ECOLE DOCTORALE
« Mécanique, Energétique, Génie Civil, Procédés »
ED 468

Thesis proposal for a Doctoral position 2024-2027

Title	**Multi-scale simulations coupled by machine learning and application to the calculation of thermodynamic and transport properties of colloidal dispersions.**
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Laboratory	Chemical Engineering Laboratory

Research project description:

Colloidal suspensions have large-scale thermodynamic and transport properties (osmotic pressure, collective diffusion coefficient, viscosity, etc.) that are highly dependent on interactions between the nanoparticles they contain (mesoscale), these interactions being determined in turn by the nature and distribution of the ions around the particles (microscale). On one hand, molecular dynamics simulations at the micro-scale (e.g. LAMMPS, GROMACS...) are sufficiently accurate to tackle this issue, but they are only able to reach the size and time scales relevant for colloids with great difficulty. On the other hand, mesoscale particle-field methods (LGC's PoBoS code, etc.) do access relevant space and time scales but they are limited in their ability to describe the dynamics of ions, particularly multivalent ones.

The first aim of this project is to couple molecular dynamics simulations at the micro-scale with particle-field simulations at the meso-scale, in order to capitalize on the advantages of each method. The role of the microscale simulations is to determine local effective boundary conditions for the mesoscale method. In order to minimize the computational cost, machine learning methods (GPR...) will be used to manage the coupling [1]. The second objective is to use this type of simulation to study how effective interaction potentials between colloids depend on ionic correlations, and to propose simple models to be used for example in integral equations.

Environment: this thesis will be carried out at the Laboratoire de Génie Chimique (LGC Toulouse, a joint UPS-CNRS-INPT unit), in the Complex Fluids and Colloids team. Start date October 2024, duration 3 years, net salary ~1700€/month.

Profile: theoretical physics or chemistry, physical chemistry, process engineering. The person recruited will have to run simulations on supercomputers and code data exchanges between two simulation tools running in parallel. Good programming skills and a taste for programming will be capital.

[1] Zhao, L., Li, Z., Wang, Z., Caswell, B., Ouyang, J., & Karniadakis, G. E. (2021). Active- and transfer-learning applied to microscale-macroscale coupling to simulate viscoelastic flows. Journal of Computational Physics, 427, 110069.