Final report for a 6-month programme at the Isaac Newton Institute for Mathematical Sciences

Stochastic Dynamical Systems in Biology: Numerical Methods and Applications

Organizing committee:

- Radek Erban, Mathematical Institute, University of Oxford
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Brief background/historical information (114 words) Why was the programme organised on this particular topic? What were the outstanding problems in the field? How was the programme organised to address them?

Stochastic dynamical systems have been used during the last decade to model a number of biological processes, including gene regulation, molecular signalling, cell division, molecular transport and cell motility. The analysis of these models poses a number of challenging mathematical problems at the interface of stochastic processes, numerical analysis and differential equations. To address these challenges the programme started with a stimulating opening workshop. The first talk present presented eight outstanding mathematical problems in the field and the workshop resulted in establishing a number of groups working towards address those. The problems included the development of multiscale methods which can be used for efficient simulation over a vast range of spatial and temporal scales.

Programme timeliness, scope and outline (252 words) Topics addressed and research areas involved Brief summary of workshop and Satellite Meeting themes

The opening workshop was followed by a satellite meeting at ICMS, Edinburgh on *Multiscale methods for stochastic dynamical systems in biology*. One of the workshop highlights was the well attended public talk by Dr. Sarah Harris from the Astbury Centre for Structural Molecular Biology, University of Leeds, entitled *Physics meets biology in The Garden of Earthly Delights*. By using analogies between modern computational modelling of molecularbased processes and a famous painting of Hieronymus Bosch, Dr Harris explained how the interplay between order and chaos at the molecular level gives rise to the complex behaviour of biomolecules inside living cells

There were two more research workshops organised in Cambridge focusing on spatial and non-spatial stochastic processes. One of the highlights of the concluding workshop in June was the Rothschild lecturer given by Prof. Yannis Kevrekidis, Princeton University. This lecture, entitled *Mathematics for data-driven modeling - The science of crystal balls*, described a fascinating new promising directions of the research in the area by building algorithms that "jump directly" from data to the analysis of models, which are not available in closed forms, so as to make predictions about their behaviour. Another distinguished lecture was given by Prof. James Rothman, Yale University, the 2013 Nobel Prize in Physiology or Medicine. In his lecture he posed a number of open biological questions related to communication between neurons, which will require the development of new mathematical models to investigate.

* Scientific outcomes Highlights Collaborations How the programme advanced research in the field

There were three overlapping areas of scientific outcomes of the programme: (i) development and software implementation of efficient methods for stochastic simulation; (ii) analysis of dynamical behaviour of biological models; and (iii) the integration of data and models towards their successful parametrisation. Significant progress was made on all the eight of the proposed open problems. In response to programme participants, the open problem of incorporating more realistic biological features into models of cellular processes, was addressed by extending Smoldyn, a widely used software package for cell biologists. The open problem of developing multiscale methods, was addressed by a number of new collaborations. For example, new hybrid methods resolving different portions of a biological system at different spatial and/or temporal scales were developed and analysed. Future activities have been discussed and planned, including a training network for graduate students across a number of European countries, a proposed followed workshop at MATRIX@University of Melbourne, and a proposed three month programme at the Institut Henri Poincaré.

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* Multimedia Activity
Evidence of remote access to streamed lectures
Lectures delivered over the internet from other locations
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Two participants could not attend the programme due to child caring responsibilities, but thanks to the institute audio visual facilities remote seminars were arranged. These were very well received followed by discussions at the INI and electronically with the speakers. All institute seminars and lectures were with the permission of speakers recorded, streamed online and made available on the web in perpetuity. This created a unique resource for researchers worldwide, including a recorded graduate course given by David Holcman. *Publications Books planned Major papers or publications that were produced Links to multimedia items that might be included in the on-line version of the

The programme resulted in x submitted papers during the programme and many more in preparation, while it has stimulated research for the years to come. A Springer book, edited by the programme organisers, summarising the mathematics discussed at the programme has been commissioned and is due to appear in the Summer of 2017.

Illustrations

Colour illustrations or photographs, together with appropriate captions, can be include