Contribution ID: **72** Type: **Oral Presentation**

Multiscale methods for modelling intracellular processes

Monday, 9 July 2018 11:00 (30 minutes)

I will discuss mathematical and computational methods for spatio-temporal modelling in molecular and cell biology, including all-atom and coarse-grained molecular dynamics (MD), Brownian dynamics (BD), stochastic reaction-diffusion models and macroscopic mean-field equations.

Microscopic (BD, MD) models are based on the simulation of trajectories of individual molecules and their localized interactions (for example, reactions). Mesoscopic (lattice-based) stochastic reaction-diffusion approaches divide the computational domain into a finite number of compartments and simulate the time evolution of the numbers of molecules in each compartment, while macroscopic models are often written in terms of mean-field reaction-diffusion partial differential equations for spatially varying concentrations.

I will discuss the development, analysis and applications of multiscale methods for spatio-temporal modelling of intracellular processes, which use (detailed) BD or MD simulations in localized regions of particular interest (in which accuracy and microscopic details are important) and a (less-detailed) coarser model in other regions in which accuracy may be traded for simulation efficiency [1,2,3]. I will discuss error analysis and convergence properties of the developed multiscale methods, their software implementation [4] and applications of these multiscale methodologies to modelling of intracellular calcium dynamics [5], actin dynamics [6,7] and DNA dynamics [8]. I will also discuss the development of multiscale methods which couple MD and coarser stochastic models in the same dynamic simulation [3,9].

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[4] M. Robinson, S. Andrews and R. Erban (2015). Multiscale reaction-diffusion simulations with Smoldyn. *Bioinformatics* **31**: 2406-2408.
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Session Classification: Multiscale modelling and simulation

Track Classification: Minisymposium: Multiscale modelling and simulation