Proposal of M2 PCS internship

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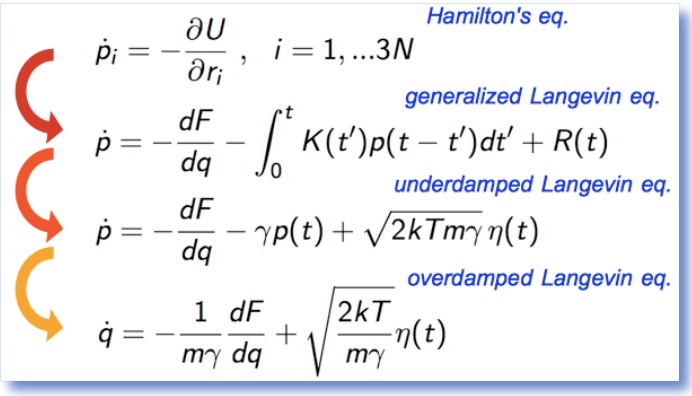
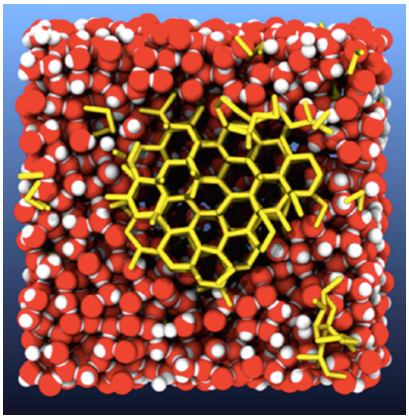
laboratory:	Sorbonne Université, IMPMC lab, campus Jussieu, 23-24 304
title:	**Theory and modeling of phase-transition mechanisms via order parameters and Langevin equations**
remuneration:	yes
possibility of PhD thesis:	yes (doctoral school grant by passing an exam)

The research work is in the context of a fundamental theoretical challenge: mastering the projection of the high-dimensional phase-space dynamics of a system of >1000 atoms on 1 order parameter, a coarse-graining procedure that leads to a mathematical description in terms of Langevin equations (stochastic differential equations). Such projection is a key tool to study phase transitions, but also other activated processes in biophysics (e.g., protein folding or protein-drug interaction), chemistry (reactions in solution), nanoscience, and so on. This tool has many advantages, since it yields a physically intuitive (no black box) and parsimonious model of a complex phenomenon, while keeping rigorous mathematical foundations and preserving the real free-energy landscape and kinetic rates.

However, to date, this theoretical approach is not routinely applied to many complex systems, due to a series of conceptual and practical challenges: How to find the optimal order parameter, and what are the consequences of adopting a sub-optimal one? What is the most accurate form of Langevin equation (non-Markovian, Markovian, overdamped...)? How to infer the parameters of the equation from a finite amount of simulation data, like molecular dynamics (MD) trajectories?





The internship builds upon an intense research activity in the host group over the last years: see, e.g., *J. Chem. Phys.* 159, 164111 (2023), *J. Chem. Theory Comput.* 19, 5701 (2023), *Proc. Natl. Acad. Sci. U. S. A.* 119, e2117586119 (2022), *Phys. Rev. Lett.* 119, 245701 (2017). The goal will be to advance the theoretical understanding and the exploitation of Langevin models as applied to a fundamental phase-transition mechanism, the nucleation of a critical solid cluster (and eventually of a solid phase) from a liquid. Notwithstanding the severe failure of simplified descriptions in terms of classical nucleation theory (in particular, the predicted rates are often spectacularly wrong), the candidate will contribute to solve the open problem of faithfully modeling the nucleation mechanism of a realistic, complex system.

The first task will be to generate MD trajectories of nucleation events in Lennard-Jones and mW water systems of thousands of atoms, exploiting a robust transition path sampling technique. This will allow, as a second task, the statistical inference of free-energy landscapes and diffusion coefficients as a function of different order parameters. The resulting Langevin models will be assessed in terms of predictive power, while the order parameters will be scored / machine learned on the basis of a recent variational principle – of fundamental importance – that prescribes kinetic rate minimization (Faraday Discussions 195, 365 (2016)). The results should lead to a first reliable

numerical approach for estimating accurate kinetic rates of nucleation, and to a publication in a scientific journal. The project is supported by the interaction with a young team of 2 PhD students and one postdoc, and by the collaboration with applied mathematicians and international leading scientists like C. Dellago (University of Vienna), P. Bolhuis (University of Amsterdam) and G. Hummer (MPI Frankfurt). The work environment is lively and multidisciplinary, with frequent interactions, weekly group meetings, visiting scientists and seminars throughout the year.

In perspective, a PhD thesis can be designed together with the candidate, aiming at substantial method development together with applications to the nucleation and dissolution of carbonate solids starting from water solutions of ions and CO_2: the latter problem is of importance for understanding and enhancing the capture of CO_2 from the atmosphere, a key urgent task that will be mandatory to avoid a climate catastrophe in the next decades.