon}_{kk}$ of the strain rate tensor will allow developing a rate-dependent continuum model. For waves, if the wavelength is comparable to a particle size, material response could be significantly different from the RVE response even for a comparable strain rate. This paper is devoted to study of shock waves, whose thickness could be just few particle diameters. Once a model is validated for both (RVE and short wavelength) types of granular flow, we can expect that it will have good predictive capabilities for complex applications, where loading is just a superposition in time of different loading conditions.

NUMERICAL APPROACH

We used GEODYN code, a multi-material Eulerian Godunov shock physics code [2] featuring material strength and adaptive mesh refinement (AMR) for direct numerical simulation. GEODYN is able to model large deformations of solids, capture shocks and track material interfaces with piecewise linear interface reconstruction (PLIC). GEODYN has a flexible material library with analytic and tabular equations of state and a wide range of constitutive models.

We performed a number of mesh convergence studies with GEODYN. We found that 28 cells per particle diameter is the acceptable for mesoscale simulations. The lower resolution gives good results for the shock position and averaged values behind the shock, but shows slightly wider shock front. Gradual density increase behind the shock due to advection errors is noticeable as well. Effects of particle "welding", which are inherent to Eulerian simulations and may not be a good representation of grain contacts, have been evaluated as well. We compared GEODYN and ParaDyn (a Lagrangian code with an autocontact algorithm) and found that Eulerian and Lagrangian results match both qualitatively and quantitatively if shock pressure

$$p_s > Y/k,$$

where Y is material yield strength and k is friction coefficient on the particle interfaces in Lagrangian simulations.

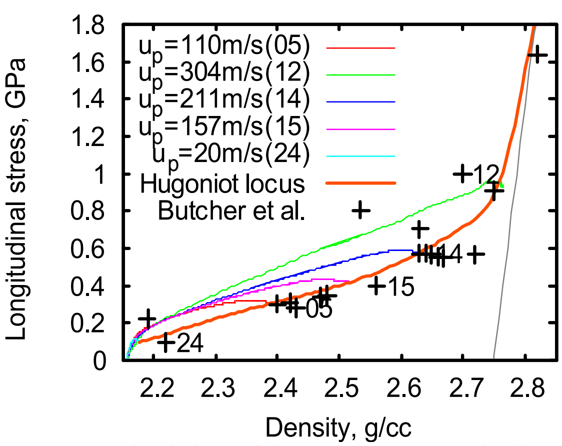

Figure 1. Simulations of sintered 22% porous aluminum and experimental data [1]. Density-stress paths for each flyer velocity are depicted with thin lines and Hugiot locus is depicted with a thick line. Experimental data is represented with crosses.

DUCTILE POWDER COMPACTION

We evaluated our approach for extensive experimental dataset on 22% porous sintered 2024 aluminum [1]. Experimental samples were hot pressed at 600°C. We repeated numerically the sample preparation with quasistatic compression at elevated temperature. After compression, material parameters (density, temperature, plastic strain) have been reset to reference values. The Steinberg model for 2024 Aluminum [3] has been used without any adjustments. Figure 1 shows experimental datapoints from ref. [1], simulated density-stress paths for flyer velocity and Hugoniot locus as a thick line. Tracing of time-dependent density-stress illustrates strong rate-dependent response of porous material.

To study morphology influence on the strain-stress curves, we studied two additional configurations. In the first one, we inverted metal and air material and shrank the sphere size to get the 22% air porosity in a "Swiss cheese"

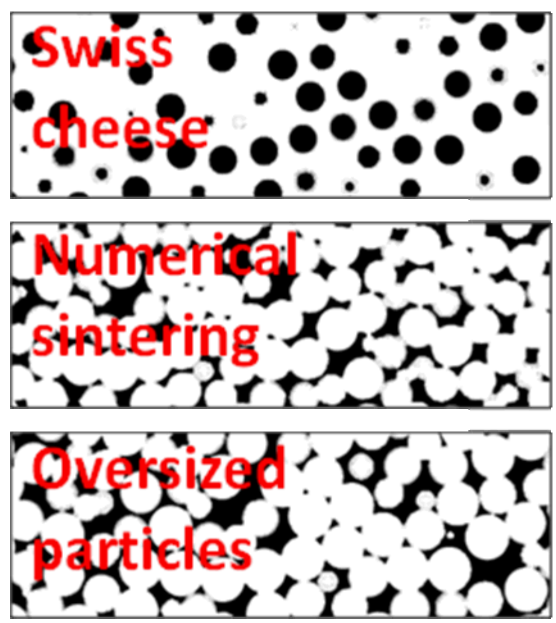

Figure 2. A 2D Slice through different initial morphologies for the shock simulations (white is solid and black is air)

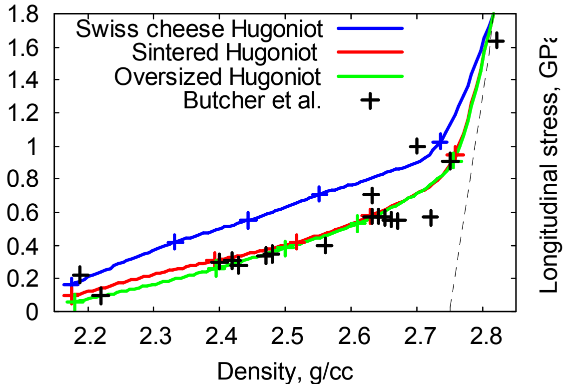

Figure 3. Hugoniot loci for different morphologies.

configuration. For another configuration, instead of plastic densification of 36% porous spheres, we "oversized" the spheres allowing them to overlap, until 22% porosity was reached. Visually this setup is almost identical to the baseline (see Fig. 2). At moderate pressures, the differences in compaction curves are proportional to differences in morphology: the "Swiss cheese" produces a significantly stiffer response curve than the other two (see Fig. 3). This can be explained by stronger arch structure of the "Swiss cheese". Surprisingly, visually barely distinguishable plastically densified and "oversized" systems gave a very different response for the low pressure regime. The magnitude of elastic precursor (measured by an inflection point on the particle velocity profile, Fig. 4) is different by 70% between both "Swiss cheese" and baseline, as well as baseline and oversized particle setup. The elastic precursor speeds are also very different (2.8, 3.7, 4.7 km/s) between 3 setups. The baseline configuration gave the best match to

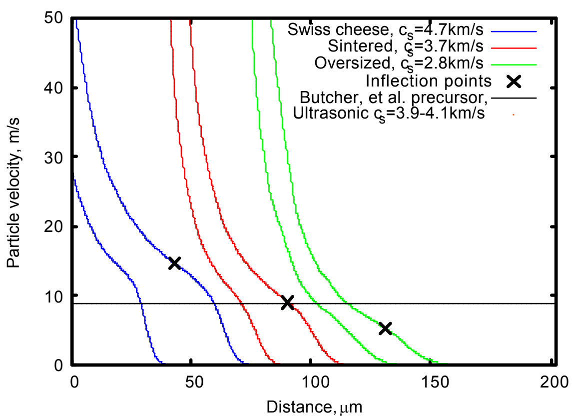

Figure 4. Zoom on elastic precursor space profiles in porous Aluminum with different morphologies.

the experiment for values of the precursor magnitude and wavespeed.

CERAMIC POWDER COMPACTION

Whereas static and dynamic compaction behaviors of ductile powders appear to be little different [1], experiments on brittle powders suggest that the quasistatic response is significantly softer than the response under shock, which is still softer than the behavior upon re-shock from an already compressed state [4]. Such complicated response features are indicative of complex history-dependent processes at the grain scale, which in addition to fracture and fragmentation could include sintering and agglomeration. The initial simulations presented here do not model all these complex phenomena. On the other side, they show what can be modeled even with overly simplistic (constant yield strength) material model. The AMR feature of GEODYN allowed simulating actual shock experiments [4] directly, to compare Hugoniot states (see Fig 5.), reshock states (Fig 7.) and a velocity record. (Fig 6.).

The experiments were performed on sifted 45% porous 20-32 mm tungsten carbide powder. Contrary to aluminum, there is a big uncertainty in properties of brittle materials. We performed parametric study on the solid parameters by varying the yield strength value it is possible to get a good

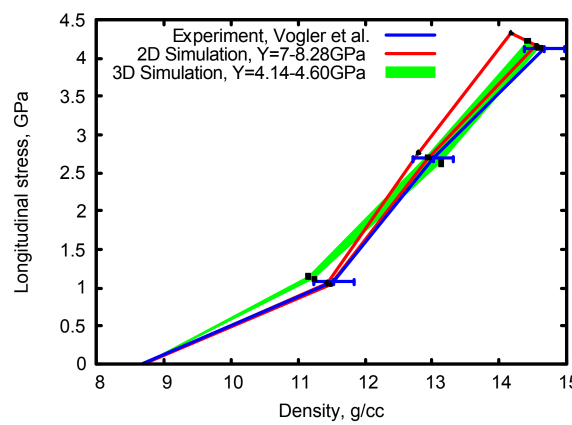

Figure 5. Hugoniot of tungsten carbide powder. Line with density error bars denote experimental data. The filled polygon shows shocked states in 3D simulations with yield strength varying from 4.14 to 4.6 GPa, and unfilled polygon shows shocked states in 2D simulations with yield strength varying from 7 to 8.28 GPa.

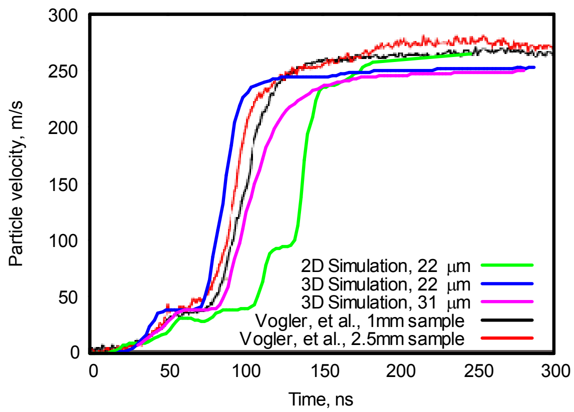

Figure 6. Experimetal and numerical VISAR velocity records are shifted to the same arrival time.

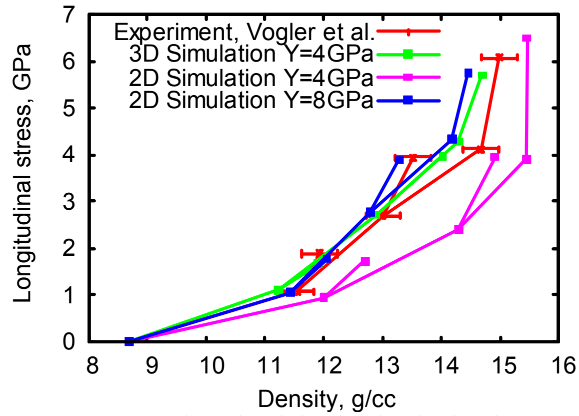

Figure 7. Experimetal and simulated reshock points.

fit to experimental points. It is important to note, that 2D and 3D simulations need very different values to match experiments. Moreover, 2D results are quite sensitive to initial positions of particles. For certain configurations (non-touching particles) it is impossible to get a good fit for the lowest experimental point. The 3D results do not show such sensitivities. Simulated velocity records (Fig. 6) show good agreement with experimental counterpart. Simulations with 22 and 31μm particles bound the experimental shock width. 2D results indicate elongated precursor, suggesting "sintered" response. We were not able to match the particle velocity level in 3D simulations, which characterize the reshock behavior of the sample. Experiments suggest a stiffer reshock, i.e. a line which connects single shock Hugoniot loci lies below the line of reshocked Hugoniots. This is unusual; for homogenous materials the trend is opposite due to more entropy production in a single shock. We did not observe "stiffer reshock" behavior in the 3D simulations. Some of 2D simulations show "stiffer reshock" behavior, while other do not. This issue has to be addressed by further computational research as well as firmly confirmed experimentally.

CONCLUSIONS

The conducted research shows that not only 2D and 3D results have substantial quantitative differences, but also that even on qualitative level the 2D results can be misleading, since use observe qualitatively behavior similar to experimental (stiffer reshock) which vanishes when we simulated more realistic 3D configuration. We demonstrated ability to build validated material response curves using only information on morphology and properties of constituents for ductile powders. We matched some characteristics of brittle powders, but still lack predictive capabilities in this area. Mechanisms of brittle damage and granular temperature generation and dissipation need to be better understood for advances in this area.

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