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RPPR Final Report

as of 31-Aug-2021

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Major Goals: This project aimed to explain how particle ruptures due to grain-scale fracture influence the energy dissipation in particulate solids subjected to rapid loading, as well as to interpret the rate-sensitivity of these materials with principles of crack growth dynamics and granular physics. To bridge length scales, a continuum law linking the rate of comminution to the failure kinetics of single particles was proposed. Direct visualization based on x-ray tomography was used to assess the evolution of the polydispersity of the material, as well as to constrain the modes of grain fracture with both the statistics and morphology of the breakage products. Such grain-scale data were used to formulate a continuum breakage model, as well as to test its performance against evidence of particle comminution. In addition, data reported in the literature regarding the rate-sensitivity of both breakage and deformation in granular packings were used to formulate a breakage kinetics applicable under both low and high strain rate regimes. Finally, the newly formulated constitutive law was implemented into a computational platform to solve boundary value problems via the Finite Element Method, detailing in this way the ability of the new framework to capture highly heterogeneous grain ruptures by means of data about the initial conditions of the packing and the fracture properties of its grains. The results of this project provide new simulation tools to quantify the influence of a range of grain-scale attributes rarely considered in continuum-scale engineering design protocols (e.g., particle size, shape, and polydispersity). As a result, findings and methods deriving from this project can assist the design of granular barriers and shock absorbers with tunable dissipative characteristics, informing at the same time the fabrication of new materials consisting of interacting units with different morphology and mechanical properties.

The abovementioned goals have been pursued through the following methods:

- 1) Comminution experiments assisted by x-ray tomography and digital image analysis aimed at quantifying grain fracture mechanisms, evolving grain morphology, and spatiotemporal patterns of breakage.
- 2) Formulation of a Discrete Element Model for crushable particles accounting for the local fracture strength of individual grains and its statistical variability, as well as allowing for arbitrary particle failure mechanisms.
- 3) Formulation of a continuum thermodynamics constitutive law quantifying energy loss at microscopic and macroscopic length scales on the basis of a dynamic fracture kinetics and by accounting for the grain-scale micro-inertia.
- 4) Implementation of the new constitutive law in computational platforms to solve boundary value problems, in conjunction with a strategy to map data from digital images into the mesh, thus better identifying the causes of spatially heterogeneous breakage fields.

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Accomplishments: 1) Inspection of confined comminution due to grain-scale fracture with x-ray micro-tomography:

This project has conducted comminution experiments in packed granular samples. In particular, x-ray tomography and digital image analysis were used to bridge grain scale fracture mechanisms to macroscopic deformation.

The experiments were conducted through a portable compression device suitable for x-ray tomography scans. Sands with similar grain size but different particle shape were used in the tests. The experiments were accompanied by the development of a particle tracking algorithm designed to quantify the 3D kinematics of grains and their evolving morphology. The algorithm compares digital images from successive scans by searching for a match between particles. If no match is found, such as in the case of crushing, further detection criteria are used to identify the fragments generated by the rupture of a grain. This procedure facilitates the discovery of relations between different generations of fragments.

The new algorithm enabled the quantification of the statistics of crushed fragments and the determination of their mode of fracture. The results show that the degree of grain shape evolution depends on the initial morphology, with rounded particles exhibiting the most severe shape alterations. However, it was found that at high compressive stress all morphological indices approach similar values. Such a tendency is achieved when crushing involves primarily the finer fractions – that is, when cushioning hinders the rupture of larger particles. A quantitative assessment of the mode of particle failure also revealed that comminution is not achieved abruptly, but is rather attained by way of successive stages of splitting and chipping. These findings suggest that in crushable solids the initial grain shape plays a key role during the first stages of loading, but its influence vanishes at high pressure, when cushioning mitigates the role of initial morphological differences and hinders further breakage.

The algorithm also enabled an examination of the evolution of particle shapes. This analysis was accomplished by combining particle tracking with fitting procedures based on geometric approximations of the grains. Such strategy allowed the quantification of the three principal lengths of each particle. The results pointed out a strong correlation between the aspect ratio of parent and child particles. This finding can inform geometric models describing the shape of grains undergoing size reduction and was used to build an enhanced breakage constitutive law.

Finally, the experiments prompted the formulation of a Discrete Element Model (DEM) able to replicate the observed multiplicity of grain fracture mechanisms. This 3D DEM approach was aimed at reproducing the size-dependence of the fracture strength, while allowing for an arbitrary geometry of the crushing mechanisms. This goal was accomplished through a bonded particle framework able to simulate grain ruptures through the disintegration of agglomerates made of bonded spheres. The good agreement between experiments and DEM results, combined with the inherent dynamic formulation of this method, suggest that it is a valid virtual testing tool to study the response of granular materials at varying strain rates and perform synthetic computations of energy dissipation due to comminution.

2) Continuum thermodynamics modeling of high-strain-rate comminution in granular solids:

The project tested the possibility to link dynamic grain-scale fracture models and continuum breakage mechanics. This connection was first tested for quasi-static crack growth models. By using a crack growth kinetics characterized by an activation threshold, it was possible to establish an analogy with yielding in packed assemblies. The proposed formulation retains the benefits of the original model (i.e., the ability to account for the initial grading of the material and track its evolution), while incorporating rate effects through subcritical crack growth properties. The model was tested against quasi-static comminution experiments with a stage of creep. The performance was satisfactory, in that both the deformation response and changes in grain size distribution were replicated for a range of applied stresses and test durations.

To test the ability of the rate-dependent breakage model under a wider range of conditions, high-strain rate data from Split-Hopkinson bar tests were used for validation. Although the model was able to capture the first-order features of the response, the analysis found that stationary values of viscosity do not lead to a fully satisfactory performance. In fact, while improvements are possible by adjusting the breakage fluidity as a function of the imposed rate of deformation, the study showed that a more versatile framework is required to encompass dynamic loading. For this purpose, the breakage model was augmented by: (i) modifying the breakage kinetics on the basis of dynamic crack growth laws; (ii) incorporating grain-scale micro-inertial effects based on granular hydrodynamics theories. This formulation led to non-stationary levels of fluidity and allowed the constitutive model to replicate the

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crushing response of sand at both low and high strain rates. The model was tested for two datasets and it was found that the predicted evolution of the macroscopic fluidity was similar to that obtained from the optimized viscous-breakage law, but without need of parameter adjustment. During the last stages of the project, this framework was extended to mixed shear and compression loading, as well as to varying packing density.

Finally, to account for the findings of the x-ray tomography experiments, the effect of grain shape alteration due to comminution was taken into account. This activity was conducted by providing a geometric interpretation for the similarity between the shape of the fragments and of their parent particles. This interpretation was based on a 3D prism preserving its aspect ratio upon successive splits. By observing that this prism had an aspect ratio consistent with that of crushed grains found at planetary impact sites, it was postulated that its value can be used as an attractor for the ultimate shape of crushed particles. This hypothesis was incorporated into an augmented breakage model in conjunction with two enhancements: (i) the definition of a strain energy potential dependent on the shape of the particles; (ii) the formulation of a co-evolution law linking changes in particle shape with the breakage growth rate. The continuum simulations resulting from this model are consistent with those obtained with computationally more expensive DEM approaches. Most importantly, the model predicts distinct regimes to attain the attractors for particle size and shape, an aspect that has never been examined until now neither in experiments nor in simulations.

3) Numerical simulation of heterogeneous grain breakage through rate-dependent continuum models:

To use the proposed breakage models in engineering applications, they were implemented in numerical simulation platforms. Their initialization was based on spatially distributed data of particle packing and grain size distribution. If x-ray tomography imagery is available, this procedure results in a full-field characterization of the initial system heterogeneity. This approach was tested against the full field deformation/breakage data collected through during the experiments. For this purpose, the testing setup used was replicated numerically by accounting not only for material heterogeneity, but also for system constraints such as friction at the loading platens and along the confining ring. The simulations show that the formulated numerical model captures satisfactorily the field of porosity evolution, as well as the heterogeneity of the breakage index.

Training Opportunities: The project supported the research training of one postdoctoral scholar (Dr. Jose Lizarraga) and three Ph.D. students (Dr. Changbum Sohn, Ms. Dawa Seo, and Ms. Ritaja Ray). Dr. Sohn was awarded his doctoral degree during the course of the project, while Ms. Seo and Ms. Ray are expected to defend their doctoral dissertations in early 2022. In addition, an undergraduate research assistant (Mr. Alexander Gallard) was mentored and trained in conducting research in engineering mechanics through the financial support of an URAP supplement associated with this project.

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Results Dissemination: The project led to the following international journal publications:

- 1) Sohn, C., Buscarnera, G. (2019). Measurement and simulation of comminution rate in granular materials subjected to creep tests. *Granular Matter*, 21(3), 1-14.
- 2) Marinelli, F., Buscarnera, G. (2019). A Generalized Backward Euler algorithm for the numerical integration of a viscous breakage model. *International Journal for Numerical and Analytical Methods in Geomechanics*, 43(1), 3-29.
- 3) Seo, D., Sohn, C., Cil, M. B., Buscarnera, G. (2020). Evolution of particle morphology and mode of fracture during the oedometric compression of sand. *Géotechnique*, 1-13.
- 4) Cil, M. B., Sohn, C., Buscarnera, G. (2020). DEM modeling of grain size effect in brittle granular soils. *Journal of Engineering Mechanics*, 146(3), 04019138.
- 5) Ray, R., Buscarnera, G. (2021). Simulation of High-Strain-Rate Comminution through a Breakage Model with Adaptive Rate Dependence. *Journal of Engineering Mechanics*, 147(6), 04021030.
- 6) Buscarnera, G., Einav, I. (2021). The mechanics of brittle granular materials with coevolving grain size and shape. *Proceedings of the Royal Society A*, 477(2249), 20201005.

In addition, the following publications are in preparation and are expected to be submitted shortly after the conclusion of the project activities (titles are provisional):

- A) Xue, D., Shahin, G., Seo, D., Lu, X., Buscarnera, G. (2021). Modeling breakage heterogeneity in crushable sands through a CT-FE mapping scheme. In preparation for *Computers and Geotechnics*.
- B) Seo, D., Buscarnera, G. (2021). Sequential shape affinity during confined comminution. In preparation for *Mechanics Research Communications*.
- C) Ray, R., Buscarnera, G. (2021). Continuum modeling of dynamic rate effects in dilative sand through a pseudo-viscous micro-inertial potential. In preparation for *Granular Matter*.

The project outcomes were also disseminated through the following conference and workshop presentations:

- 1) Sohn, C., Cil, M., Buscarnera, G. (2018). Multi-scale assessment of the effect of particle shape on soil crushability, *Engineering Mechanics Institute (EMI) Conference, MIT, May 29-June, 1, 2018*.
- 2) Buscarnera, G. (2019). Constitutive laws for crushable solids accounting for grain-scale processes, *ALERT Geomaterials Workshop, 30th – 2nd October, 2019, Aussois, France*.
- 3) Seo, D. (2019). Tracking grain-scale kinematics in crushable granular materials. *International NSF workshop on Granular and Particulate Networks (PARNET19), Dresden, Germany (July 2019)*.
- 4) Seo, D., Buscarnera, G. (2021). A tracking algorithm to quantify grain fracture mechanisms during compaction, *Engineering Mechanics Institute (EMI) Conference, Virtual Event, May 25-28, 2021*.
- 5) Ray, R., Buscarnera, G. (2021). Simulation of partially drained deformation processes in fluid-saturated crushable sand, *The Biot-Bazant Conference on Engineering Mechanics and Physics of Porous Materials, Virtual Event, June 1-3, 2021*.

Honors and Awards: Ph.D. student Dawa Seo received national and international awards for her research excellence. These include the Chateaubriand Fellowship by the Embassy of France in the United States, the KSEA Scholarship by the Korean American Scientists and Engineers Association, and the IS-ASCE Scholarship by the Illinois Section of the American Society of Civil Engineers.

The research work of Ph.D. student Ritaja Ray was recognized by the *Journal of Engineering Mechanics* by including her paper "Simulation of High-Strain-Rate Comminution through a Breakage Model with Adaptive Rate Dependence" in the Editor's choice list.

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Participant Type: PD/PI

Participant: Giuseppe Buscarnera

Person Months Worked: 1.00

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Project Contribution:

National Academy Member: N

Participant Type: Graduate Student (research assistant)

Participant: Dawa Seo

Person Months Worked: 2.00

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Project Contribution:

National Academy Member: N

Participant Type: Graduate Student (research assistant)

Participant: Ritaja Ray

Person Months Worked: 12.00

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Project Contribution:

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Participant Type: Undergraduate Student

Participant: Alexander Gallard

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Article Title: A Generalized Backward Euler algorithm for the numerical integration of a viscous breakage model

Authors: Ferdinando Marinelli, Giuseppe Buscarnera

Keywords: continuum breakage mechanics, finite element method, integration algorithms, Perzyna viscoplasticity, rate effects

Abstract: This paper discusses the formulation and numerical performance of an implicit algorithm used to integrate a rate-dependent breakage model. For this purpose, a Generalized Backward Euler (GBE) algorithm has been implemented according to two linearization strategies, the former derived by a direct linearization of the constitutive equations, while the latter introduces rate effects through a consistency parameter. The accuracy and efficiency of the GBE algorithm have been investigated by performing material point analyses and solving initial boundary value problems. In both cases, the performance of the algorithm is inspected for a range of loading rates, thus simulating comminution from slow to fast dynamic problems. As the viscous response of the breakage model can be recast through a viscous nucleus function, the algorithm can be considered as a general framework to integrate constitutive equations relying on the overstress approach typical of Perzyna-like viscoplastic models.

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Article Title: Measurement and simulation of comminution rate in granular materials subjected to creep tests

Authors: Changbum Sohn, Giuseppe Buscarnera

Keywords: Comminution · Subcritical crack growth · Creep · Constitutive modeling · Breakage mechanics

Abstract: The subcritical growth of particle cracks and their consequent rupture are responsible for creep in granular solids. Here, a framework inspired by the physics of delayed crack growth is used to interpret creep measurements through continuum variables. Creep experiments were conducted on water-saturated materials with different particle size and shape. The experiments were interpreted and simulated with a kinetics model characterized by a power law expression similar to those used in subcritical crack growth theories. The results show that the model is able to replicate the phenomenology of delayed breakage. The power law coefficient linking the breakage growth rate to the elastic stored energy was found independent of the size of the grains and characterized by values within the range reported the stress corrosion index of quartz. By contrast, the timescale of comminution was size-dependent, thus signaling an increase of elapsed creep time in materials with larger grains.

Distribution Statement: 3-Distribution authorized to U.S. Government Agencies and their contractors

Acknowledged Federal Support: Y

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as of 31-Aug-2021

Partners

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I certify that the information in the report is complete and accurate:

Signature: Giuseppe Buscarnera

Signature Date: 8/22/21 3:56PM

**Final Report: Bridging Dynamic Particle Fracture and High-Strain Rate
Comminution of Granular Continua**

Contract Number: W911NF-18-1-0035
Principal Investigator: Giuseppe Buscarnera

Report submitted by:

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Major Goals

This project aimed to explain how particle ruptures due to grain-scale fracture influence the energy dissipation in particulate solids subjected to rapid loading, as well as to interpret the rate-sensitivity of these materials with principles of crack growth dynamics and granular physics. To bridge length scales, a continuum law linking the rate of comminution to the failure kinetics of single particles was proposed. Direct visualization based on x-ray tomography was used to assess the evolution of the polydispersity of the material, as well as to constrain the modes of grain fracture with both the statistics and the morphology of the breakage products. Such grain-scale data were used to formulate a continuum thermodynamic breakage law, as well as to test its performance against evidence of particle comminution. In addition, data reported in the literature regarding the rate-sensitivity of breakage and deformation in granular packings were used to formulate a breakage kinetics applicable under both low and high strain rate regimes. Finally, the newly formulated constitutive law was implemented into a computational platform to solve boundary value problems via the Finite Element Method, detailing in this way the ability of the new framework to capture highly heterogeneous grain ruptures based on data about the initial conditions of the packing and the fracture properties of its grains. The results of this project provide new simulation tools to quantify the influence of a range of grain-scale attributes rarely considered in continuum-scale engineering design protocols (e.g., particle size, shape, and polydispersity). As a result, findings and methods deriving from this project can assist the design of granular barriers and shock absorbers with tunable dissipative characteristics, informing at the same time the fabrication of new materials consisting of interacting units with different morphology and mechanical properties.

The abovementioned goals have been pursued through the following methods:

- Comminution experiments assisted by x-ray tomography and digital image analysis aimed at quantifying grain fracture mechanisms, evolving grain morphology, and spatiotemporal patterns of breakage.
- Formulation of a Discrete Element Model for crushable particles accounting for the local fracture strength of individual grains and its statistical variability, as well as allowing for arbitrary particle failure mechanisms.
- Formulation of a continuum thermodynamics constitutive law quantifying energy loss at microscopic and macroscopic length scales on the basis of a dynamic fracture kinetics and by accounting for the grain-scale micro-inertia.
- Implementation of the new constitutive law in computational platforms to solve boundary value problems, in conjunction with a strategy to map data from digital images into the mesh, thus better identifying the causes of spatially heterogeneous breakage fields.

In the next sections, further details are provided about the findings resulting from this.

Accomplishment Under Goals

Inspection of confined comminution due to grain-scale fracture with x-ray micro-tomography

Dynamic penetration and impact on granular beds are known to cause large deformation and severe microstructural alterations. These processes usually trigger a highly rate-sensitive response of the bed subjected to disturbance. Considerable evidence suggests that grain breakage is a major cause of such rate-sensitive response, in that it may involve pervasive fracture of the bed constituents. To examine this hypothesis, this project has bridged two scales of analysis, namely the grain scale (at which microscopic fracture occurs) and the continuum scale (which focuses on the macroscopic deformation resulting from particle interactions). For this purpose, the project conducted confined comminution experiments in packed granular samples, used x-ray tomography to examine the link between grain scale fracture and macroscopic deformation, and analyzed the collected x-ray scans via digital image analysis. The findings from the testing program were eventually used to formulate a continuum-scale constitutive law based on the mechanics of grain-scale fracture, as well as to test the model performance in the context of full-field numerical analyses.

The experiments were conducted through a portable miniaturized compression device suitable for x-ray tomography scans. Testing was conducted on two sands characterized by similar grain size but different particle shape (i.e., angular and round particles, respectively; Figure 1). The testing program led to a depiction of the deformation within the specimens, as well as of the corresponding changes in particle size gradation. High-resolution imaging also enabled the quantification of grain shape alterations. It was found that particle angularity promotes contact fracture and pervasive fragmentation. This effect was nearly absent from the initial scans of round particles and revealed an important role of contact indentation in affecting the magnitude and rate of breakage.

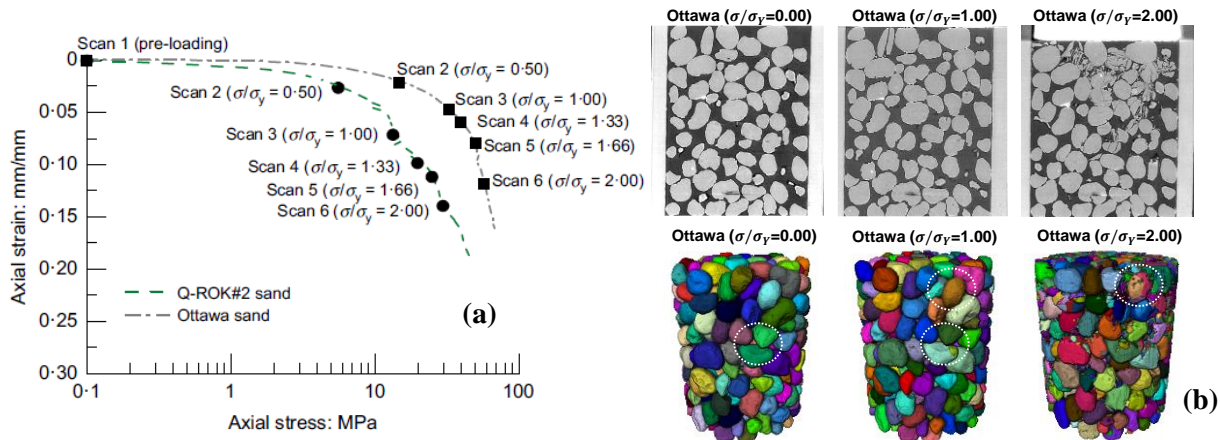


Figure 1. (a) Compression experiments on two sands (angular Q-ROK#2 and rounded Ottawa) with x-ray tomography scans performed at selected stresses; (b) examples of radiographs acquired during the experiments, along with a 3D rendering of the packing after segmentation and labelling. The images display the development of pervasive breakage in the tested specimens [after Seo et al., 2020].

The experiments were accompanied by the development of a particle tracking algorithm designed to quantify the 3D kinematics of individual grains (i.e., displacements and rotations) and their

morphology (Figure 2). The algorithm operates by comparing digital images from successive scans. This is accomplished by searching for a match between particles within a control window defined based on the movement of the particles across the volume of interest. The match is finally pursued by setting strict tolerances for the size and shape of the particles within the test area. If a match is found, incremental kinematic quantities are computed, which can later be used to define local and homogenized deformation measures. Instead, if no match is found, such as in the case of crushing, further detection criteria are used to identify the fragments generated by the rupture of a grain. Such procedure relies on a cumulated volume matching between the original particles and their fragments and enables to cluster the particles into classes on the basis of their order of appearance. This procedure facilitates the discovery of relations between different generations of fragments, necessary to examine correlations between the initial morphology of the grains and the shape and number of the fracture products.

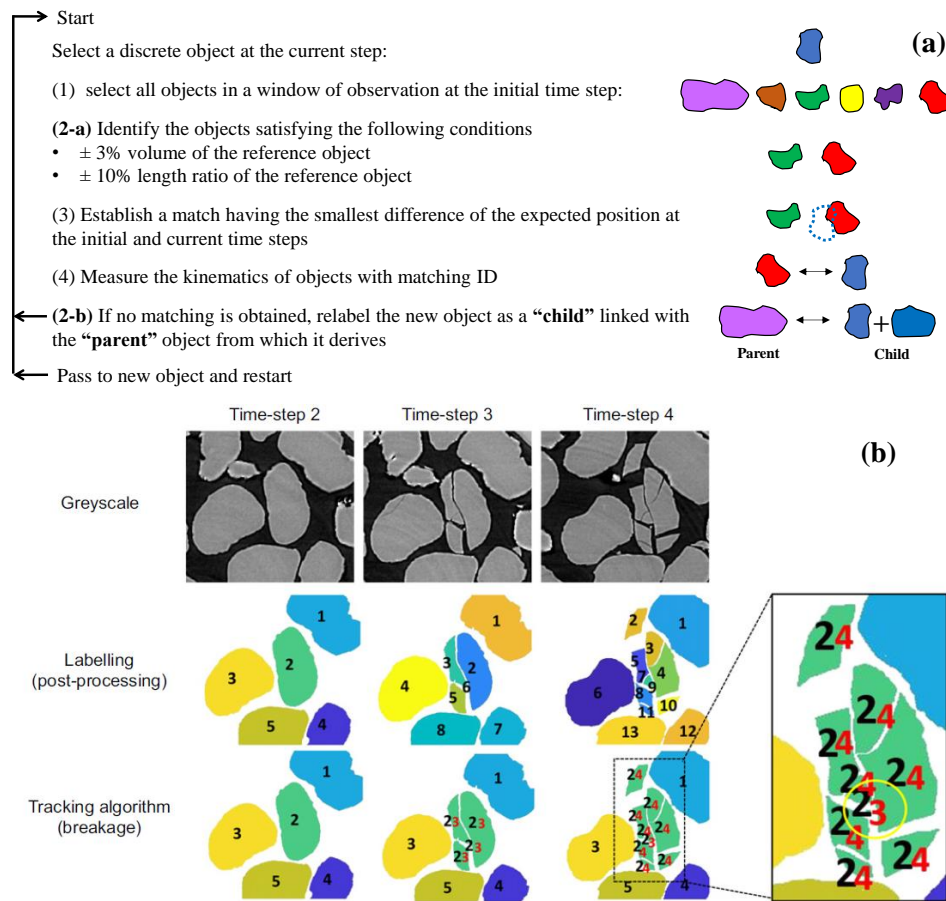


Figure 2. (a) Schematic of the tracking algorithm detailing the tolerances to identify a particle match between consecutive scans. The strategy to quantify the number and characteristics of the fragments resulting from particle ruptures, as well as the correspondence between parent and child grains is also illustrated; (b) Cross-section of images processed with the tracking algorithm. Black labels indicate the index number of the original (intact) particles. The second number indicates the time step at which crushed fragments were detected [after Seo et al., 2020].

The new algorithm enabled the quantification of the statistics of fragment generation (i.e., number of fragments generated by each fracture event) and the mode of fracture (i.e., whether particles were damaged via chipping, splitting, or comminution). Our results show that the degree of grain shape evolution depends on the initial morphology, with subrounded particles exhibiting the most severe shape alterations. However, it was found that at high compressive stress all morphological indices approach similar values. Such a tendency is achieved when crushing involves primarily the finer grain fractions – that is, when cushioning hinders the rupture of larger particles. A quantitative assessment of the mode of particle failure also revealed that comminution is not achieved abruptly in either of the two tested sands (Figure 3), but was rather attained by way of successive stages of splitting and chipping. These findings suggest that in crushable solids the initial grain shape plays a key role during the first stages of loading leading to yielding, but its influence tends to vanish at high pressure, when cushioning mitigates the role of initial morphological differences and hinders further major breakage.

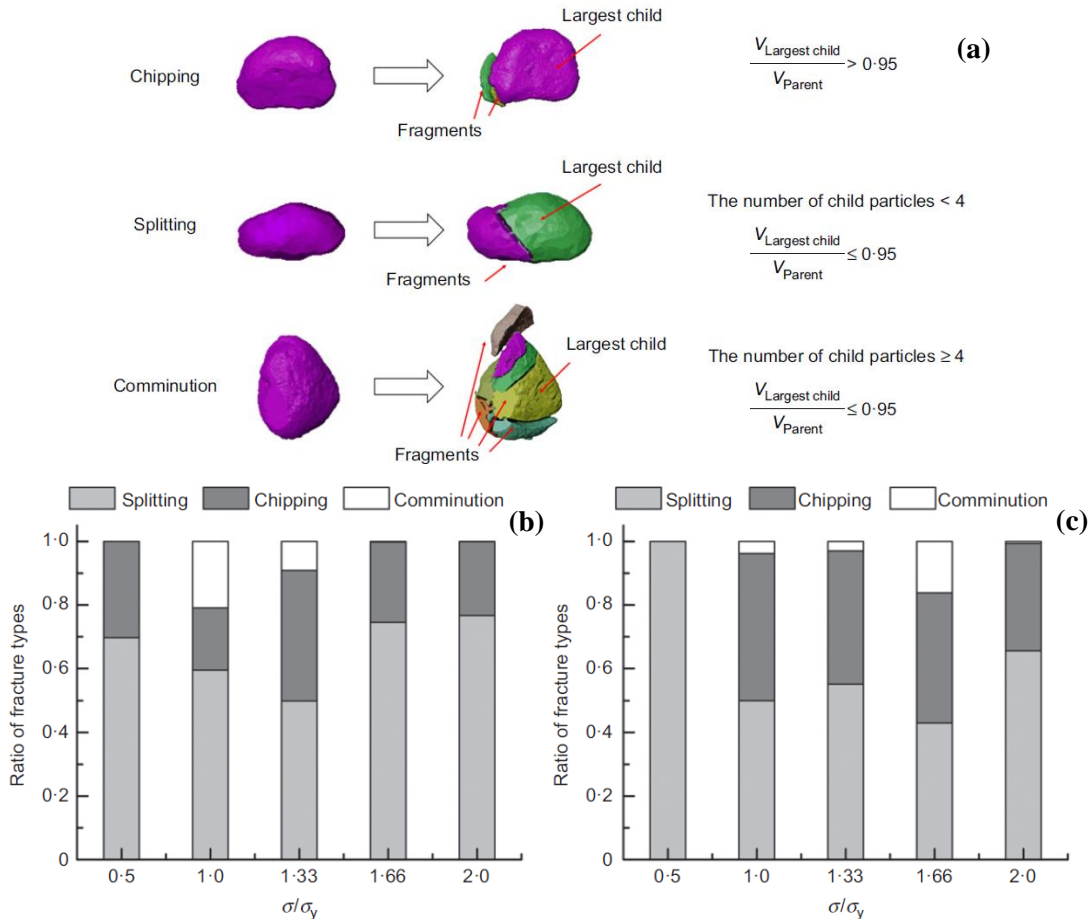


Figure 3. Mechanisms of particle failure defined on the basis of the incremental ruptures detected through digital image analysis: chipping, splitting and comminution (a); evolution of incremental fracture mechanisms for Q-ROK#2 (b) and Ottawa sand (c) [after Seo et al., 2020].

The data processed with the algorithm also allow the study of the statistics of the crushing products. The goal of this analysis is to identify relations between the different mechanisms of grain-scale

fracture and the size of the parent particle from which a given event emerged. Our analysis shows that at yielding failure events are rather uniformly distributed across the affected particle sizes for both splitting and chipping mechanisms. At higher stress levels, however, incremental splitting concentrates on the finest fractions (i.e., particles with equivalent size smaller than 0.075 mm), which display the highest values of relative frequency (85% in Q-ROK#2 and 51% in Ottawa). This result suggests presence of cushioning at high compressive stress (i.e., small grains hindering rupture of large grains). Most notably, it is apparent that cushioning affects more significantly the splitting rather than the chipping events. In fact, while for splitting the frequency peaks are identifiable both for Q-ROK#2 and Ottawa sands, in the case of chipping the frequency peaks for events affecting the finest grain fractions are either weaker (Q-ROK#2) or missing (Ottawa).

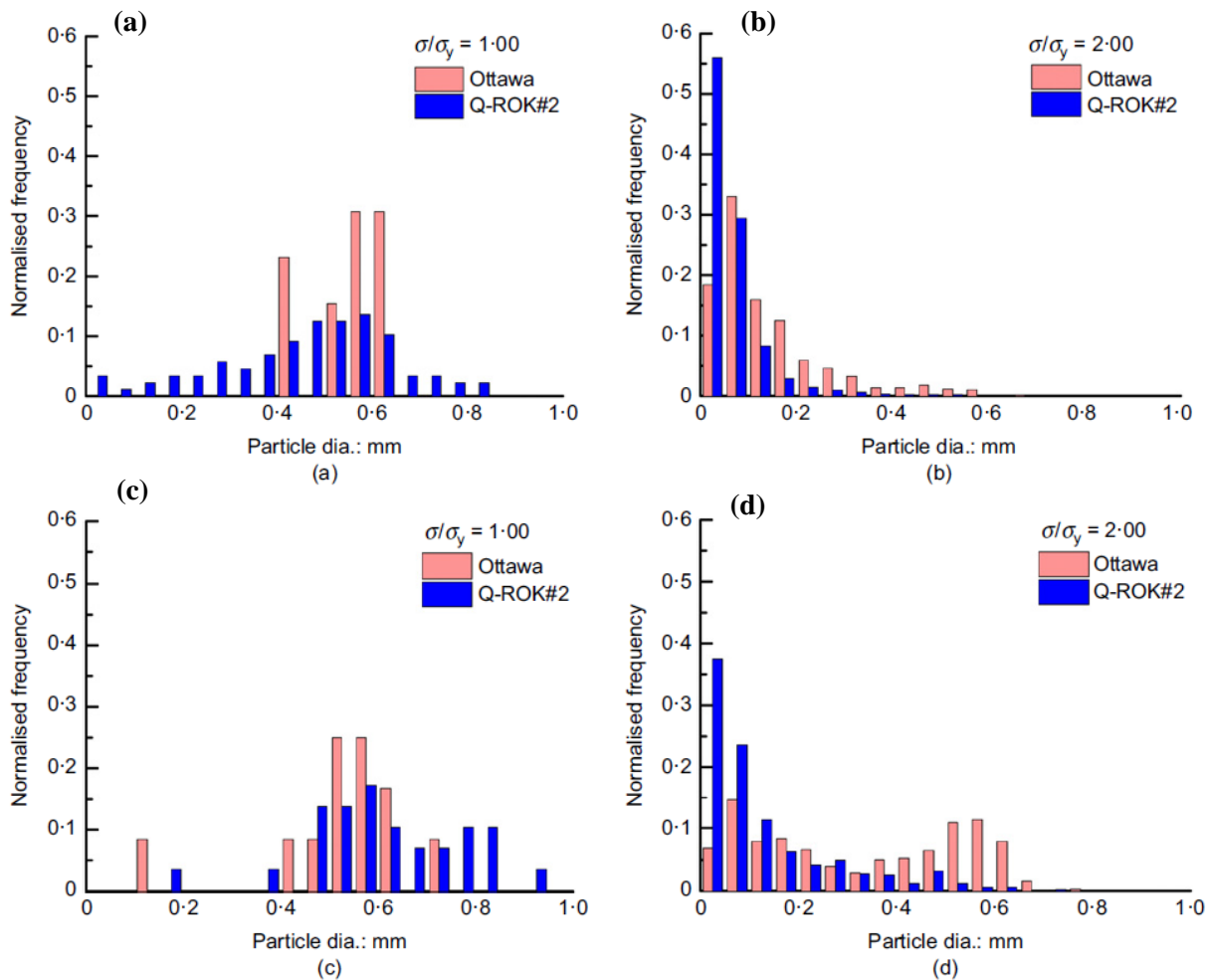


Figure 4. Normalized frequency plot of incremental failure mechanisms plotted as a function of the diameter of the parent particle: splitting at (a) $\sigma/\sigma_y = 1.00$ and (b) $\sigma/\sigma_y = 2.00$; chipping at (c) $\sigma/\sigma_y = 1.00$ and (d) $\sigma/\sigma_y = 2.00$ [after Seo et al., 2020]. The symbol σ_y indicates the yielding stress of the two sands, here used to normalize the applied stress ($\sigma_y = 15$ MPa for QROK#2; $\sigma_y = 29$ MPa for Ottawa) [after Seo et al., 2020].

The algorithm also enabled an examination of the evolution of particle shapes upon fracture. This analysis was accomplished by combining the outcomes of individual particle tracking with a set of fitting procedures based on geometric approximations of the grains (Figure 5). Such strategy enabled the quantification of the three principal lengths of each particle (i.e., shortest, intermediate, and longest dimension) and of non-dimensional ratios depending on these values (e.g., aspect ratio, flatness, and elongation). In addition to quantifying how these attributes evolve upon loading, our results point out a remarkable correlation between the aspect ratio of parent and child particles. This finding can inform geometric models describing the shape of grains undergoing size reduction and was used in subsequent stages of this project to build an enhanced continuum breakage model.

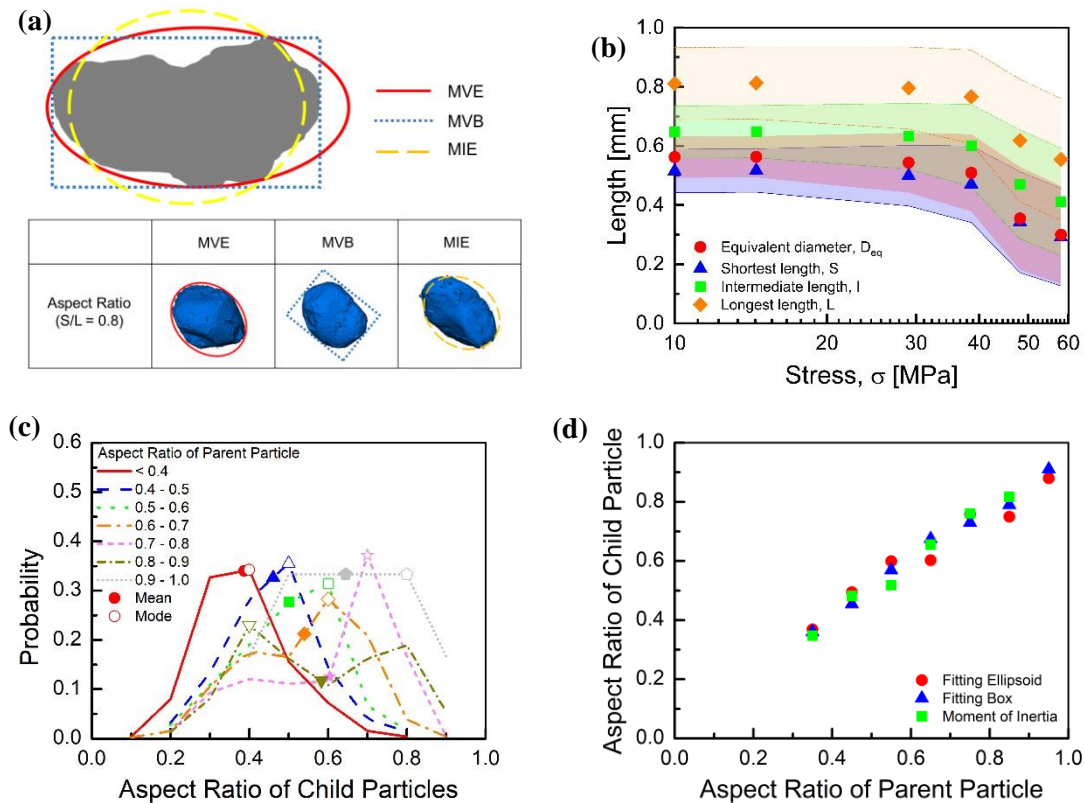


Figure 5. (a) Fitting of 3D particle morphology with three strategies: Minimum Volume Ellipsoid (MVE), Minimum Volume Box (MVB), and Moment of Inertia Ellipsoid (MIE); (b) Evolution of the average principal dimensions of crushed particles within an assembly (example based on the MVE fitting strategy); (c) frequency plot of the aspect ratio of several families of fragments (child particles) grouped in terms of the aspect ratio of the corresponding parent particles; (d) Correlation between the modal values of the statistics of the breakage products and that of their parent particles.

Finally, the complexity of the particle failure mechanisms detected by the experiments prompted the formulation of a Discrete Element Model (DEM) able to replicate the statistical variability of the particle strength, as well as the multiplicity of the potential grain fracture mechanisms. The 3D DEM approach formulated by this project is therefore aimed at reproducing the size-dependence of the particle fracture strength, while allowing for an arbitrary geometry of the resulting failure mechanisms. This goal was accomplished through a bonded particle framework able to simulate grain ruptures through the disintegration of agglomerates made of bonded spheres (Figure 6). Such

strategy enables the representation of general initial shapes for the grains and poses no restrictions for the ensuing morphology of the fragments, allowing for chipping or splitting events depending on the computed magnitude and location of inter-particle forces. The model was tested against diametric loading tests on single particles and oedometric compression experiments on packed granular specimens. The size effect and variation of the particle strength were evaluated in terms of stress and energy measures and interpreted via Weibull statistics. It was shown that our DEM approach successfully captures the particle strength variability and the size-dependence of the failure and yielding strength at particle- and assembly-scale, respectively. The breakage levels computed upon confined compression were compared with those measured in the experiments by means of a relative breakage index (Figure 7). The agreement between experiments and numerical results suggests that the proposed DEM approach can be employed to simulate the comminution of crushable granular solids, thus being useful to study size reduction processes when direct testing is impractical. In addition, given the inherently dynamic nature of DEM techniques, the model is a valid virtual testing platform to study the response of granular solids at varying strain rates, as well as to compute energy dissipation contributions at multiple length scales.

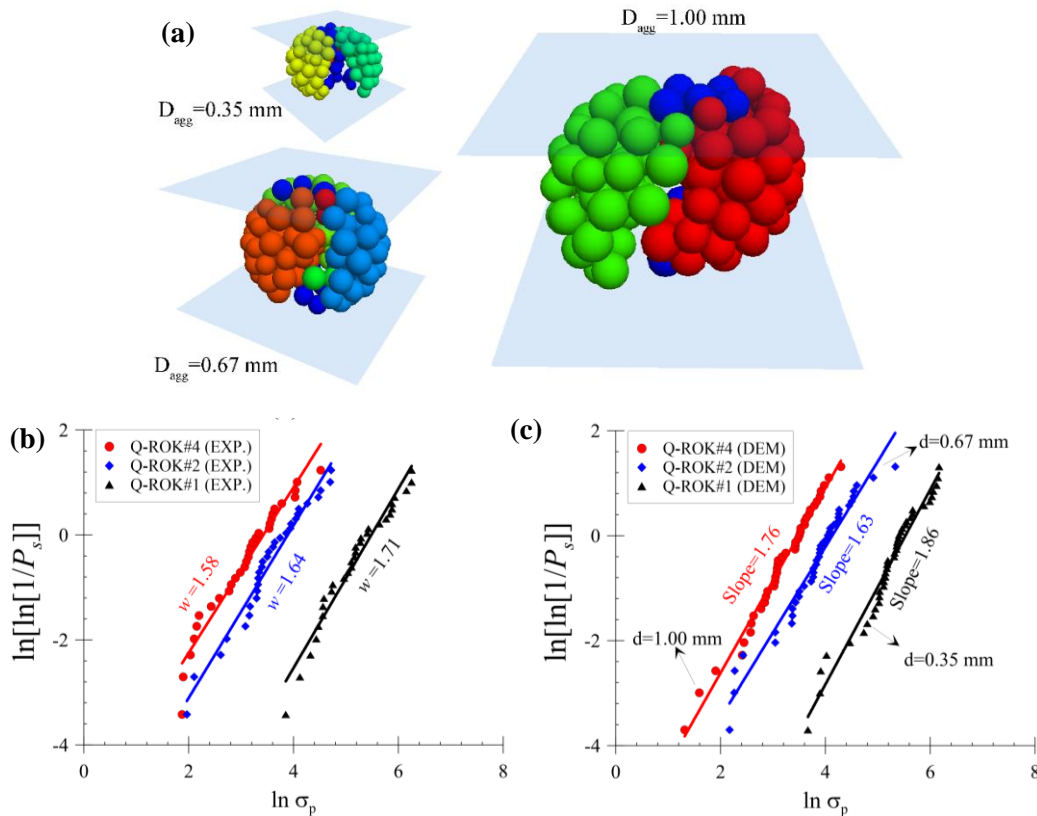


Figure 6. (a) View of bonded particle agglomerates of different size after diametric compression simulation. In the simulations, particle failure emerges from the rupture of the bonds making up the agglomerate. Different colors represent separate newly formed fragments after crushing; Weibull plots of particle strength measured in experiments on QROK sands (b) and computed via DEM simulations (c) [after Cil et al., 2020].

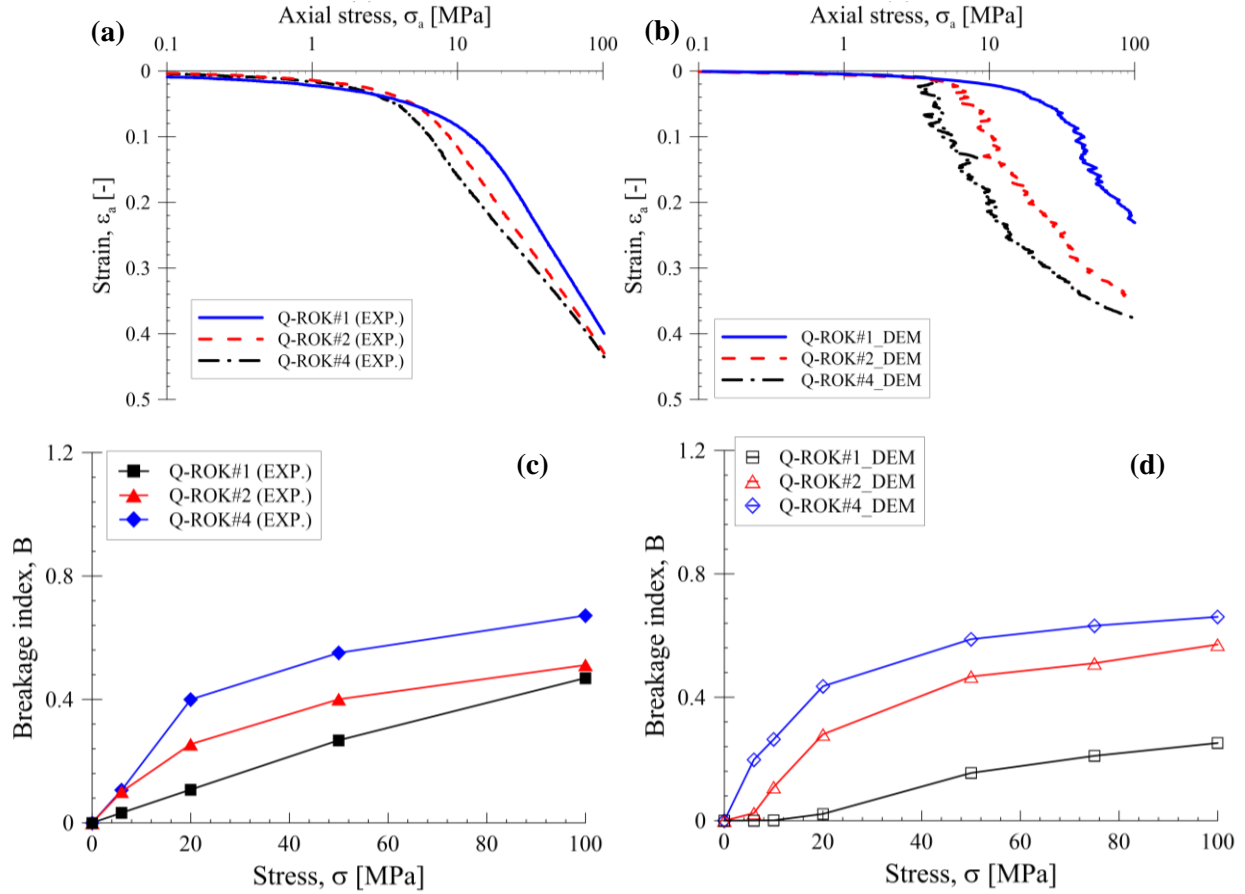


Figure 7. Axial stress-strain response relative to oedometric compression experiments on angular QROK sand (a) and DEM simulations (b); Evolution of the breakage index, B , during oedometric compression experiments (c) and simulations (d) for Q-ROK sands with different initial grain sizes. The results illustrate the ability of the DEM model to replicate breakage growth patterns measured in on particle assemblies solely on the basis of a calibrated grain-scale fracture model [after Cil et al., 2020].

Continuum thermodynamics modeling of high-strain-rate comminution in granular solids

The findings of the experimental program summarized above, along with evidence available in the literature, constituted the basis for the formulation of augmented breakage models able to capture multiple sources of dissipation in granular solids subjected to rapid loading. Breakage Mechanics is a continuum thermodynamics framework conceived to account for the energetics of particle breakage due to high-pressure loading in granular packings. In analogy with Damage Mechanics models, it encapsulates strain energy release and consequent dissipation into an internal variable associated with distributed fracture. However, at variance with the micro-cracking simulated by damage models, the release of strain energy is associated with the fracture of particles, and hence with the shift of the grain size distribution towards finer gradings. To examine the possibility to extend such approach to rate-dependent settings, the project tested the validity of the link between grain-scale fracture and macroscopic breakage for a quasi-static crack growth kinetics. For this purpose, the breakage evolution equation was constructed by setting up an analogy with the rate

of crack growth in grains subjected to diametral compression (Figure 8). This is possible by referring to subcritical crack growth models, widely used to simulate the propagation of flaws in brittle solids at stress concentration levels lower than those leading to instantaneous fracture. By using a crack growth kinetics characterized by an activation threshold, it was possible to establish an analogy with yielding in packed assemblies. Since in breakage models yielding is given in energy terms, this analogy led to a breakage kinetics characterized by a power law relation similar to that of subcritical crack growth laws, but dependent on the variables controlling the onset of comminution in an otherwise rate-independent granular continuum. In other words, the formulation is mathematically consistent with that of classic overstress viscoplastic approaches, with the main difference that the overstress violation is now computed in terms of breakage energy. The proposed formulation retains the key benefits of the original model (i.e., the ability to account for the initial grading of the material and track its evolution), while incorporating rate effects as a function of the subcritical crack growth properties embedded in the breakage kinetics (i.e., stress corrosion coefficient and breakage energy threshold). The model was tested against quasi-static comminution experiments with a stage of loading followed by creep. The performance of the model was satisfactory, in that the deformation response was replicated for a range of applied stresses and test durations. Most notably, the model was found able to capture changes in grain size distribution (GSD) during both compression and creep, in that changes in GSD were naturally reflected by the evolution of the breakage index, B .

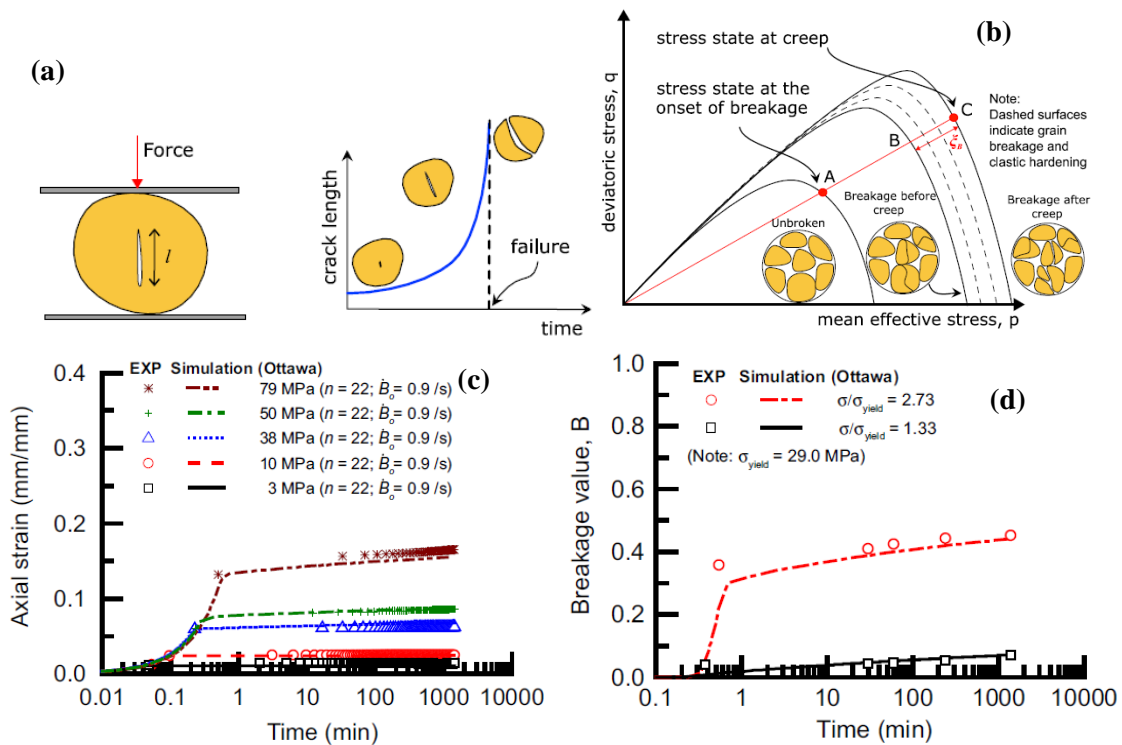


Figure 8. Schematic of subcritical crack growth in grain subjected to diametral compression (a) and continuum generalization in terms of overstress due to a violation of the rate-independent breakage yielding criterion (b). Model performance in capturing the compression and creep response of sands subjected to high-pressure compression. The model is shown capable of replicating both compression response (c) and breakage growth (d) with a set of parameters based on the subcritical crack growth properties of the particles [after Sohn and Buscarnera, 2019].

To test the ability of the rate-dependent breakage model under a wider range of loading conditions, high-strain rate experiments available in the literature were used as a part of the validation strategy. For this purpose, data from Split-Hopkinson bar compression tests on different granular materials were used. Although the model was able to capture the first-order features of the compression response, the analyses found that the use of stationary values of macroscopic viscosity leads to unsatisfactory performance upon strain rate increase (Figure 9). Specifically, quasi-static breakage kinetics relations were unable to capture the rate-sensitivity of the response at both low and high strain rates with a unique set of parameters. As a result, improved simulations had to be based on adjusted values of breakage fluidity expressed as a decreasing function of the rate of deformation. This practice was found to reduce the range of applicability of this class of rate-dependent breakage models and may result in ad-hoc strain-rate-dependent fluidity functions.

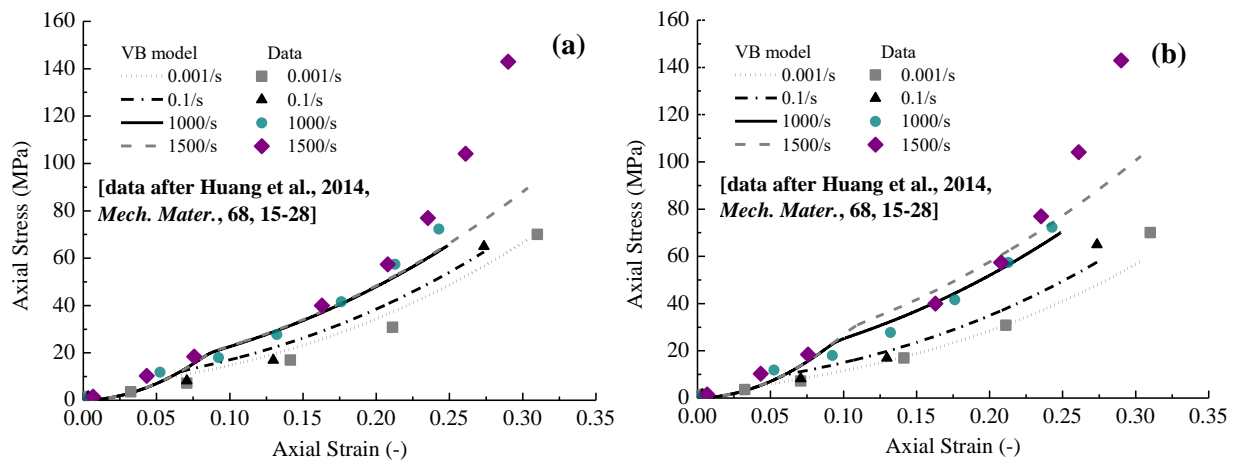


Figure 9. Performance of different viscous-breakage (VB) constitutive laws against evidence of rate-dependent compression behavior in quartz sand subjected to Split Hopkinson Bar compression tests: (a) VB model with stationary fluidity; (b) VB model with values of stationary material fluidity optimized for each imposed strain rate. The results show the ineffectiveness of stationary fluidity, especially at high strain rate. While the use of optimized values of fluidity for each test mitigates the problem, this example illustrates the need to improve the breakage kinetics for dynamic loading [after Ray and Buscarnera, 2020].

We found that improved simulations can be achieved by using an adaptive fluidity. Such result was achieved by: (i) modifying the breakage kinetics on the basis of dynamic crack growth theories; (ii) incorporating micro-inertial effects on the basis of granular hydrodynamics models. While the former enhancement resulted into an augmented power law expression of the breakage kinetics, the latter was pursued by expressing the breakage fluidity as a function of the granular temperature, i.e., a measure of the frequency of particle collisions in a granular system. This choice led to an evolution equation for the breakage fluidity reflecting micro-inertial effects due to the application of high strain rates. This formulation led to non-stationary macroscopic fluidity (i.e., values of fluidity which not only changed with the imposed strain rate, but that also evolved during a single test as a function of changes in microstructural state variables). Such modifications allowed the constitutive law to replicate successfully the crushing response of sands tested at both low and high strain rates. Specifically, at low strain rates the predictions were found to converge

to those provided by the progenitor viscous-breakage model. By contrast, when used under high strain rates spikes of granular temperature led to a transient growth of the macroscopic viscosity, as well as to delays in the accumulation of inelastic deformation. The model was tested for two datasets available for quartz sands tested at varying strain rates (Figure 10). It was found that the evolution of the granular temperature yielded changes of fluidity similar to those obtained from the optimization of the viscous-breakage law with stationary viscosity. In addition, the new model was found to provide a more realistic prediction of the compression behavior by eliminating the sharp transition from elastic to viscoplastic response characteristic of the progenitor model.

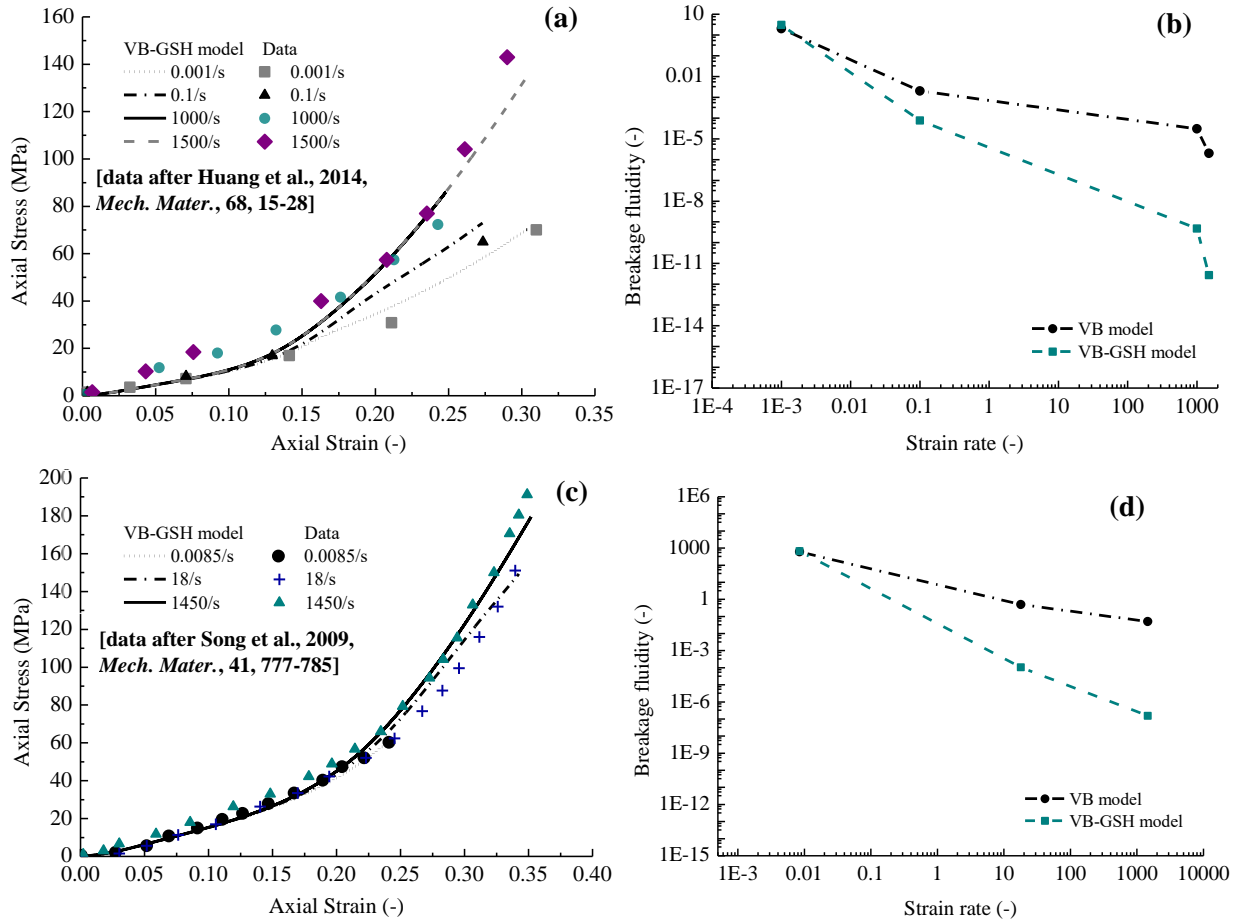


Figure 10. Simulation of compression response for sands subjected to a wide range of strain rates in Split Hopkinson bar compression tests. The results show that the adaptive fluidity leads to improved results across the entire spectrum of imposed strain rates (a, c). Most notably, the variation of the fluidity (b, d) associated with granular temperature evolution (VB-GSH model) is found to provide similar trends to those obtained via optimization of the model with stationary fluidity (VB model). This prediction corroborates the fluidity evolution law, which was formulated independently of the optimized results obtained through the original model [after Ray and Buscarnera, 2021].

During the last stages of the project, this framework was extended to encompass mixed shear and compression loading, as well as varying packing density. For this purpose, scenarios characterized by energy dissipation without grain crushing were simulated by implementing a recently proposed

approach allowing for dilative volumetric response at low pressure (i.e., without particle breakage) and plastic compaction coupled to breakage at high pressure. Also in this case, the formulation was extended to simulate rate-dependent deformation responses by incorporating dissipative terms linked to micro-inertial effects. The dependence of these terms on the breakage rate once again led to adaptive rate dependence in the high-pressure loading regime. Figure 11 illustrates selected examples of model performance relative to triaxial compression tests conducted at a range of high strain rates. The analysis shows the ability of the augmented rate-sensitive model to capture HSR responses for different confinement levels and initial density conditions.

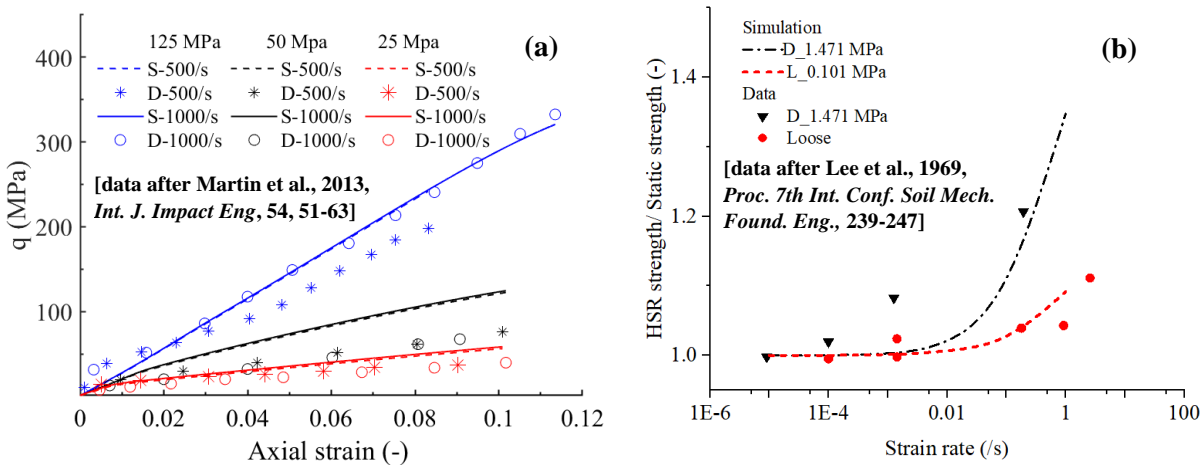


Figure 11. Model performance in simulating undrained HSR triaxial tests under varying confinement pressures; model performance in simulating changes in the ratio between the dynamic and static shearing resistance of sand subjected to varying strain rates for different levels of packing density.

Finally, to account for the findings of the x-ray tomography experiments conducted in this project, grain shape evolution was incorporated by means of a thermodynamic formulation with additional dissipative state variables. Such variables were linked to the current grain shape, thus introducing new dissipative terms reflecting how grain-scale fracture modifies the particle morphology. This activity was conducted by developing a geometric interpretation for the experimentally observed similarity between the shape of the fragments generated by particle rupture and that of their parent particles (Figure 5). Figure 12 provides a schematic depiction of a 3D prism fulfilling this property upon successive splitting events. Such property can be shown to be satisfied when the splits occur at the center and the aspect ratio has a specific value, referred to as silver ratio. Interestingly, the value of this ratio was consistent with the aspect ratio of heavily crushed particle systems found at planetary impact sites. Given the extreme crushing suffered by these systems, we postulated that such critical value of aspect ratio serves as attractor for the particle shape, similar to how power law relations are widely accepted attractors for the size polydispersity of crushed grains. These hypotheses were incorporated into an augmented continuum breakage model along with two other key elements: (i) the definition of a strain energy potential dependent on the shape of the particles; (ii) a co-evolution law linking changes in shape with the breakage growth rate. The treatment of the particle shape as a new state variable lead to a more complex energetics of comminution, which involved corrective terms taking into account the underlying variability of the mode of fracture.

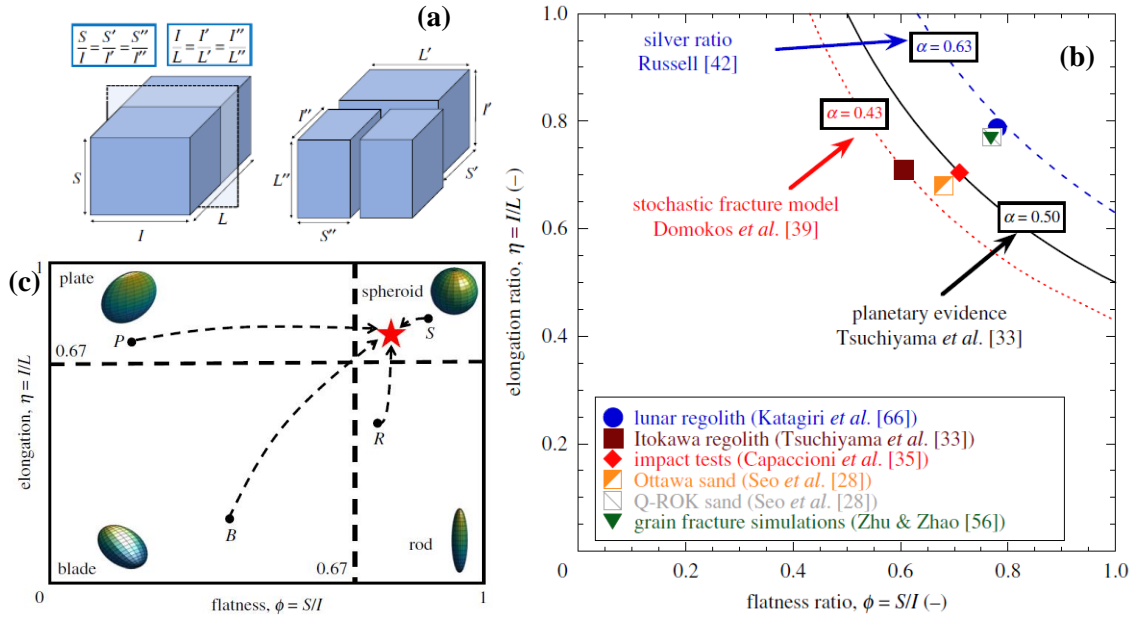


Figure 12. (a) Splitting events in a 3D prism with specific aspect ratio (*silver prism*). The aspect ratio of the prism is preserved in the crushing products if the initial aspect ratio is $2^{2/3}$ and fractures occur through the center; (b) data for heavily crushed systems. The aspect ratio is found within a small range regardless of the mechanism that caused fragmentation; (c) morphometric plane describing the evolution of the 3D shape towards an attractor [after Buscarnera and Einav, 2021].

The continuum-scale simulations resulting from this model are shown in Figure 13 with reference to virtual and physical experiments. The results illustrate the ability of the model to simulate changes in particle shape due to compression. Notably, the results are consistent both qualitatively and quantitatively with those obtained with computationally more expensive DEM approaches. Most importantly, the model predicts distinct regimes to attain the attractors for particle size and shape, an aspect that has never been examined until now neither in experiments nor in simulations.

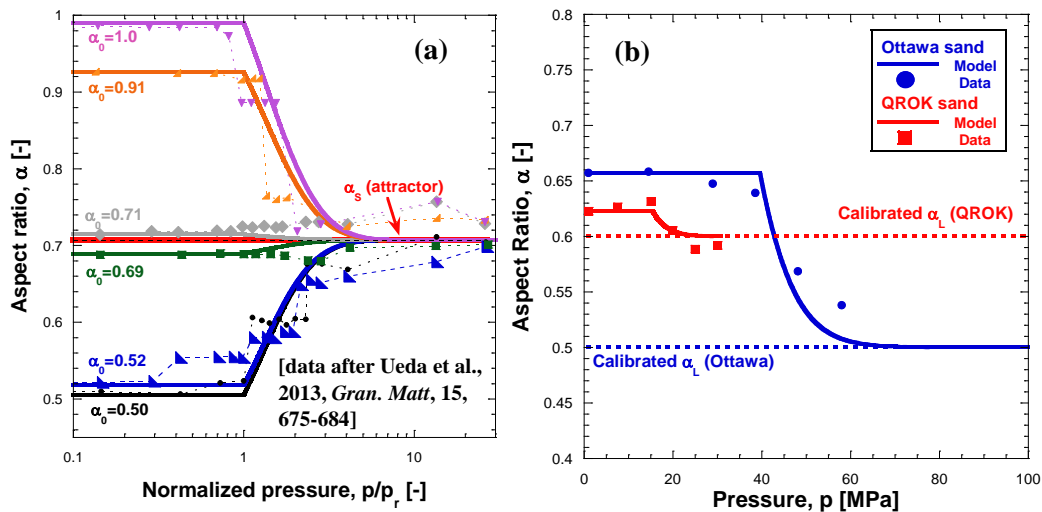


Figure 13. Continuum simulation of shape evolution (solid lines) due to comminution compared with DEM numerical results (a) and laboratory experiments (b) [after Buscarnera and Einav, 2021].

Although the shape-dependent constitutive model formulated in the final stage of this project was designed with reference to compressive quasi-static loading, the incorporation of its new elements into advanced model formulation such as those discussed for HSR loading is straightforward. The combination of such formulations may therefore lead to hierarchical models in which different sets of capabilities can be activated or not depending on the goals of a simulation or the availability of data. Regardless of the details of the formulations, the possibility to ask new questions that these models offer, especially with reference to geometric attractors, constitutes a fundamental scientific finding which can open new avenues to understand the behavior of particulate matter subjected to mechanical extremes, as well as to the design of improved material fabrication technologies aimed at controlling microscale fracture and achieve desired targets for the macroscopic properties.

Numerical simulation of heterogeneous grain breakage through rate-dependent continuum models

To apply the proposed constitutive laws in engineering applications, the proposed breakage models were implemented into numerical simulation platforms. This activity focused on the development of a user defined UMAT subroutine applicable for the general-purpose Finite Element (FE) code ABAQUS. Since a key benefit of the proposed class of breakage models is the use of state variables with a clear physical interpretation, model initialization for numerical analyses was combined with the use of spatially distributed data of initial packing and grain size distribution prior to loading. The benefits of this strategy are evident if x-ray tomography imagery is available, in that it results in a full-field characterization of the initial system heterogeneity. This procedure is illustrated in Figure 14, with reference to laboratory experiments on compressed granular solids. Specifically, to define initial porosity and grain size distribution across the volume of interest, the initialization procedure formulated in this project uses the concept of Reference Elementary Volume (REV). Once the REV on the basis of the statistical fluctuations of pre-selected physical properties (e.g., porosity), its value is used to set the size of a control window. Such window is then centered in correspondence of each Gauss point of the computational mesh and used to compute the local value of the state variables required for model initialization. This procedure is applied throughout the domain to fully define initial conditions prior to loading.

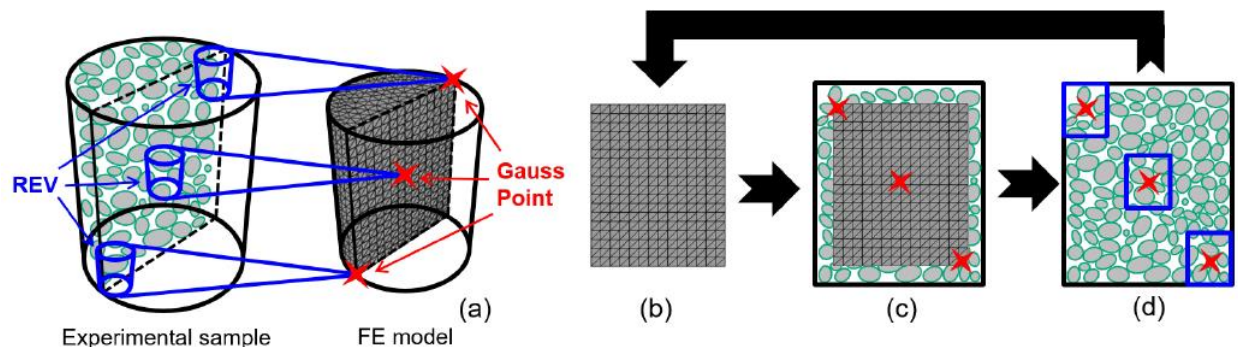


Figure 14. Illustration of the computed-tomography to finite-element (CT-FE) mapping scheme used in this project: (a) conceptual schematic; (b) extraction of Gauss integration point coordinates; (c) projection of the coordinates onto a digital image embedding measurements; (d) superposition of the REV window at each Gauss integration point, over which averaged variables are computed.

This procedure has been tested against the full field deformation/breakage data collected through the experiments conducted in this project. For this purpose, the setup used in the experiments was replicated numerically by accounting not only for material heterogeneity, but also for system constraints such as friction at the loading platens and along the confining ring. The outcomes of simulations based on constitutive model parameters calibrated in accordance with the procedures detailed in the previous sections are shown in Figure 15. The results show that the formulated numerical model captures satisfactorily the field of porosity evolution, as well as the heterogeneity of the breakage index, which is predicted to concentrate in the upper portion of the domain because of arching processes shielding the bottom of the specimen.

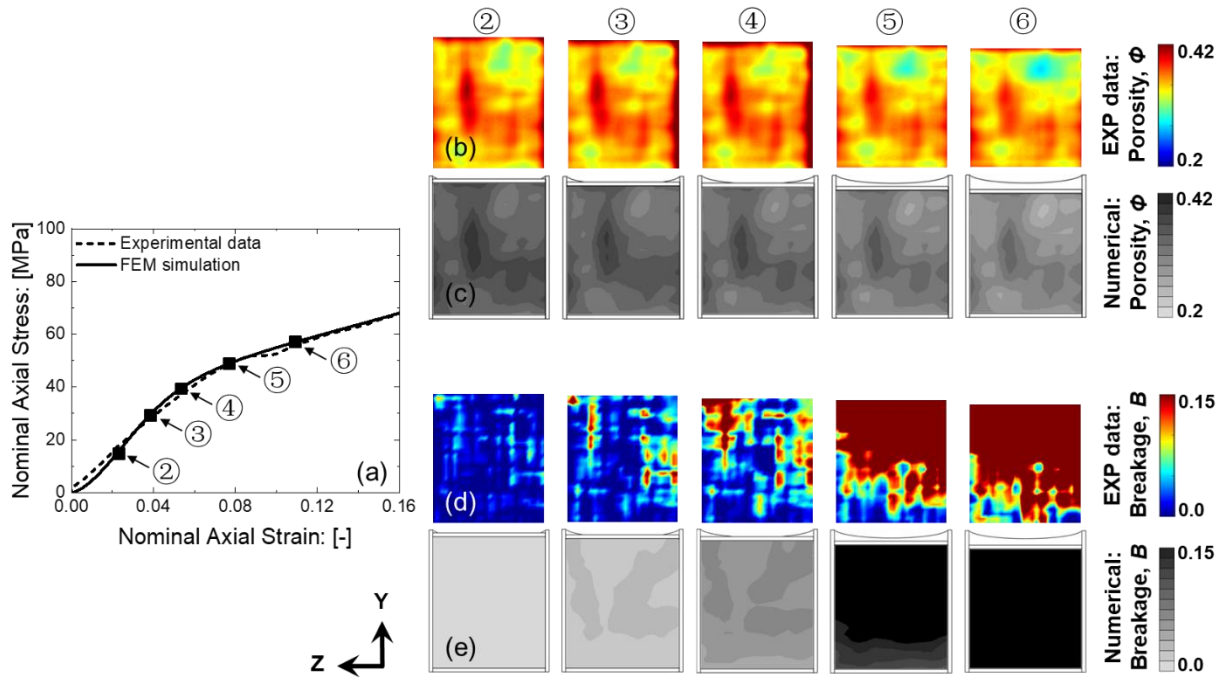


Figure 15. Comparison between measurements and full-field oedometric compression simulations based on an initially heterogeneous sand specimen: (a) mechanical response; (b) porosity field mapped from digital images; (c) porosity field obtained from numerical simulations; (d) breakage field mapped from digital images; (e) breakage field obtained from numerical simulations.

Training Opportunities

The project supported the research training of one postdoctoral scholar (Dr. Jose Lizarraga) and three Ph.D. students (Dr. Changbum Sohn, Ms. Dawa Seo, and Ms. Ritaja Ray). Dr. Sohn was awarded his doctoral degree during the course of the project, while Ms. Seo and Ms. Ray are expected to defend their doctoral dissertations in early 2022. In addition, an undergraduate research assistant (Mr. Alexander Gallard) was mentored and trained in conducting research in engineering mechanics through the financial support of a URAP supplement linked to this project.

Results Dissemination

The project led to the following international journal publications:

- Sohn, C., Buscarnera, G. (2019). Measurement and simulation of comminution rate in granular materials subjected to creep tests. *Granular Matter*, 21(3), 1-14.
- Marinelli, F., Buscarnera, G. (2019). A Generalized Backward Euler algorithm for the numerical integration of a viscous breakage model. *International Journal for Numerical and Analytical Methods in Geomechanics*, 43(1), 3-29.
- Seo, D., Sohn, C., Cil, M. B., Buscarnera, G. (2020). Evolution of particle morphology and mode of fracture during the oedometric compression of sand. *Géotechnique*, 1-13.
- Cil, M. B., Sohn, C., Buscarnera, G. (2020). DEM modeling of grain size effect in brittle granular soils. *Journal of Engineering Mechanics*, 146(3), 04019138.
- Ray, R., Buscarnera, G. (2021). Simulation of High-Strain-Rate Comminution through a Breakage Model with Adaptive Rate Dependence. *Journal of Engineering Mechanics*, 147(6), 04021030.
- Buscarnera, G., Einav, I. (2021). The mechanics of brittle granular materials with coevolving grain size and shape. *Proceedings of the Royal Society A*, 477(2249), 20201005.

In addition, the following publications are currently in preparation and expected to be submitted shortly after the conclusion of the project (titles are provisional):

- Xue, D., Shahin, G., Seo, D., Lu, X., Buscarnera, G. (2021). Modeling breakage heterogeneity in crushable sands through a CT-FE mapping scheme. In preparation for *Computers and Geotechnics*.
- Seo, D., Buscarnera, G. (2021). Sequential shape affinity during confined comminution. In preparation for *Mechanics Research Communications*.
- Ray, R., Buscarnera, G. (2021). Continuum modeling of dynamic rate effects in dilative sand through a pseudo-viscous micro-inertial potential. In preparation for *Granular Matter*.

The project outcomes were also disseminated through the following conference and workshop presentations:

- Sohn, C., Cil, M., Buscarnera, G. (2018). Multi-scale assessment of the effect of particle shape on soil crushability, Engineering Mechanics Institute (EMI) Conference, MIT, May 29-June 1, 2018.
- Buscarnera, G. (2019). Constitutive laws for crushable solids accounting for grain-scale processes, ALERT Geomaterials Workshop, 30th – 2nd October, 2019, Aussois, France.
- Seo, D. (2019). Tracking grain-scale kinematics in crushable granular materials. International NSF workshop on Granular and Particulate Networks (PARNET19), Dresden, Germany (July 2019).

- Seo, D., Buscarnera, G. (2021). A tracking algorithm to quantify grain fracture mechanisms during compaction, Engineering Mechanics Institute (EMI) Conference, Virtual Event, May 25-28, 2021.
- Ray, R., Buscarnera, G. (2021). Simulation of partially drained deformation processes in fluid-saturated crushable sand, The Biot-Bazant Conference on Engineering Mechanics and Physics of Porous Materials, Virtual Event, June 1-3, 2021.

Honors and Awards:

Ph.D. student Dawa Seo was awarded several national and international awards for her research excellence. These include the Chateaubriand Fellowship by the Embassy of France in the United States, the KSEA scholarship by the Korean American Scientists and Engineers Association, and the IS-ASCE scholarship by the Illinois Section of the American Society of Civil Engineers.

The research work of Ph.D. student Ritaja Ray was recognized by the Journal of Engineering Mechanics by including her paper “*Simulation of High-Strain-Rate Comminution through a Breakage Model with Adaptive Rate Dependence*” in the Editor’s choice list.

Participants

Dr. Giuseppe Buscarnera, PI

Dr. Jose Lizarraga, postdoctoral scholar

Dr. Changbum Sohn, Ph.D. student

Ms. Dawa Seo, Ph.D. student

Ms. Ritaja Ray, Ph.D. student

Mr. Alexander Gallard, Undergraduate research assistant