Fluid-solid coupling simulations in nano-granular materials: application to solid bridges formation

Master thesis (M2) internship + funded PhD

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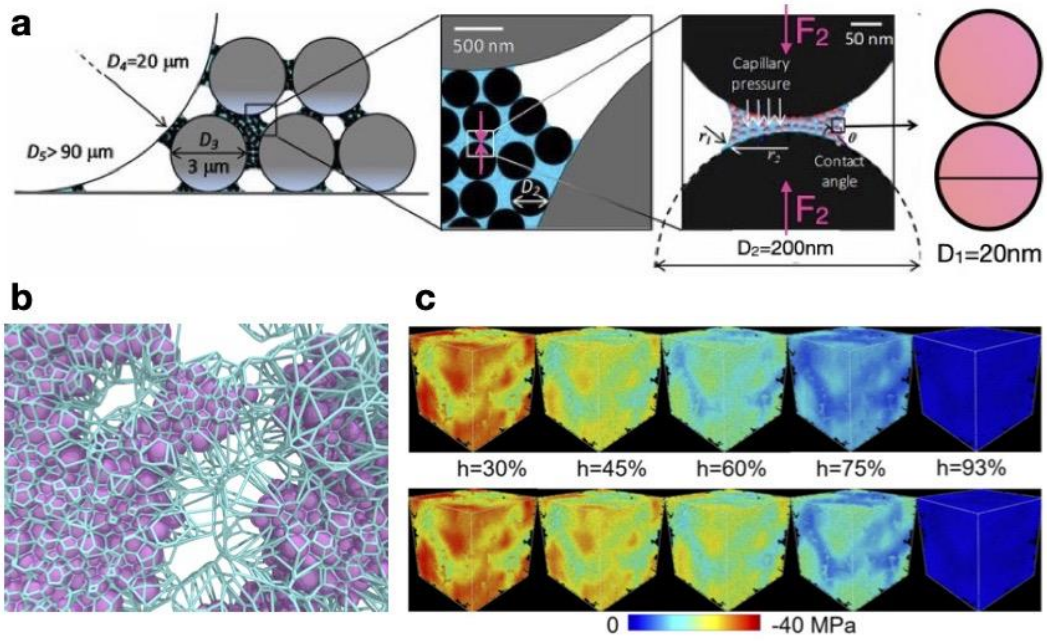

Figure. **a**) Formation of solid bridges induced by capillary forces at the nanoscale stabilize polydisperse size aggregates at the macroscale. **b**) Computation of capillary forces using voronoi tessellation. **c**) Local variation of capillary pressure of a porous sample of cement with increasing/decreasing relative humidity.

Drying of colloidal suspensions can lead to formation of out-of-equilibrium aggregates. This phenomenon, which is not well understood, contributes to the cohesive strength and stability of various geological, biological and industrial granular materials. Such systems usually are characterised by size polydispersity and effective interparticle interactions based on electrostatics, chemical bonding, capillary adhesion or solute precipitation. In a mixture consisting of particles of different sizes, the presence of small particles can cause cohesionless larger grains to be joined together by filling the gaps between them, resulting in the formation of aggregates (Fig. a).

The aim of this project is to gain novel insights on how capillary forces provide cohesion to colloidal assemblies of large size polydispersity by simulation techniques such as Molecular Dynamics and Density Functional Theory. The starting point of this work are recent simulation studies proposing a framework for coupling fluid-solid interactions and induced deformations in porous solids such as cement paste. More generally, our approach provides novel methodologies to rationalize through multiscale simulations, the interplay of fluid-solid forces in porous and granular materials, which is key for process ranging from drying of cement, CO2 sequestration, crack formation after drying in aqueous electrodes of Li-ion batteries to soil erodibility and water actuation of plant seeds.

We are looking for a student strongly motivated by numerical work and with strong a background in physics (statistical physics, soft matter, mechanics) or physicochemistry. This internship is funded by the ANR project DYNAME and can be followed by a PhD thesis.

References

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