M2 STAGE

**Multi-scale modelling of cellular environment with support of AI**

Biological processes in cellular environment involve a spread range of space- and time-scales, and a variety of actors from macromolecules (proteins, RNA, DNA, lipid, metabolites) to solvent.
In our lab, by applying a multi-scale approach capable to introduce solvent mediated correlations (hydrodynamics) in the simulations of coarse-grained models of macromolecules, we have explored important processes like protein diffusion under cellular crowding, pathological amyloid aggregation, fluid mediated organisation of membrane-less organelles, structural organisation of enzymes clusters.

In this stage we aim to explore methodologies to further develop our multi-scale strategy. We are interested in two problems:

1. Define a protocol to change resolution of the description of the macromolecules actors, namely back-map from highly coarse-grained description (e.g. density distribution) back to molecular-like description. This procedure can be supported by ML/AI tools.
2. Use the large data set of simulated systems to develop an AI training for the on-the-fly generation of fluid forces acting on solvent-free coarse-grained molecular simulations. This will help to speed up the simulations of complex cellular processes.

The student will work in the group of F. Sterpone at the Laboratoire de BiochimieThéorique (IBPC) in Paris (CNRS UPR9080).

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Presently there is not available funding for a PhD, but f the internship is successful the candidate will be supported to apply for PhD fellowships.

References

1. S. Timr, S. Melchionna, P. Derreumaux, F. Sterpone, "Optimized OPEP Force Field for Simulation of Crowded Protein Solutions", JPCB (2023), 27, 16, 3616–3623
2. D. Di Bari, et al, "Diffusive Dynamics of Bacterial Proteome as a Proxy of Cell Death", ACS Central, (2023), 9, 1, 93–102.
3. M. Chiricotto, S. Melchionna, P. Derreumaux, F. Sterpone, «Multiscale Aggregation of the Amyloid Aβ16–22 Peptide: From Disordered Coagulation and Lateral Branching to Amorphous Prefibrils», J. Phys. CHem. Lett. (2019), 10, 1594–1599.