'Physique et Chimie des Matériaux' – ED 397 – année 2022

PhD project for funding, to send by 28/02/2022 to

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Research unit (full name + acronym) : Inst. de Minéralogie, Physique des Matériaux, Cosmochimie IMPMC

Team if applicable : PHYSIX

Address : Couloir 23-24, salle 304, 4 Place Jussieu, 75005 Paris

Project leader (PI): Fabio Pietrucci HDR? yes Position : Lecturer SU

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Nber of phD under supervision 1.5 Participation to supervisor training? no Year

Co-supervisor : HDR? select Position : select

Tel email :

Research unit :

International co-supervision ? select

Keyword 1 : statistical mechanics Keyword 2 : machine learning

Keyword 3 : phase transitions Keyword 4 : biophysics

Select co-funding programme if applicable : select

Project title : Modeling the dynamics of complex systems with stochastic processes and machine-learned coordinates

Project Description :

Recent advances in algorithms as well as computer hardware allow today to simulate the behavior of advanced materials and biosystems in atomic detail on the scale of 100 000 atoms and microseconds using approximate force fields, or 1000 atoms and nanoseconds using quantum mechanical forces. These figures are insufficient to characterize free energy landscapes and kinetic rates of important processes like phase transitions, conformational changes of proteins, or chemical reactions, characterized by rare transitions between metastable states, unless smart techniques are employed to circumvent the limitations of Boltzmann statistics. Most of such techniques, however, require the judicious choice of a reaction coordinate or order parameter, able to monitor the progress of the transformation as well as the kinetic fate of each atomic configuration [1]. Only the optimal generalized coordinate, in principle, allows an accurate calculation of free energy profiles and kinetic rates. Such optimal coordinate is customarily identified with the committor function, associating each atomic configuration to the probability to reach the final metastable state before the initial one. Albeit widespread in current literature, such identification has important shortcomings in connection with high-barrier processes, due to the practical impossibility to estimate the committor far from the barrier top.

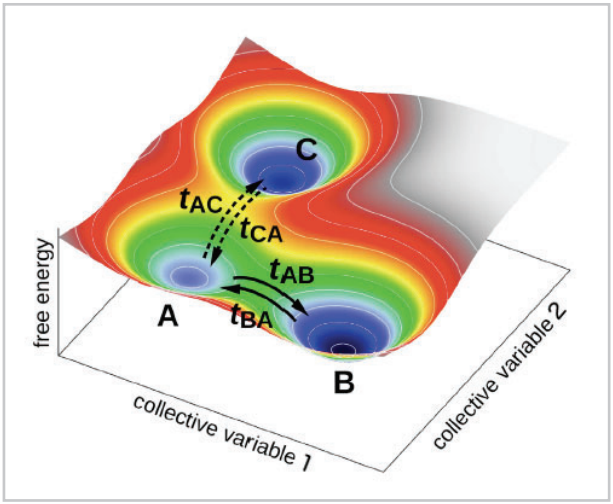
The proposed PhD thesis will tackle the problem of identifying the optimal reaction coordinate / order parameter for several important processes employing machine-learning techniques [2] and an original criterion, different from customary committor-based one. The idea consists in optimizing the kinetic rates, computed via Langevin models, as a function of the parametrization of putative reaction coordinates. This is made possible by the work of a previous PhD student (Karen Palacio-Rodriguez) who recently demonstrated a new approach

to the likelihood optimization of stochastic models from short unbiased molecular trajectories [3]. The Langevin model provides a fast and accurate access to kinetic properties, normally very difficult to achieve, opening the way to an automatic iterative optimization of coordinates.

Within the project we will develop the new approach starting from transition path sampling trajectories for benchmark systems, and subsequently tackling challenging problems. The first consists in protein-protein interaction: as of today, available numerical techniques can predict the binding free energy and dissociation rate only for special cases and at a very large computational cost. We will employ trajectories for different complexes provided also by the D.E. Shaw research group in New York [4], comparing with their own thermodynamic/ kinetic results and with those obtained from metadynamics simulations [5].
The second problem is the homogeneous nucleation of crystalline nanoparticles or bulk systems (including Lennard-Jones as well as mW water models) from the liquid phase in presence of large barriers, based on classical force fields: currently it is unclear how to predict reliable nucleation rates, despite many efforts in the literature, and in this context our approach combining machine-learned coordinates and optimal Langevin models [6] should provide a robust solution. The research will be conducted within a network of international collaborations including the University of Vienna, the University of Amsterdam, and the Freie Universität of Berin. The PhD student will be proposed to spend several weeks in some of the corresponding foreign institutions.

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

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



References:

[1] C. Camilloni, F. Pietrucci, Adv. Phys. X 3, 1477531 (2018)
[2] P. Gkeka... F. Pietrucci et al, J. Chem. Theory Comput. 16, 4757 (2020)
[3] K. Palacio-Rodriguez & F. Pietrucci, arXiv:2106.05415 (2021)
[4] A.C. Pan, D. Jacobson, K. Yatsenko, D. Sritharan, T.M. Weinreich, D.E. Shaw Proc. Natl. Acad. Sci. U. S. A. 116, 4244 (2019)
[5] K. Palacio-Rodriguez, H. Vroylandt, L.S. Stelzl, F. Pietrucci, G. Hummer, P. Cossio, arXiv:2109.11360 (2021)
[6] H. Vroylandt, L. Goudenège, P. Monmarché, F. Pietrucci, B. Rotenberg, Proc. Natl. Acad. Sci. U. S. A. (in press, 2022).