M2 Internship proposal:
Coupling proteins and nucleic acids coarse-grained models

DNA, RNA and proteins are life's essential molecules.
Despite advances in experimental methods, many questions remain open concerning the dynamics and thermodynamics of these molecules. Numerical studies can complement the experimental information, but they are limited by the size of the systems and by the time-scales characteristic of the processes. In recent years, coarse-grained models have been proposed to alleviate this problem by using simplified representations of molecules while striving to keep the important details.
Two such programs are our in-house developed OPEP and HiRE-RNA models, which, maintaining a good level of resolution and lacking conformational constraints, are able to give access to the dynamics and thermodynamics of nucleic adics and proteins folding and assembly.
Up to now the two models have been developed independently from one another, allowing to perform simulation either on proteins alone, or on nucleic acids alone, but not of the two systems together. However the main simulation code used to run simulation is the same, and the two systems could be easily coupled through the development of an appropriate interaction force field.
In this internship we propose to take the first step in this direction by developing a simple interface allowing to simulate systems composed of both proteins and nucleic acids, accounting for occupied volume, electrostatics and Van der Waals interactions.

We are looking for a candidate holding an undergraduate ("Licence") degree in chemistry, physics, or bioinformatics, with excellent programming skills, and good analytical understanding of force fields. The work will be supervised jointly by Philippe Derreumaux and by Samuela Pasquali at the Laboratoire de Biochimie Theorique, at the Institut de Biologie Physico-Chimique (IBPC) in central Paris.

If interested, please send your CV, copy of your undergraduate records, as well as a motivation letter to Samuela Pasquali : samuela.pasquali@ibpc.fr.

References

S. Pasquali, P. Derreumaux, **HiRE-RNA: a high resolution coarse-grained energy model for RNA**, J Phys Chem B., 114, 11957-11966 (2010)

T. Cragnolini, P. Derreumaux, S. Pasquali, **Coarse-grained simulations of RNA and DNA duplexes**, J Phys Chem B, 117, 8047-8060 (2013)

F. Sterpone, S. Melchionna, P. Tuffery, S. Pasquali, N. Mousseau, T. Cragnolini, Y. Chebaro, J-F. Saint-Pierre, M. Kalimeri, A. Barducci, Y. Laurin, A. Tek, M. Baaden, P.H. Nguyen, P. Derreumaux, **The OPEP coarse-grained protein model: from single molecules, amyloid formation, role of macromolecular crowding and hydrodynamics to RNA/DNA complexes**, Chem Soc Reviews, **43**, 4871-4893 (2014)

T. Cragnolini, Derreumaux, S. Pasquali, **Ab initio RNA folding**, Journal of Physics: Condensed matter, 2015, 23, 233102

T. Cragnolini, Y. Laurin, P. Derreumaux, S. Pasquali (2015), **Coarse-grained HiRE-RNA model for ab initio RNA folding beyond simple molecules, including noncanonical and multiple base pairings**, JCTC, 11, 3510-5322

S. Doutreligne, C. Gageat, T. Cragnolini, A. Taly, S. Pasquali, P. Derreumaux, M. Baaden (2015), **UnityMol: interactive and ludic visual manipulation of coarse-grained RNA and other biomolecules**, Virtual and Augmented Reality for Molecular Science (VARMS@ IEEEVR).