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Title of the project Bridging the gap between particulate systems and continuum theory

Project aim

The gap between discrete (micro) and continuum (macro) concepts for the modelling and understanding of particulate systems is bridged by micro-macro transition methods. Modern discrete particle-based models describe the particles in detail, but are of limited value for studying industrial processes and natural phenomena since too many particles are involved. Continuum methods, on the other hand, are readily applied in engineering applications. However, continuum methods rely on empirical constitutive laws with phenomenological parameters that disregard both the discrete nature of particles and the micro-structure. Micro-macro transition methods are being developed to combine the advantages of discrete and continuum models.

Furthermore simulations of realistic granular systems are extremely difficult due to huge computational costs. A significant proportion of these cost is associated with the detection of (possible) contacts. Different state of the art methods for contact detection are only suitable for mono dispersed systems. However realistic granular examples usually consist of particles with hugely varying radius.

Progress

Constitutive modelling

A novel local constitutive model based on observations from discrete element simulations has been developed for small-scale deformations of a quasi steady bi-axial geometry. The model consists of non-linear evolution equations for both shear stress and anisotropy, where the anisotropy is used to model the history dependence of the material. The main advantage of the model is that it only consists of 5 material parameters, where comparable constitutive usually require many more. Several discrete particle simulations were performed to test the models accuracy for various deformation modes. In (Krijgsman and Luding 2013) paper this has been done for small cyclic pure shear, where it has been shown that the model is able qualitatively model the transient as well as the limit cycles. For larger scale cycle shear the work is still in progress (Krijgsman and Luding 2013). In this paper also a comparison with different other constitutive models (e.g. granular solid hydrodynamics) will be given. Future work will include extending the model to generic three-dimensional cases and implementing it in a finite element method. The objective is to predict stresses and strains in macro scale applications, taking into account the evolution of the microscopic material structure.

Contact detection

A contact detection method based on a hierarchical grid is developed. The improvement of the algorithm stems from the fact that in granular media most interactions between particles is short ranged. Therefore it is not necessary to test the interactions for particles pairs which are quite distant. This idea for monodisperse flows is incorporated in the Linked Cell method, where the domain is partitioned in different cells (which sizes equal to the particle diameters). In each cell the number of particles is low ($O(1)$) for all possible parameters. For polydisperse flows however the cells have to be as big as the biggest particle in the system. Therefore the number of particles in each cell increases with increasing polydispersity, rendering the algorithm useless for polydisperse flows.

The idea of the new method is to use different grids to partition the particle (i.e. use a grid with small spacing for the small particles and a grid with large spacing for larger particles). Due to this multiple grid the average number of particles per cell is kept low and the method performs excellent for all kinds of particle simulations. For the algorithm to perform optimally the correct number of levels and their sizes have to be determined. In (Krijgsman, Ogarko et al. 2014) we describe the method and suggested four different methods of choosing the number of levels and their sizes.

Mercury DPM

The quick contact detection methods described in the previous chapters is implemented in MercuryDPM (Thornton, Krijgsman et al. 2013, Thornton, Weinhart et al. 2013). MercuryDPM is an open-source code for particle simulations developed within the MultiScale Mechanics group and is actively developed by Thomas Weinhart, Anthony Thornton and Dinant Krijgsman. MercuryDPM is a very versatile, easily understandable code. Thus, it enables the transition of scientific knowledge to users in industry and academia.

References

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