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Editorial

Use of DEM in geomechanics: Special issue associated with the DEM 8 conference

Computers and Geotechnics has a strong track record of publishing high quality research papers associated with the discrete element method (DEM). Referring to Fig. 1(a) there 400 papers including DEM as a keyword were published in Computers and Geotechnics between 1998 and 2020. Since 2008 there has been a rapid increase in the number of papers published each year, as indicated by the exponential best-fit line in Fig. 1(a). Fig. 1(b) indicates the rate of publication of papers documenting use of DEM across all scientific disciplines (following the approach suggested in Zhu et al., 2007), and shows that high rate of growth in DEM related research in geomechanics reflects a broader research trend. Some of the most highly cited DEM publications in *Computers and Geotechnics* have considered model developments including development of contact models and algorithms for contact detection. However there has been a greater emphasis on application of DEM to improve understanding of the material behaviour of soil, or to simulate the behaviour of rock mass. A relatively small number of papers have considered boundary value problems.

The 8th International Conference on Discrete Element Methods (DEM 8) took place at the University of Twente in the Netherlands from 21st to 26th July 2019. This conference was inherently multidisciplinary, bringing together physicists, mechanical engineers, process engineers, chemical engineers, and civil engineers. A number of mini-symposia were convened during the conference. This special issue of Computers and Geotechnics emerged from a mini-symposium entitled "Achieving innovation in geomechanics applications" that was convened by Prof. Catherine O'Sullivan to showcase recent activity using DEM specifically within the geomechanics community. Following the conference, Prof. Catherine O'Sullivan, Dr. Hongyang Cheng and Prof. Jidong Zhao acted as joint editors of this special issue. Invitations to submit papers were extended to the 14 groups who had presented at the Mini-Symposium. All papers were subject to the standard, rigorous peer review required for publication in *Computers and Geotechnics*, resulting in the final 10 papers in this special issue.

The papers themselves can be classified into 4 categories: (i) Developments in the DEM method (Duriez and Bonelli, 2021; Li et al., 2020) (ii) Application of DEM to advance understanding of material behaviour (Otsubo et al., 2020; Ahmadi et al., 2020; Huang et al., 2020), (iii) Use of DEM to simulate problems involving coupled fluid-particle interactions (Hu et al., 2021; Li et al., 2020; Xu and Dong, 2021; Yamashiro and Tomac, 2021) (iv) Application of DEM to boundary value problems (Pol and Gabrielli, 2021; Zhang et al., 2021). These categories broadly reflect our analyses of DEM papers in Computers and Geotechnics, however there is a clear interest in coupled CFD-DEM simulations in this special issue.

Accurately representing grain shapes poses a significant challenge to using DEM in simulations of granular media of relevance to engineering practice. Realistic shape descriptions in DEM simulations are commonly accompanied by significant computational costs. Duriez and Bonelli (2021) address this issue as they presented a significant extension of the level-set DEM (LS-DEM) to model arbitrary grain shapes. They developed a technique of storing the distance to surface in a grid for each discrete element in conjunction with boundary nodes pertaining the discrete element surface, in conjunction with parallel computing techniques, to improve the accuracy and computational efficiency of their LS-DEM. This paper along with the contribution by Li et al. (2020) (which is discussed below in relation to the coupled contributions are examples of the fundamental DEM development work has been documented in *Computers and Geotechnics* over the last 4 decades.

From a geomechanics perspective, one motivation to use DEM is that it enables us to study the origins of the complexity of the mechanical behaviour of soil in physical regimes ranging from quasi-static to dynamic. There are three examples of use of DEM in this way in this special issue: Ahmadi et al. (2020) focused on internal stability, Otsubo et al. (2020) analyzed wave propagation and Huang et al. (2020) considered liquefaction. Otsubo et al. (2020) investigated the anisotropy of small-strain stiffness by simulating elastic wave propagation in granular soils under a K_0 stress-state; they considered particles with different aspect ratios and varied the particle major axis orientation. Their results show that, for a given particle orientation, a lower aspect ratio results in a greater stress wave anisotropy and for a given aspect ratio, both the compression and shear wave velocities increase as the propagation direction becomes more aligned with the particle major axis orientation. An analytical expression for P-wave velocities in simple cubic (SC) packings that consist of ellipsoids and clumps is derived, which qualitatively captures the dependence of wave velocity ratio on the particle aspect ratio in random packings. Otsubo et al. (2020) highlighted the importance of selecting a sensible contact law when non-spherical particles are adopted. Ahmadi et al. (2020) presented a DEM study on the influence of relative density on the internal stability of gap graded soils. Based on their numerical study, they showed that for some cases, a gap-graded soil which is initially unstable can become internally stable by increasing the relative density. Fine-coarse contacts are found to govern the soil behaviour in the transitional zone, with fine-fine contacts being dominant when the soil become internally stable. A regime map is created to visualize three types of transitions in the internal stability of gap-graded soils (see Fig. 13 in Ahmadi et al. (2020)). Another key characteristic of soil microstructure is the spatial variability or randomness that is always present at the mesoscale (i.e., representative volume elements). Huang et al. (2020) quantified and related the evolution of stress variability and local stress fluctuations (deviation of per-

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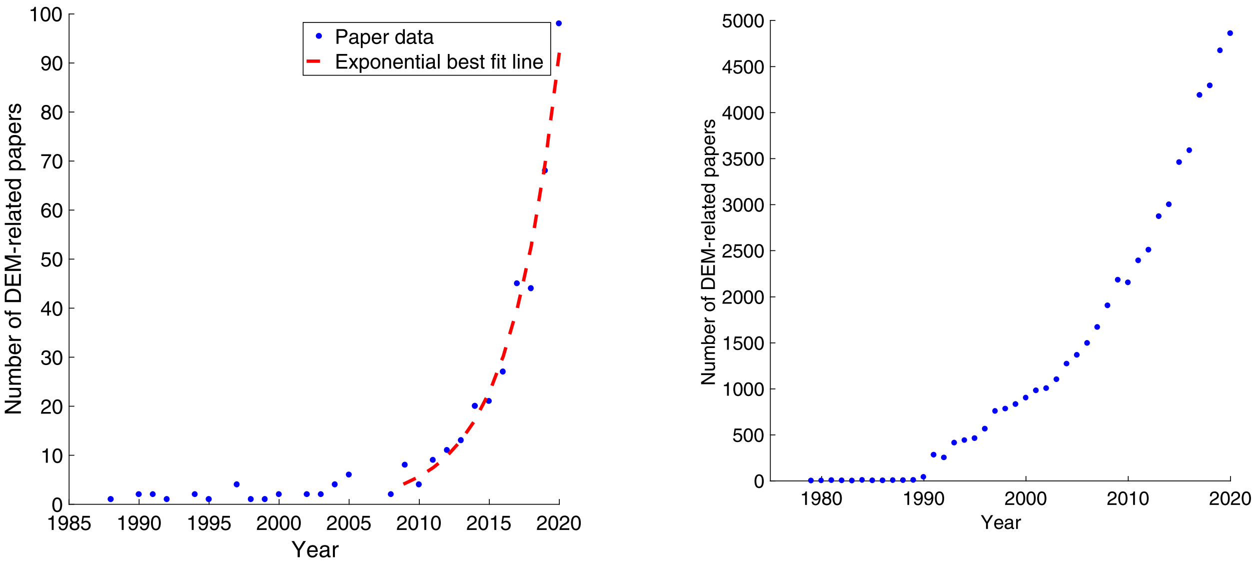
particle stress tensor from the bulk stress tensor) to characteristic states in the process of liquefaction. The tensor-based approach allows also quantification of the coaxiality between local stress, global stress and global fabric tensor. They observed a decrease in the fluctuation of stress values about the mean. Notably, liquefaction is characterized by the progressive degradation of coaxiality between the aforementioned tensors, resulting from an increasing heterogeneity in local stress tensors.

Amongst the papers on coupled analysis using DEM the basis for both DEM coupled with CFD (Yamashiro and Tomac, 2021) and DEM coupled with SPH (Xu and Dong, 2021) are outlined; both papers focus on validation and application and provide useful insight into how users should run coupled simulations using these frameworks. Yamashiro and Tomac (2021) considered the application of coupled DEM-CFD to study the mechanics of proppant transport within fractures, specifically considering the effect of particle clusters on the behaviour of the flow of the slurry that comprises the particles suspended in the fluid. The paper outlines the basis for coarse-grid DEM-CFD coupling. They used LIGGGHTS coupled with the OpenFOAM fluid solver and their contribution includes a direct comparison of the Model A and Model B approaches used in DEM-CFD coupling. Their contribution shows that the clustering of particles depends upon injection rate, and concentration and that this clustering has a large effect on particle settling and conveyancing. Hu et al. (2021) also used CFD-DEM based on LIGGHTS coupled with OpenFOAM in their study on suffusion. In contrast to Yamashiro and Tomac (2021), their contribution focusses purely on the application of CFD-DEM. Their contribution which considered simulation of suffusion in a gap-graded sample followed by undrained triaxial compression illustrates how DEM can be used to simulate conditions that cannot easily be attained in the laboratory. Xu and Dong (2021) analysed systems that are significantly larger in scale by coupling DEM with SPH. Again the coupling approach used is detailed. The paper documents simulation of experiments for validation purposes as well as simulations of landslide-induced tsunamis which demonstrate that the shape and motion of the landslide have a considerable effect on the tsunami generated. Their contribution includes a discussion on the need to consider the DEM particle size to the characteristic size of the slide simulated as well as the ratio of the SPH particle and DEM particle size. While also considering the issue of coupled DEM modelling, the contribution by Li et al. (2020) is more theoretical and looks at an alternative approach to coupling in which the continuum fluid is simulated using the finite element method, either using a locally averaged Navier-Stokes (as in CFD-DEM) or Darcy's Law. The focus is on imposing the boundary conditions on the RVE so that the Hill-Mandel energy equivalence condition between the macro- and meso-scales is ensured. Coupling DEM with a model to simulate fluid flow is non-trivial and the CFD-DEM approach is not without its limitations and so detailed analysis of an alternative approach to coupled analysis is important both as an indicator of the possibility of exploring different approaches and as an example of the thorough way in which any new approach should be considered.

Two papers in this special issue were devoted to simulating boundary value problems by DEM. To investigate the use of an anchored wire mesh system to protect a debris slope, Pol and Gabrieli (2021) used DEM and a cylinder-wire based approach to model a wire mesh system and further calibrated the wire model parameters by simulating standardized punch tests, before applying it to the simulation of a secured drapery mesh system for debris retaining applications in weathered rock slopes. Based on the data they generated, they examined the characteristics of the force–displacement of the drapery mesh on failure conditions and identified the failure pattern and failure mechanism of mesh panel in the debris layer. They further discussed the force transmission mechanism in the steel wire to the anchors and the stress distribution within the wire surrounding the anchor. The study provides a valuable reference for analytical evaluation of protective measures with an anchored wire mesh system for slopes with granular debris. It may offer a basis for further development of incorporating water into the consideration for more realistic simulation of practical slope stability analysis. The second paper, Zhang et al. (2021), addresses a practically important problem of standard penetration tests in geotechnical engineering. They employed DEM to simulate a virtual calibration chamber with rods to replicate the standard penetration test in sand. By considering energy transfer among the penetrating rods and the discrete particles in the chamber, they confirmed that the energy-based field interpretation method on SPT offers an equivalent penetration resistance with a static cone penetration test. The study offers a promising approach to perform economical virtual SPT in partially replacing expensive dynamic field tests in geotechnical practice.

The papers included in this special issue give an indication of the



(a) Number of DEM papers per year published in Computers and Geotechnics Since 1988

(b) Number of DEM papers per year across all disciplines identified in Web of Science

Fig. 1. Data publication of DEM-related papers.

current use of DEM in geomechanics and it is useful to draw out some key observations. A summary of some key features of the way DEM has been used in these papers is presented in Table 1. PFC3D was the most popular code, used in three of the contributions, which is unsurprising given the long association of PFC2D/PFC3D with the geomechanics DEM community. However it is clear that researchers are using open source codes (LIGGGHTS, Yade and LAMMPS). It is interesting to note that only three of the papers use LIGGGHTS/LAMMPS which can be compiled to run on large distributed memory, high performance computers. However, the largest simulations documented in this special issue were carried out by Ahmadi et al. (2020) using the windows-based code PFC3D.

In DEM simulations to study soil behaviour it is important to achieve a representative element volume (REV). Unless periodic boundaries are used, simulations should be sufficiently large so that boundary effects are minimized. Both of these issues motivate DEM users to exploit available computing resources to consider large system sizes. The papers documented here considered between 8,000 and 758,281 particles. Fig. 2 gives an indication of the numbers of particles considered in DEM publications in selected geomechanics journals. There is an upward trend when the largest system sizes simulated each year are considered, however the average number of particles in documented across a calendar year is not obviously increasing. Each year we see a broad range of numbers of particles in simulations, reflecting the fact that large numbers of particles are not always needed to achieve good science. The minimum number of particles required to achieve a REV is both dependant on the distribution of particle sizes and the nature of the problem considered, reflected in the smaller number of particles considered in the narrowly graded samples considered by Huang et al. (2020) when compared with the very large systems simulated in the study of gap-graded materials by Ahmadi et al. (2020). Ahmadi et al. (2020) have correctly highlighted the need for DEM codes to include efficient contact detection algorithms for highly polydisperse gap-graded size distributions.

The arguments in favour of using non-spherical particle geometries are well rehearsed in the literature. Amongst the more highly cited DEM papers that have been published in *Computers and Geotechnics* there have been contributions that have considered shape. It is interesting then to see that 8 of the studies included in this special issue used spherical particle geometries, indicating that use of non-spherical particle geometries is still not routine in geomechanics DEM simulations. Some contributions have used rolling resistance to account for the moment transmission that occurs between contacting non-spherical particles. The slow uptake of non-spherical particle geometries must reflect both the increased computational cost and also the fact that, as acknowledged

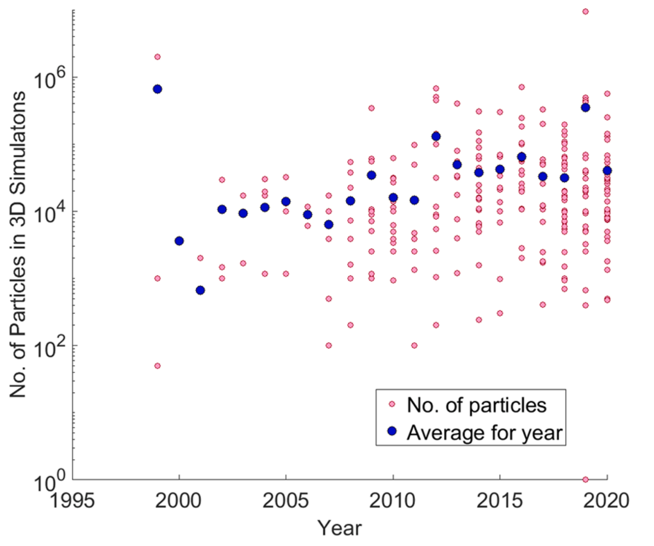


Fig. 2. Size of DEM simulations reported in publications in selected geomechanics journals (*Géotechnique*, the *International Journal for Numerical and Analytical Methods in Geomechanics*, the *Journal of Geotechnical and Geoenvironmental Engineering* (ASCE), *Soils and Foundations*, the *Canadian Geotechnical Journal*, *Computers and Geotechnics* and the *International Journal of Rock Mechanics and Mining Sciences*).

by Cundall (2001), simulations with spheres can capture a lot of the complex phenomena we associate with granular material behaviour. Considering the special issue papers, it is interesting that while simple spheres remain popular, researchers are willing to engage with computationally complex and expensive coupled CFD-DEM simulations, reflecting the significance of fluid-particle interactions in many phenomena and problems of interest in geomechanics. All of the coupled simulations considered in this special issue considered unresolved CFD-DEM. It is important to acknowledge the key challenges in CFD-DEM; these include the lack of robust drag models for highly polydisperse systems, the lack of drag models for non-spherical particles, and a need to better understand the appropriate CFD grid resolution to use in unresolved CFD-DEM simulations. As noted above, Xu and Dong (2021) considered the optimal SPH to DEM particle size ratio in their coupled simulations.

In the interest of including well documented research in the scientific record, it is important that researchers clearly include key information when reporting their work, perhaps the most basic information is the

Table 1
Summary overview of papers contained in special issue.

	Code	Max no particles	Contact Model	Particle geometry/PSD	Verification/link to experimental/ theoretical data	Boundary conditions
Otsubo, et al. (2020)	LAMMPS	226,817	SHM, no rolling resistance	Clumps, mono-sized	Theoretical validation	Periodic
Ahmadi et al. (2020)	PFC3D	758,218	SHM, no rolling	Spheres, gap-graded	Experimental validation	Rigid walls
Huang et al. (2020)	PFC3D	19,449	SHM, no rolling resistance	Spheres, size distribution of Toyoura sand	Validation not considered in this paper.	Cylindrical rigid walls
Xu and Dong (2021)	CoSim, in-house	8,345	Linear, rolling resistance	Spheres, polydisperse	Experimental validation	free
Li et al. (2020)		93 per 2D RVE	Linear, rolling resistance	Spheres, mono-sized	Validation not considered in this paper.	periodic
Yamashiro and Tomac (2021)	LIGGGHTS	n.a.	SHM + no rolling	Spheres, mono-sized	Experimental and validation	Inlet, periodic
Zhang et al. (2021)	PFC3D	69,166	SHM + rotation fixed	Spheres, Scaled to size distributino of Fontainebleau sand	Experimental validation	Rigid walls
Hu et al. (2021)	LIGGGHTS	40,000+	n.a. + rolling	Spheres, gap-graded	Validation not considered in this paper.	Rigid Walls
Pol and Gabrielia (2021)	Yade	45,000	Linear + rolling resistance	Spheres, polydisperse	The drapery system model is calibrated with experimental data.	Free
Duriez and Bonelli (2021)	Yade	8,000	Linear, no rolling	Irregular shape	Validation not considered in this paper.	Rigid walls

particle density, size, and shape, the contact model (including parameters) and the numbers of particles in their system. Table 1 gives a summary of the key data reported in the papers included in this special issue. Important information is often omitted in published DEM papers (e.g. the time-step used, number of particles per CFD cell, drag expression in CFD-DEM, etc.). As an example of good practice, Hu et al. (2021) provide data on the inertial number to achieve quasi-static loading during compression, this information is critical to enable use of the simulation data to develop constitutive models. An indication of DEM model verification/validation is important; many of the contributions here included experimental validation, and some used code whose validation is discussed elsewhere. We note that Duriez and Bonelli (2021) showed how a synthetic dataset obtained from DEM simulation using spherical shapes can be used to verify implementation of their level set algorithm.

Looking into the future, and specifically reflecting upon the papers included in this Special Issue, we can identify some future trends in DEM research and use in geomechanics:

(i) Further development of CFD-DEM including use of fully resolved simulations to develop drag expressions for use with non-spherical particles and polydisperse systems.
(ii) Increased uptake of DEM software that can exploit large-distributed memory high performance computing systems to enable simulation of boundary value problems.
(iii) Improvements to the contact detection algorithms in new and existing DEM codes to enable more efficient simulation of non-spherical particles and highly polydisperse systems.
(iv) Increase in the use of non-spherical particles in applied DEM studies to improve understanding of material behaviour and mechanisms.
(v) Expansion of coupled DEM simulations to consider thermal effects, reactive flow and multi-phase fluids.
(vi) Continued development of algorithms to link discrete and continuum analyses, considering coupled simulations in particular.

The editors would like to thank all the authors for engaging in this collaborative exercise, while also expressing gratitude to all of the reviewers who generously gave their time to provide technical insight that has ultimately improved all of the manuscripts. We are delighted with our final set of 10 articles and hope that grouping these articles together will enable readers of *Computers and Geotechnics* to get a snapshot of current research trends considering the development of DEM and its application to geomechanics problems.

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