Suggested title of dissertation:

From Molecular Dynamics to Brownian Dynamics

Dissertation supervisor:

Prof Radek Erban

Description of the proposal:

Molecular dynamics (MD) methods studied in this project are based on classical mechanics and are sometimes called molecular mechanics approaches in the computational chemistry literature [4]. The growing importance of MD has been recognised by the award of the Nobel Prize in Chemistry to pioneers of this approach [5]. In applications, MD approaches are used to study how complex biomolecules move, deform and interact over time. In mathematical terms, MD can be described by systems of ordinary differential equations (ODEs) or stochastic differential equations (SDEs) for the positions and velocities of atoms or beads (representing collections of atoms), which can be also subject to algebraic constraints [1]. At much coarser level, biomolecules and their interactions can also be modelled by Brownian dynamics (BD) approaches stochastic reaction-diffusion models, which are studied in course B5.1 (essential prerequisite).

In this project, the candidate(s) will investigate mathematical limits in which a fine MD description converges to a coarser BD model. There are different types of simple MD models, where an analytic progress can be made and mathematically oriented candidates can focus on a particular theoretical MD model in more detail. More computationally oriented candidates can focus their work on realistic MD models used in biological applications. Analysis of the MD to BD limit is useful for developing modern multi-scale (multi-resolution) methods [2,3].

Possible avenues of investigation:

- derivation of BD from MD systems with short-range interactions
- derivation of BD using a theoretical MD model based on harmonic oscillators
- multi-resolution (multi-scale) methods: using a detailed MD model only in a small part of the computational domain (where this level of detail is necessary) and a coarser BD modelling description in the remainder of the computational domain
- parameterization of the generalized Langevin equation from MD simulations
- numerical methods for MD and for solving (generalized) Langevin equation
- thermostats – controlling temperature in MD simulations
- applications to modelling ions, DNA, proteins and intracellular processes

Pre-requisite knowledge:

Essential: material from course B5.1 Stochastic Modelling of Biological Processes (`https://courses.maths.ox.ac.uk/node/36382`)

Useful: depending on an avenue of investigation, candidates might find useful some of the material (but not everything) covered in other optional Part A (2nd year) and Part B (3rd year) courses, for example:
Part A Numerical Analysis (`https://courses.maths.ox.ac.uk/node/37682`),
Part B Further Mathematical Biology (`https://courses.maths.ox.ac.uk/node/36417`)
Part B Applied Probability (`https://courses.maths.ox.ac.uk/node/36568`)

Useful reading:

[1] B. Leimkuhler, C. Matthews, *Molecular Dynamics. With deterministic and stochastic numerical methods*, Springer, 2016

[2] R. Erban, "From molecular dynamics to Brownian dynamics", *Proceedings of the Royal Society A* **470**, 20140036 (2014)

[3] R. Erban, "Coupling all-atom molecular dynamics simulations of ions in water with Brownian dynamics, *Proceedings of the Royal Society A* **472**, 20150556 (2016)

Further references:

[4] E. Lewars, *Computational Chemistry*, 3rd edition, Springer, 2016

[5] `http://www.nobelprize.org/nobel_prizes/chemistry/laureates/2013/`

[6] D. Frenkel, B. Smith, *Understanding Molecular Simulation*, 2nd edition, 2002

[7] P. Attard, *Non-Equilibrium Thermodynamics and Statistical Physics*, OUP, 2012

[8] M. Allen, D. Tildesley, *Computer Simulation of Liquids*, 2nd edition, 2017

[9] M. Tuckerman, *Statistical Mechanics: Theory and Molecular Simulation*, OUP, 2016