Monthly informal seminar series on

Integrative Modelling in Biophysics

presented by

Molecular Biophysics Unit, IISc

Challenges in RNA simulations

RNA molecules are now known to play a central role in the cell's life and have become the subject of intensive experimental and theoretical research both to understand the behavior of their structures and to target them with drugs. Unlike most proteins, a single RNA molecule can adopt a multitude of 3-dimensional structures, which makes its investigation particularly tricky. In this presentation I will discuss the challenges posed by RNA molecules such as ribozymes, riboswitches, and regulatory RNAs in general, the peculiar features of their structures, and why we need to develop specific tools to study them through modeling. I will present different enhanced simulation techniques, which coupled with both atomistic and coarse-grained models, can shed light onto the molecule's polymorphism. Because of the variability of their structures and their sensitivity to environmental conditions, different experiments can give apparently incompatible results. Modeling guided by experimental data can then help gather a coherent view on the molecule's behavior. I will discuss how experimental constraints and environmental conditions can be implemented onto our coarse-grained model to obtain structures that are compatible with experimental data.

Prof. Samuela Pasquali

University of Paris

Samuela Pasquali is professor at the University of Paris in the Pharmacy department. She's a theoretical physicist specialized in modeling of biomolecules in particular. She received international training with a bachelor's degree from the University of Milan and a Ph.D. from New York University and arrived in Paris as postdoc in 2005. After working on statistical mechanical problems, in 2008 she was hired by UP in the Biology department and focused her research on modeling RNA systems. She first developed a coarse-grained RNA model considering the specificity of nucleic acids and coupled it to environmental conditions (temperature, pH). Since joining the Pharmacy department in 2016, she has worked in close collaboration with experimentalists and developed methods to integrate experimental data onto the simulations. She collaborates closely with the University of Cambridge to develop energy landscape exploration methods adapted to RNA systems, both at the coarse-grained and atomistic description level.

Date: 14-Sep-2021 (Tuesday)
Time: 17:30 hours (IST)

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Link: http://mbu.iisc.ac.in/IMSS/index.html