

Pore collapse during impacts in granular materials

Sohanjit Ghosh^{1,*}, Mohamad Thakur^{2,3}, and Ryan Hurley^{1,2}

¹Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD 21218

²Hopkins Extreme Materials Institute, Johns Hopkins University, Baltimore, MD 21218

³Earth and Environmental Sciences Division, Los Alamos National Laboratory, Albuquerque, NM 87545

Abstract. The rapid compaction of grains and pores during the initial stages of impact into granular materials controls crater formation and ejecta release. In hydrocode modeling of these impacts, pore collapse is assumed to occur homogeneously throughout the material, with no consideration of local variations in porosity, microstructure, pressure, and volumetric strain. In this work, we employ the methodology of [1–3] to infer the kinematics and kinetics of the grains subjected to impact by combining *in-situ* X-ray imaging of impact with numerical modeling of a “digital twin” of the same material. We then use the validated numerical model to quantify pore space evolution in 3D with excellent temporal and spatial resolution. Our results demonstrate that porosity evolution is indeed heterogeneous, and local porosity evolution can deviate significantly from the average porosity evolution due to the intricacies associated with the granular microstructure. Pore pressures and volumetric strains computed in simulations allow us to verify the efficacy of these two popular pore collapse models at lower length scales – the $P-\alpha$ and $\epsilon-\alpha$ models. The $P-\alpha$ model was determined to be able to capture the statistical distributions of evolving pore pressures. In contrast, the $\epsilon-\alpha$ model was shown to have limitations due to its functional form. Our work is the first to investigate pore collapse using validated digital twin models. This study advances our understanding of the complexities involved in rapid granular compaction.

1 Introduction

It is critical to understand the complex phenomena associated with impact in granular materials to predict natural and man-made processes. For instance, impact in granular materials occurs during planetary impacts, projectile penetration in defense applications, and pharmaceutical manufacturing processes. More recently, the DART (Double Asteroid Redirection Test) mission [4] involved impacting an asteroid covered in granular regolith to cause course deflection. During such projectile entry into a granular target, mechanisms including grain rearrangement, pulverization, breakage, and dilation occur in the cratering region [5]. A significant fraction of the impact energy is also consumed in the collapse of the pores (or voids) during compaction in regions directly below the projectile, which experience almost purely uniaxial strain, similar to planar impacts. The large volume fraction occupied by pores in granular materials results in the macroscopic (or bulk) response being heavily dependent on the pore collapse phenomena. Understanding pore collapse phenomena is the main goal of this work.

Impact in the velocity ranges considered in this study (on the order of 1 km/s) typically occurs on timescales on the order of microseconds. Traditional X-ray tomography imaging can provide *in-situ* information on the pore deformation in 3D but require long timescales. Based on our previous work [1–3], we see in figure 1 that the X-ray Phase Contrast Imaging (XPCI) technique during plate im-

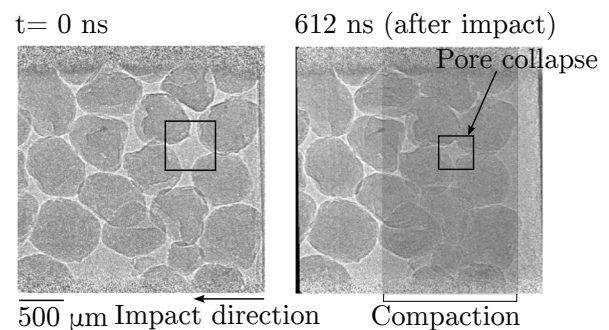


Figure 1. XPCI revealing the collapse of pores during planar impact in single layer of Ottawa sand (OS) grains at 714 m/s.

pect experiments can capture the deformation of individual pores at such short timescales with high spatial resolution. Individual pores collapse until complete closure and the material reaches its solid volume fraction. Despite this *in-situ* visualization, XPCI only provides 2D through-thickness information and cannot be directly used to understand the 3D microstructure evolution. Therefore, combining these experiments with mesoscale modeling, which resolves local microstructure from a single grain to hundreds of grains, is essential to obtain full 3D information.

Using the methodology in [1], we developed a numerical finite element method (FEM) digital twin of the experiments using an X-ray Computed Tomography (XRCT) image of the material prior to impact. The XRCT image resolved grains and pores at a resolution of $10 \mu\text{m}/\text{voxel}$. The mesoscale simulations provided pore kinematics and kinetics in 3D and provided access to pressure, P , and vol-

*e-mail: sghosh29@jhu.edu

umetric strain, ϵ , in the pores. The time evolution of these variables and the pore sizes given by distension α , where $[\alpha = 1/1 - \phi]$, and ϕ being the local porosity, were used to determine the efficacy of continuum and phenomenological models such as P - α [6] and ϵ - α [7], respectively, in predicting pore collapse and its associated heterogeneity [8]. Here, we aim to characterize this heterogeneity among all the pores in the system and its dependence on local micro-structural variables [9]. Finally, we comment on the applicability of the P - α and ϵ - α models to capture pore collapse at different length scales and some of their limitations.

The remainder of the paper is organized as follows. Sec 2 describes the methodology used to obtain the variables P , ϵ , and α for the individual pores from the mesoscale model. We compare the P - α and ϵ - α response of the pores with theoretical predictions in Sec 3. Finally, we discuss our findings and conclude in Sec 4.

2 Methodology

In our previous work [1–3], we demonstrated that experiments, although useful in visualization and providing qualitative information regarding pore collapse, cannot be directly used to quantify variables such as pressures, stresses, strains, and temperatures that are required to understand the physics of the phenomenon. Therefore, we must couple the experiments with modeling that would allow us to probe these variables and their evolution during pore collapse in 3D. We have shown in [1–3] that we can accurately capture the deformation of grains and pores with the choice of simple material models for our sand grains and accurate representations of grain shapes based on XRCT imaging. This section discusses the setup of our mesoscale simulations and the quantification of variables relevant to understanding P - α and ϵ - α response from these simulations.

2.1 Simulation Setup

The simulations performed in this work are performed using the FEM software ABAQUS/Explicit. Often, when modeling in the Discrete Element Method (DEM), grains are approximated as spheres, leading to the loss of intricacies caused by irregular particle shapes and sizes in real granular systems. For our simulations, we capture the exact grain shapes, sizes, and their arrangement using XRCT, which provides the most accurate initial conditions for our simulations, as shown in figure 2. The XRCT scans can then be imported into mesh generation software *Simpleware*, which, for around 500 Ottawa Sand grains in our sample, generated a mesh with C3D4 tetrahedral elements containing approximately 500,000 nodes and 1.8 million elements.

In the impact experiments, which were performed at the Dynamic Compression Sector (DCS) of the Advanced Photon Source (APS) using a single-stage gas gun, a polymeric box was necessary to provide grain confinement. However, in our previous work, [1–3], we observed that

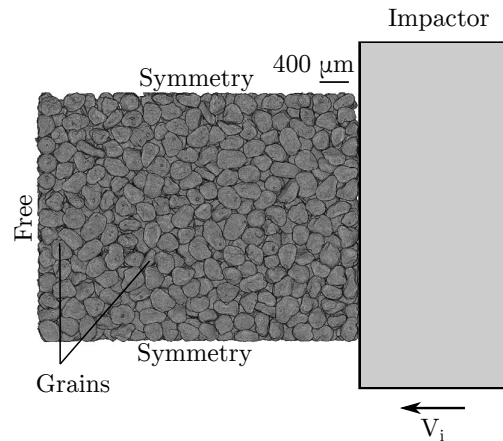


Figure 2. Schematic of the simulation setup in ABAQUS/Explicit. The granular assembly was captured through XRCT. The boundary conditions and the material models used in the simulations are described in the main text.

the large deformation of the box leads to dilational flow of the grains close to the impactor. This dilational flow caused deviation from uniaxial strain loading scenario typically locally in large-scale impacts. In the current simulations, we therefore do not explicitly model the box and instead allow the Lithium Fluoride (LiF) tipped impactor to directly impact the sample as shown in figure 2.

For our simulations, we define the boundary conditions on the impactor and the granular assembly. For the impactor, we assign it a constant velocity equal to the impact velocity of 714 m/s to replicate one of our impact experiments with Ottawa sand (OS) grains. The face of the grains farthest from the impact was unconstrained, while the lateral boundaries were assigned symmetry boundary conditions, which prevented dilational flow [1]. The grains also interact through Coulombic frictional sliding with friction coefficient $\mu = 0.3$.

At sufficiently high pressures, the volumetric response of the solid becomes significant along with the deviatoric response. For capturing the volumetric response of both the grains and the impactor, a Mie-Grüneisen Equation of State (EOS) was employed, given by a linear shock velocity U_s and particle velocity u_p relationship. Instead of explicitly modeling the brittle nature of sand grains characterized by cracking and fracturing, we approximate their material response with an elastic-perfectly plastic model with Cowper-Symmonds strain rate hardening. This choice was motivated by the good match with experimental images for brittle materials such as Soda Lime Glass (SLG) and OS [2, 3]. In this work, we focus only on pore collapse due to the compaction of the grains and not due to the breakage of the grains, which typically occurs at much longer timescales than the observation window of the experiments (1-2 μ s post-impact). To this end, we run the simulations up to 6 μ s, sufficiently long enough for all the pores in the sample to collapse.

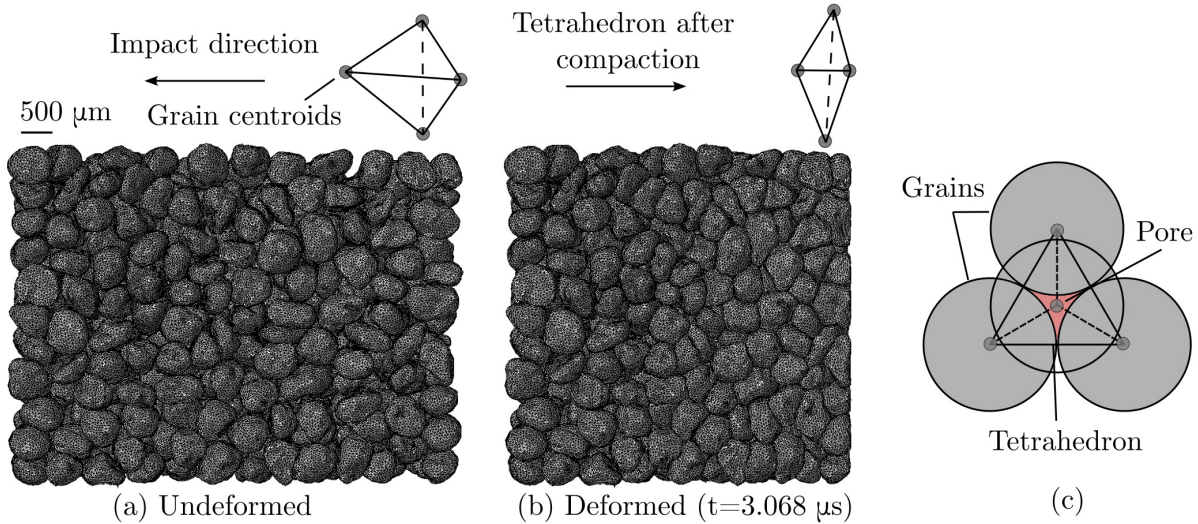


Figure 3. The discretization of the domain into tetrahedrons for (a) the undeformed configuration at $t = 0$ and (b) at $t = 3.068\mu s$ after impact, as captured in FEM. The evolution of the tetrahedron shapes is tracked, and pore size is estimated in (c).

2.2 Estimation of α , P and ϵ

The simulations provide the full 3D kinematics and kinetics of the grains with time. A measure of the pore space is given by the distension α . As the grains compact, the pore space between them collapses until it reaches the solid volume fraction, given by $\alpha = 1$.

The initial microstructure representing the undeformed configuration, as shown in figure 3(a), is discretized using Delaunay triangulation into tetrahedrons, with vertex points at the centroids of neighboring grains. As the material is compacted in figure 3(b), the tetrahedron collapses as the centroid of the constituent grains moves toward one another. The pore space inside each tetrahedron, as shown in figure 3(c), is calculated using the relative ratios of the solid volume fraction V_S and the total volume of the tetrahedron V_T , from which the porosity is determined as

$$\phi = 1 - \frac{V_S}{V_T}. \quad (1)$$

Distension α can be calculated from ϕ by $\alpha = 1/1 - \phi$. The average of all nodal pressures within a particular tetrahedron gives an approximation of P that will be used to test the P - α response. For the volumetric strain, ϵ_V , the strain arises due to the compaction of the grains and the evolving microstructure and is estimated using the large deformation strain formulation of [10]. The locations of the moving centroids and linear shape functions provided the strain tensor ϵ , from which the volumetric component ϵ_V is obtained as $tr(\epsilon)$. This ϵ_V is obtained for all the tetrahedrons in the granular assembly at each time instant and is used in the ϵ - α analysis.

3 Results and Discussions

Having quantified α , P , and ϵ for all tetrahedrons in the simulations, we now check how these variables evolve with time and compare against continuum and phenomenological predictions from the Carroll-Holt P - α and

ϵ - α models, respectively. The theoretical framework for these models has been elaborately discussed in our previous work [1]. Due to the fluctuations in the microstructure and grain rearrangements during compaction, pores can also sometimes open, rather than demonstrating monotonic closure with time [1]. In this work, we consider only the pores that exhibit monotonically decreasing α , from $\alpha = \alpha_0$ to $\alpha = 1$.

3.1 P - α response

In the theoretical calculation of the Carroll-Holt P - α model, two quantities can be obtained from the mesoscale simulations. First, the initial distension $\alpha = \alpha_0$ for each tetrahedron can be obtained from the XRCT scans based on the relative void and solid fractions around each pore. During the simulations, the shock rise time τ denotes the time it takes for the shock pressure to reach from 0 to the equilibrium pressure [1]. This quantity is a microstructure-informed quantity, which means it varies for each tetrahedron in the granular assembly and can be obtained from the simulations. Using α_0 and τ from our simulations in the theoretical formulation of the Carroll-Holt model leads to the predictions of pore collapse in each tetrahedron shown in figure 4(a). On the other hand, figure 4(b) demonstrates significantly more heterogeneity and fluctuations in the systems due to the granular microstructures as opposed to the idealized boundary value problem pore collapse assumed in the Carroll-Holt model.

Statistical analysis of the distribution of the pressures at pore collapse in figure 4(c) shows that the P - α theoretical model using actual variables representing the microstructure (α and τ) provides an accurate prediction of the mean response, with simulations reflecting a broader spread of final pressures.

3.2 ϵ - α response

The ϵ - α model uses a predefined functional form and requires fitting parameters. The ad hoc parameter κ was

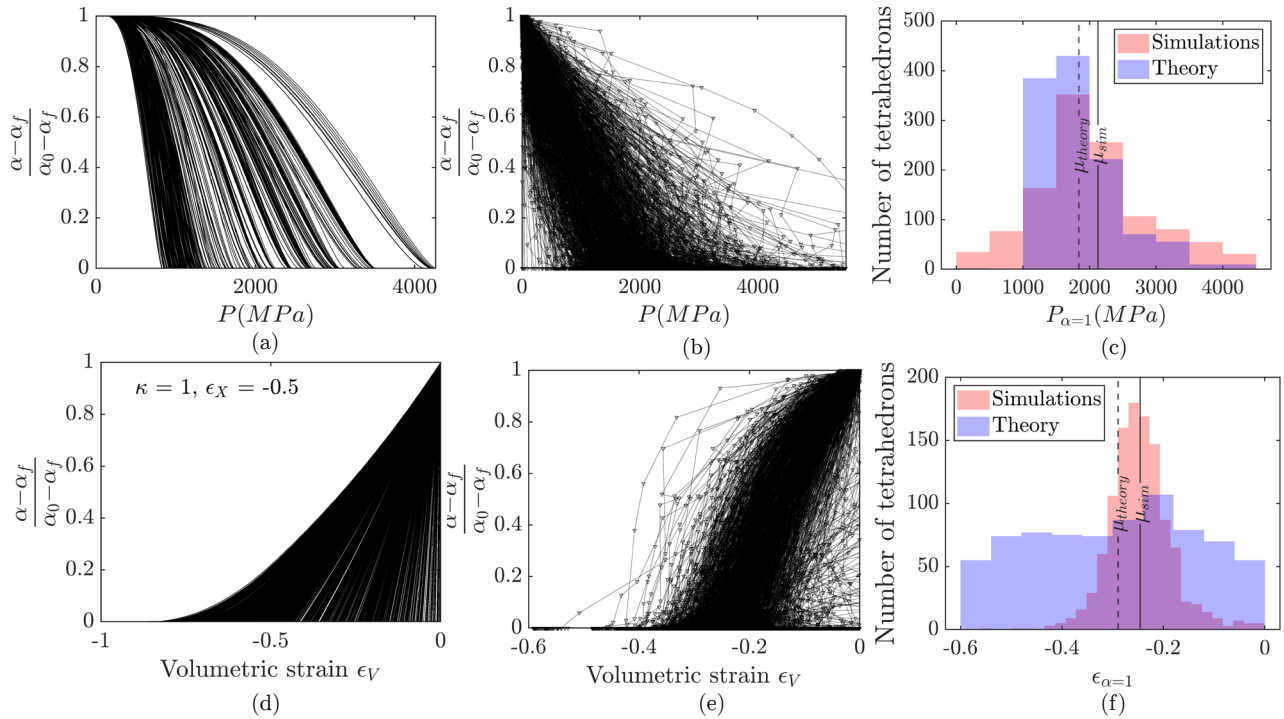


Figure 4. P - α predictions for each tetrahedron from the (a) theory, (b) simulations, and (c) a statistical comparison. (d)-(f) is the corresponding response for the ϵ - α model. α_0 and α_f represent the initial and final distension, respectively.

introduced to control the compaction rate without explicitly considering the effects of compression of the solid or the grain rearrangement during compaction. Figure 4(d) shows the evolution of ϵ - α from the theoretical framework, using α_0 from the initial configuration as above for P - α .

The simulations again show the heterogeneity in the ϵ - α evolution among different tetrahedrons in figure 4(e). Deviations between the distributions of the volumetric strain at full pore collapse $\alpha = 1$ are apparent in figure 4(f), although the mean response is similar. Unlike parameter τ used in P - α , there is no quantity in the theoretical framework of the ϵ - α model based on microstructure. The parameter κ , which controls the compaction rate, cannot be assumed to be the same for all tetrahedrons or pores. Pores in different regions of the granular assembly compact at different rates, arising from the local microstructural conditions. Therefore, the empirical fitting approach in the ϵ - α model cannot account for the heterogeneity at the pore scale during pore collapse. Fitting κ to each pore's response would be the ideal way to match the simulation data. However, predicting it a priori based on microstructure is impossible due to the heterogeneity in pore collapse.

4 Conclusions

Mesoscale simulations are useful tools for investigating processes such as pore collapse, which dictate the macroscopic response of granular materials subjected to rapid compaction. We demonstrated that simulations that accurately capture grain shapes and use simple material models provide accurate estimates of pressures, strains, and porosity evolution. We showed that the P - α and ϵ - α responses from the simulations were heterogeneous, and the

P - α model, with its parameters α_0 and τ derived from simulations, provided an accurate estimate of the average pressures at pore collapse, as well as their heterogeneity. However, the ϵ - α model cannot predict the pore scale response due to the assumption of a single parameter κ for all pores. κ is a function of the local conditions and varies from pore to pore.

This work advances our understanding of pore collapse in granular materials and the need to develop accurate models that capture the stochasticity arising from the microstructure of the granular system.

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