Informing continuum models of clay via particle scale simulation.

**Principle Supervisor:** Catherine O’Sullivan (Civil and Environmental Engineering, Imperial College)

**2nd supervisor:** Stefano Angioletti-Uberti (Materials, Imperial College London)

**Collaborator:** Paul Tangney (Materials, Imperial College London)

**Abstract**

Clay is a type of soil with very small particle sizes and a specific mineralogy (chemical composition). Geotechnical engineers need to be able to understand and predict the behaviour of clay in the ground in order to design foundations to buildings, dams, tunnels etc. No matter how a clay deposit is formed the clay particles will have a particular geometrical arrangement (a fabric) and there may be bonding or cementation between the particles. This combination of fabric and bonding is called the structure of a clay.

Experimental research (e.g. Cotecchia and Chandler, 2000), that considers clay at the macro scale as a continuum material, has shown that the strength and stiffness of structured clays differs from the equivalent destructured clay. This is important as engineering understanding about how clay behaves when loaded due to construction of buildings and infrastructure has been developed largely by considering destructured clay. This research will achieve a more comprehensive theoretically-based understanding using particle-scale models based on molecular dynamics. Advancing the recent research of Ebrahimi et al. (2016), the novel aspect of the proposed work will be incorporating structure effects in the model. Simulations using the model will be compared with the continuum models and frameworks that have been proposed in geotechnical engineering.


**What is the multi-scale nature of the project?**

There are two scales:

1. The scale of the clay particles which is generally accepted to be < 2mm.
2. The scale of a conventional soil mechanics element test (where soil is considered to be a continuum), this will be < 10 mm

We aim to assess whether the features assigned to continuum consistutive models can be reproduced via particle scale simulation and to identify the particle scale phenomena associated with aspects of the continuum scale behaviour descriptors.

**How do the expertises of the supervisors complement each other?**

O’Sullivan is a geotechnical engineer. She has some experience of particle scale simulation of sand. However sand particles are larger (> 100 micron) and so their interactions are simpler than is the case for clay particles. Angioletti-Uberti is an expert on soft matter and will bring his experience of researching colloids to the project. We have discussed the project idea with Tangney and feel the collaboration would benefit from his periodic involvement which will draw on his on his experience with molecular dynamics and silicates.

**Literature Review**

Particle scale simulation of the mechanical behaviour of clay


**MSc Project**

In the initial period the objective will be to create a model of destructured clay, with a view towards introducing structure in the later doctoral research.

A sample of non-contacting randomly orientated particles will be created to simulate a remolded clay which has no fabric bias. The basic unit considered will be a clay platelet. The Gay-Berne (GB) potential will be used and the LAMMPS MD code will most likely be the software used. A single GB ellipsoid will represent one clay platelet. The five GB parameters will be systematically tuned to capture the response observed in published one dimensional compression and shearing tests on kaolinite.

Pore fluid will be considered implicitly, as a modification of interactions between clay particles, and hydrodynamic drag effects will be neglected. To constrain the problem domain we will not vary the particle size distribution and will not consider temperature effects, creep or rate effects. Sample sizes of the order of 5000-10000 particles will be used. The models will be created in a periodic cell, i.e. a representative element volume (REV) will be considered and deformation will be controlled using the servo-controlled algorithms implemented in the granular LAMMPS package that have been used by O'Sullivan and her students.