SCIENCES SORBONNE UNIVERSITÉ

2021-2022

Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22
Director: A. Marco Saitta

Title:
Modeling the dynamics of complex systems with Langevin equations and machine-learned coordinates

Keywords:
statistical mechanics, stochastic models, machine learning, phase transitions, biophysics, computer simulation

Scientific description:
One of the major challenges in the theory and simulation of complex systems consists today in the prediction of free energy landscapes and kinetic rates for phase transitions, biomolecular processes, and chemical reactions. A unified theoretical framework allows tackling many different systems: the high-dimensional phase-space dynamics is projected/coarse grained with the help of a few generalized coordinates (or order parameters), whose dynamics is modeled using Markovian or non-Markovian Langevin equations, that allow accessing the desired properties (free energy, diffusion coefficients, transition rates). The master thesis will pursue the development and application of machine learning techniques both for the identification of optimal coordinates and for the parametrization of the evolution equations. The starting data set is represented by molecular dynamics simulations (transition path sampling) generated by collaborators in our group, while applications of the new methods include protein folding/interaction and ice nucleation. The research will be conducted within a network of international collaborations including the University of Vienna, the Max Planck Institute for Biophysics in Frankfurt, and the Freie Universität of Berin. There will also be a fruitful interaction with the MAESTRO team (formed by mathematicians, physicists and chemists) at the Sorbonne ISCD lab. Recent related works in our team:
* K. Palacio-Rodriguez & F. Pietrucci, arXiv:2106.05415 (2021)
* P. Gkeka et al, J. Chem. Theory Comput. 16, 4757 (2020)
* C. Camilloni & F. Pietrucci, Adv. Phys. X 3, 1477531 (2018)

Techniques/methods in use:
Likelihood maximization techniques, Langevin and Fokker-Planck equations, transition path theory, computer simulations.

Applicant skills:
Solid background in statistical physics and theoretical physics or chemistry, computer programming, interest in collaborating with a lively team of young researchers

Industrial partnership:
No

Internship supervisor:
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Internship location:
Sorbonne Université, IMPMC Lab, Campus Jussieu

Possibility for a Doctoral thesis:
Yes