



EPSRC DTG Centre in Complex Systems and Processes — Available PhD Project

Multiscale Computational Methods for Complex Granular Systems

Dr Kris van der Zee, School of Mathematical Sciences, Faculty of Science, kg.vanderzee@nottingham.ac.uk

Dr Xia Li, Dept. Chemical and Environmental Engineering, Faculty of Engineering, xia.li@nottingham.ac.uk

“Throughout the sciences [...] there is emerging a common recognition that a universe of chance and chaos is not unruly (anarchic) but merely complex, exhibiting through its natural operation the emergence of higher-order lawfulness.”

—Nicholas Rescher [1, p. 204]

Granular media are materials consisting of a large collection of solid particles, examples being coffee, corn, coal, sand and tablets. Research into such materials is crucial to the operation and efficiency in many industrial sectors. It is also particularly important to geo-hazardous processes such as *erosion*, *landslide disasters* and *plate tectonics*.

Emergent phenomena are a paramount characteristic of general complex systems of interacting discrete entities. Granular media exhibit a range of such phenomena when observed at macroscopic length scales: *nonlinear stress-strain behaviour*, *static and dynamic arching*, and *shear banding* [2]. These critical emergent phenomena are often the trigger or companion to system failure or process blockage.

Computational modelling is very challenging. On the one hand, *macroscopic computational methods* completely neglect the discrete nature of granular media. It is extremely difficult to embed the complicated constitutive relationship of granular materials in such modelling. It is also complicated when dealing with *strain localisation and material discontinuity issues*. On the other hand, *microscopic discrete models* demand massive particle-scale inputs and, moreover, they are *computationally intractable*. The PhD project aims to address these challenges.

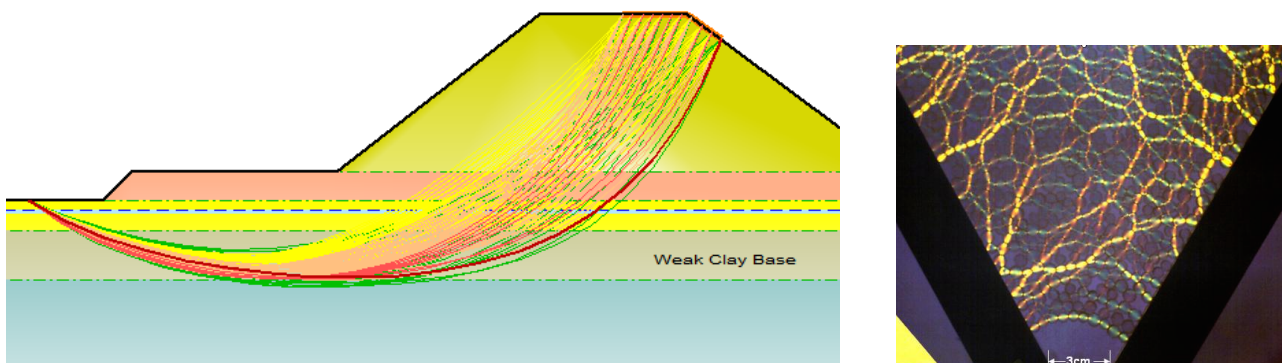


Figure: Complex granular phenomena visualized: (a) slope failure and (b) hopper jamming

PhD project: The objective of the PhD project is to develop *multiscale* computational methods for complex granular systems, which will allow for accurate, and computationally tractable, predictions of critical failure mechanisms in granulate systems. The focus will be on resolving singular events by considering, simultaneously, models at different scales in a partitioned-domain manner [3]. Important ingredients are scale relations [4], particle–continuum coupling [5] and modelling-error analysis [6].

Student profile: We are seeking a talented, highly-motivated PhD student who is inclined to work in an exciting interdisciplinary field combining engineering, mathematics and computation. A can-

didate with a strong background in continuum mechanics, computational engineering and applied mathematics will have an advantage. We also expect exceptional writing skills and a strong interest in computer-code development.

Applications details: <http://nottingham.ac.uk/complex-systems>

References

- [1] N. Rescher. *Complexity: A Philosophical Overview*. Science and Technology Studies. Transaction Publishers, New Brunswick, New Jersey, 1998.
- [2] J. D. Goddard. Continuum modeling of granular media. *Appl. Mech. Rev.*, 66:050801-1–18, 2014.
- [3] Weinan E. *Principles of Multiscale Modeling*. Cambridge University Press, Cambridge, UK, 2011.
- [4] X. Li, H. S. Yu, and X. S. Li. Macro–micro relations in granular mechanics. *Internat. J. Solids Structures*, 46:4331–4341, 2009.
- [5] E. B. Tadmor and R. E. Miller. *Modeling Materials: Continuum, Atomistic and Multiscale Techniques*. Cambridge University Press, Cambridge, 2011.
- [6] J. T. Oden, S. Prudhomme, A. Romkes, and P. T. Bauman. Multiscale modeling of physical phenomena: Adaptive control of models. *SIAM J. Sci. Comput.*, 28(6):2359–2389, 2006.