Correlating computationally derived particle surface stress-strain states to mesoscale shock response

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Abstract. The results of FE simulations are presented, correlating the continuum and mesoscale shock response of a particulate system with particle surface stresses-strains. The objective of this work is to gain insight into how the complex responses at the meso/sub-mesoscale manifest to quantities that could be experimentally measured without perturbing the material, informing the design of possible mesoscale diagnostics. Three simulation setups were analyzed. First, the normal plate impact of monolithic silica quartz for continuum comparison purposes. Second, the normal plate impact of a 2D representative volume element (RVE) of randomly packed disks. Third, the normal plate impact of a 3D RVE of randomly packed spheres. In each of the RVEs a small coupon corresponding to an assumed mesoscale "sensor" was attached to the surface of a particle in the center of the RVE. Stress quantities from the sensor and existing continuum diagnostics were analyzed. The mesoscale quantities are highly heterogeneous and differ significantly from the continuum quantities. Difficulties regarding correlation of surface quantities to the average particle and system response are also discussed.

1. Introduction and Objectives

Literature pertaining to the shock response of continuum materials is extensive and well-defined. In contrast, a thorough understanding of the shock response of particulate materials is lacking. Experimentally, diagnostics typically used for continuum materials have been applied to particulate mediums. Such methods include free surface velocity profiles and input/propagated stress gauges. Data from such diagnostics can be used to calculate the bulk response of the medium. Computationally, simulations can be performed utilizing traditional Equations of State (EOS) modified to account for initial porosity (e.g., p-α, p-σ, and p-λ models). While this method has been shown to produce accurate results [1], the fundamental assumption in such work is that the particulate medium can be described as a homogeneous material, neglecting the interactions and features at the meso/sub-mesoscale.

In order to address these shortcomings, new experimental diagnostics that operate on the mesoscale need to be coupled with accurate mesoscale simulations to gain an understanding of the mesoscale phenomena (e.g., particle contact, rearrangement, and fracture) that drive the continuum response. While experimental methods of probing mesoscale events are an area of active interest, usable and well-characterized diagnostics are not yet available. Computational simulations can play a key role in such developments, as many existing computational methods can be extended to model systems at the appropriate spatial scale.

To that end, the focus of this work is to perform mesoscale simulations using the Finite Element Method in order to gain a qualitative understanding of the potential response of a
theoretical surface-mounted mesoscale sensor. The sensor design is based on a surface-mounted coupon, on the same scale as the constituent particles in the particulate medium. The sensor would give information regarding the surface stress-strain state of the particle, which could then be correlated to the internal and overall average response of the particle to a shock loading event.

2. Microstructure Generation
The defining characteristic of heterogeneous mediums, and of particulate materials specifically, is the microstructure. Consequently, a reasonably accurate digital representation of such microstructures is necessary in order for mesoscale simulations to produce valid results. There are many different methods to generate digital microstructures, generally falling under two categories: mathematical generation of synthetic microstructures via algorithms, and generation of real microstructures using x-ray tomography. For the present study, an algorithmic approach was chosen. A random packing of identical spheres was obtained using the commercial FEM code Abaqus [2]. While real-world particulate materials are not composed of monodisperse spheres, such a simplifying assumption is a common practice when simulating particulate materials, and fits objective of this work. Each sphere/disk was meshed, assigned a rigid body constraint (which greatly reduced the time of the simulation) and a gravity force. The simulation was then run, allowing the particles to settle in a container, with a static friction coefficient set for the entire domain. The settled particles resulted in the simulation representative volume element (RVE) discussed below.

3. Simulation Setup

3.1. Geometry
Three simulations were performed, with initial configurations shown in figure 1. Abaqus was chosen as the FEM code for the simulations due to its easy availability and powerful automatic contact algorithm (general contact). While these features were of use, significant time was spent in the post-processing, which may have been less cumbersome with a more customizable and open code.

![Figure 1. Schematic of 2D and 3D simulations - (a) particulate sample treated as monolithic continuum material, (b) 2D mesoscale RVE with 100 disks (75% density), and (c) 3D mesoscale RVE with 1000 spheres (45% density).](image-url)

For all three simulations, the components were (in order from top to bottom): impacter plate, buffer plate, sample (either monolithic or particle RVE), and backer (window) plate. All components were modeled as silica quartz. For the mesoscale sensor, a small PMMA (polymethylmethacrylate) coupon was attached to the surface of a particle (figure 2), which was embedded in the center of the generated RVE.
3.2. Boundary Conditions
The boundary conditions applied at the RVE boundaries for each of the simulations varied due to the features available in Abaqus. The 2D monolithic simulations utilized plane strain conditions with the two vertical boundaries of all the four components constrained in the horizontal X-direction.

For the 2D particulate simulation, plane strain conditions had to be manually enforced. In Abaqus, general contact is only available for 3D models, requiring manual surface pairing in 2D. As the number of particles in the 2D RVE increased, the number of potential contacts required excessive surface pairing, substantially slowing down preprocessing of the simulation input file. To avoid this issue, 3D prism elements were used to make thin disks/plates with their faces constrained in the Z-direction. This permitted use of general contact while performing 2D simulations. The vertical boundaries of the plates are constrained in the horizontal X-directions, while the 2D particles are constrained horizontally by two rigid surfaces constrained in all directions. Periodic boundary conditions cannot be implemented in the simulations as designed, and as a result wave reflections from the sides of the RVE are present. Similarly, the 3D simulations have the plates constrained in the horizontal directions, and four rigid surfaces (forming the RVE boundaries) to constrain the 3D particles in the horizontal directions.

3.3. Material Properties
The silica quartz is modeled as elastic-perfectly plastic with the Mie-Gruneisen equation of state [3, 4], while the PPMA is modeled as perfectly elastic. Simulations were carried out at 500 m/s normal impact velocity. Table 1 summarizes the materials properties and table 2 provides other parameters used in the simulations.

| Table 1. Material properties. |
|-----------------------------|
| **Silica Quartz**[3, 4] |  |
| $\rho$ | 2648.5 kg/m$^3$ |
| $G$ | 46.92 GPa |
| $\sigma_y$ | 2.353 GPa |
| $\gamma$ | 0.675 |
| $C_0$ | 2209 m/s |
| $S$ | 1.5686 |
| **PMMA** |  |
| $\rho$ | 1170 kg/m$^3$ |
| $E$ | 2.2 GPa |
| $\nu$ | 0.35 |

| Table 2. Simulation information. |
|-----------------------------|
| **Parameters** |  |
| Impact Velocity | 500 m/s |
| Friction Coefficient (constant) | 0.2 |
| **Details** |  |
| Prism Elements/Particle (2D) | 270 |
| Coupon Particle Elements (2D) | ~1,000 |
| Coupon Elements (2D) | ~2,400 |
| Tetrahedral Elements/Particle (3D) | ~2,500 |
| Coupon Particle Elements (3D) | ~20,000 |
| Coupon Elements (3D) | ~10,000 |
| Simulation Time | 0.7 $\mu$s |
4. Results and Discussion

4.1. Monolithic and Particulate RVE Comparison

A comparison of two common continuum diagnostics (backer free surface velocity and input/propagated stress gauges) for both the monolithic and 3D particulate simulations are shown in figure 3. The dimensions of the 2D monolithic and 3D geometries are identical.

![Graphs showing comparison of input, propagated stress, and free surface velocity](image)

**Figure 3.** Comparison of (a) input (buffer) stress, (b) propagated (backer) stress, and (c) free surface velocity for 3D mesoscale simulation with those obtained considering sample as monolithic.

Typical of the shock response of particulate materials, the propagated stress gauge and free surface velocity show longer rise times and attenuated peaks compared to monolithic materials due to energy loss from particle interactions and deformation. The input gauge shows a lower peak stress and width, most likely caused by the release wave from the pores at the buffer/RVE interface. These results indicate that the relevant phenomena of shock in particulate materials are captured in these simulations.

4.2. Mesoscale Response

A local coordinate system was defined (based at the center of the coupon), with the $Z'$-axis normal to the coupon and pointing away from the particle. The $X'$-axis and $Y'$-axis point along the width and length of the coupon, respectively. Figure 4(a) shows the coupon stress components along the local axes. Figure 4(b) compares the mean stress in the particle with the mean stress in the coupon.

The stress observable at the coupon is significantly lower than the stress observed at the continuum level. As a result, the maximum strain observed in the coupon is less than 1.0%. The choice of material for the experimental mesoscale sensor will play a significant role in the ability to extract meaningful data from this local stress/strain state. Additionally, there is little temporal correspondence at the mesoscale with both the average particle response (figure 4(b)) and the continuum shock response of the system (e.g., primary pressure wave arrival and release).

A potential explanation for this discrepancy is illustrated in the contour plot shown in figure 5. The loading of the particle is highly heterogeneous and dependent upon the initial configuration of the packing. Finally, the stress spike at approximately 0.4 $\mu$s is due to a neighboring particle contacting the sensor particle in close proximity to the coupon. Features pertaining to such external interactions will need to be identified to aid in the interpretation of the experimental data.
Figure 4. Results from 3D mesoscale simulations showing temporal variation of (a) coupon stresses in local axes, and (b) coupon mean stress compared with particle mean stress.

Figure 5. Heterogeneous mean stress in coupon particle coupled with wave reverberation in the coupon responsible for the heterogeneous response of the coupon.

It should be noted that the mesoscale data has been smoothed significantly, as substantial reverberation was present in the results of the simulations. It is assumed that excessive wave reflections from multiple free surfaces is the cause, but a thorough analysis was not undertaken in this work.

4.3. 2D/3D Comparison
For reasons of computational efficiency, it is preferable to use 2D simulations whenever possible, with the requirement that the 2D results are representative of what would be obtained with a full 3D simulation. Figure 6(a) compares the backer stress obtained from the 2D and 3D mesoscale simulations. The coupon stresses (in local axes) obtained from the 2D simulation are shown in figure 6(b). The continuum responses (i.e., the backer stresses) are qualitatively similar. Comparison of figure 4(a) and figure 6(b) indicates that the mesoscale responses from the 2D and 3D simulations are significantly different, resulting in differences in the coupon stresses.

5. Conclusion and Future Work
The challenges in developing an experimental mesoscale sensor are significant. The present work shows that the response of an individual particle in a particulate system is complex, and the correlation of measurable surface quantities (without perturbing the mesoscale) to the actual
response of the particle (and the system as a whole) is a challenge. The 2D and 3D simulation results show that though the continuum responses are qualitatively similar, the responses at the mesoscale are significantly different. This needs to be investigated further. The future work is focused on improving the accuracy and usefulness of the simulations, by (a) varying the material and dimensions of the mesoscale sensor to reduce the impedance mismatch between the sensor and the particle and help control wave reverberation, (b) increasing RVE size to minimize the influence of wave reflections from the boundaries, and (c) implementing more rigorous material models (including thermal effects). Finally, other computational methods capable of modeling fracture should be investigated. With such improvements, the accuracy of these mesoscale models will be greatly enhanced.

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