Proposal of M2 ICFP internship

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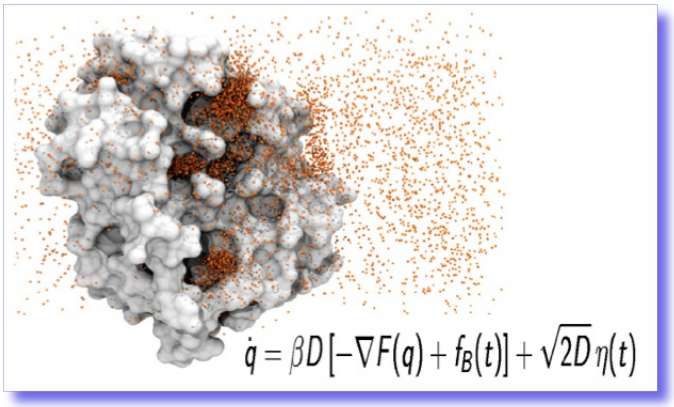
laboratory:	LBT, IBPC, 13 rue Pierre et Marie Curie, et IMPMC, place Jussieu
title:	**From biased molecular simulations to unbiased free energy landscapes**
remuneration:	yes
possibility of PhD thesis:	yes (doctoral school grant by passing an exam)

Computing free-energy landscapes is a very effective approach for describing complex systems. Unfortunately, free energies reconstructed from short simulations can suffer from large uncertainties, requiring very long and costly simulations, or making them simply impossible to obtain. However, simulations can be made much more efficient by adding specially designed external forces (“biases”).

The goal of this project is to compute reliable, unbiased free-energy landscapes and longtime kinetics from local statistics collected in biased MD simulations. The approach builds upon work from the group of Fabio Pietrucci at IMPMC and Jérôme Hénin at Laboratoire de Biochimie Théorique, IBPC.

We will start from an existing approach to fit Langevin models to unbiased dynamics [J. Chem. Theory Comput. 18, 4639, 2022]. This approach will be extended to simple cases with known static external potentials to validate the principle of the approach. To that effect, the local dynamics will be corrected to remove the effect of the external bias, to recover the properties of the underlying unbiased dynamics. Once that approach is validated, it can be extended to adaptive biasing methods used in applications to complex materials and biological molecules, like the dissociation of a ligand from a protein in water solution.



Techniques/methods in use: molecular dynamics simulation, statistical thermodynamics, numerical analysis

Applicant skills: classical mechanics, statistical mechanics, numerics, scripting