

Multi-resolution simulations of intracellular processes

Thursday 26 September 2024 14:30 (45 minutes)

All-atom and coarse-grained molecular dynamics (MD), Langevin dynamics (LD) and Brownian dynamics (BD) are computational methodologies, which have been applied to spatio-temporal modelling of a number of intracellular processes. I will discuss connections between MD, LD and BD, with a focus on the development, analysis and applications of multi-resolution methods, which use (detailed) MD simulations in localized regions of particular interest (in which accuracy and microscopic details are important) and a (less-detailed) coarser stochastic model in other regions in which accuracy may be traded for simulation efficiency. I will discuss applications of multi-resolution methodologies to modelling of intracellular calcium dynamics, actin dynamics and DNA dynamics.

Presenter: ERBAN, Radek (University of Oxford)

Session Classification: Multiscale Models in Cell Biology III (Chair: Franziska Matthäus)