Simplifying Assumptions in Models of Complex Systems: Break, Make, Justify

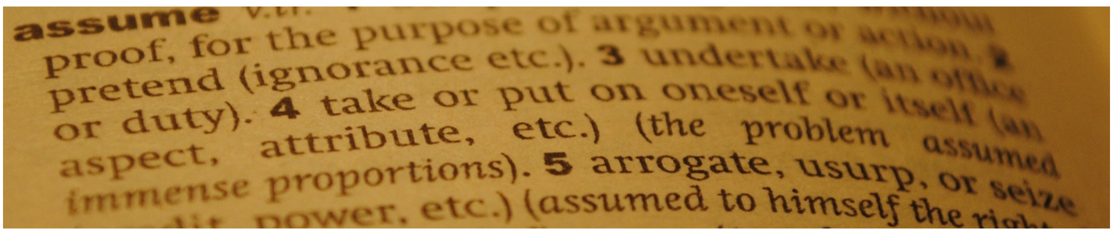
A free workshop for researchers from a wide range of scientific backgrounds interested in mathematical and computational models

Held at the

UNIVERSITY OF BIRMINGHAM

on the 7th May 2014

With kind sponsorship from the
College of Life and Environmental Sciences



Programme

The workshop will take place in the Biosciences Building (R27) of the University of Birmingham. The Undercroft is on the Ground Floor and Lecture theatre E102 is on the 1st Floor.

09:00	Registration opens, tea & coffee		Undercroft
09:25	Opening remarks		E102
09:30	Tim Benton	p. 3	E102
10:10	Samantha Dobbie	p. 3	E102
10:30	Amit Chattopadhyay	p. 4	E102
10:50	Tea & coffee, posters on display		Undercroft
11:20	Susan Lee	p. 4	E102
11:40	Paul Andrews	p. 5	E102
12:20	Buffet lunch, posters on display		Undercroft
13:20	Alan Herbert	p. 6	E102
14:00	Yan Zhang	p. 6	E102
14:20	Robert Clegg	p. 7	E102
14:40	Tea & coffee, posters on display		Undercroft
15:10	Brian Castellani	p. 8	E102
15:50	Discussion panel	p. 9	E102
16:50	Closing remarks		E102
17:00	Tea & coffee, posters on display		Undercroft

Posters on Display

Dense Chlorinated Solvents in Aquifers Under British cities: Approaches to Modelling Systems with Complex Behaviour, Data Poverty and Human Importance

Christopher Barry (University of Birmingham)

Revisiting the Evolution of Aging: Repair is the Optimal Unicellular Strategy

Robert Clegg (University of Birmingham)

Food Security: Representing Reality in an Agent-Based Model of Malawian Small Holders

Samantha Dobbie (University of Southampton)

Liveable Cities; Measuring the Performance of Cities

Susan Lee (University of Birmingham)

Large Eddy Simulations of the Airflow Around a High Sided Vehicle

Nainesh Patel (University of Birmingham)

Application of Modified Adaptive Landscapes to Product Concept Design

Brian Price (Aston University)

A Data-Driven Approach for Blood Glucose-Modelling

Yan Zhang (University of Warwick)

Complex systems, complex models and complex understanding: some issues to think about

Tim Benton (University of Leeds)

My background is in ecological systems and stochastic dynamics, but I now spend much of my time working in the policy environment associated with the complex "food system". In my talk, I'll discuss some issues around: the utility of complex models for understanding system behaviour, the generality of complex models (with respect to simple models), the issue of communicating complex models and therefore the trust in them from end-users, the matter of unknown parameters, and the generic issue of how drawing system boundaries may determine model outcomes.

I'll keep the talk non-technical and largely conceptual, so people from any discipline can access it... Essentially, the talk will be rooted in some of the philosophical debates about what models are for!

Food Security: Representing Reality in an Agent-Based Model of Malawian Small Holders

Samantha Dobbie (University of Southampton)

The inherent complexity of food security hinders its realisation. Within Malawi, the continued dependence of rural-livelihoods upon rain-fed agriculture leaves smallholders vulnerable to climatic shocks. Structural factors such as high population densities, coupled with small plot size and poor soil quality further undermine food security. It is this complex interplay between social, ecological and economic factors which lends the study of food security to agent-based modelling (ABM). Here, the emergence of system level behaviour can be explored through the interactions between agents and their environment within a computerised simulation. Application of the technique holds potential to elicit greater understanding of factors underpinning the availability, access, utilisation and stability dimensions of food security, as well as highlight knowledge gaps and prompt collaboration between scientists, policy makers and stakeholders alike. However, in order to fulfil such objectives there is a need to manage complexity effectively. How can the challenges of representing reality, technical constraints and meeting the expectations of stakeholders be overcome? The objective of this study was to explore whether participatory exercises could be used to parameterise an empirical ABM effectively; representing behavioural decisions and coping strategies of Malawian farmers accurately and allowing the impact of policy interventions on food security of rural households within Malawi to be explored. The perks and pitfalls of such an approach will be discussed with credence given to the underlying assumptions and simplifications of the resulting model.

Close Contact Fluctuations: Bonding Time and Sustenance Length in T cell Immunological Synapse

Amit Chattopadhyay (Aston University)

This is a sequel on the analysis of the strength of the T Cell immulogical synapse. Through two separate articles, we have resolved the long standing debate as to the proper time (T) and length scales of the onset of the immunological synapse (IS) bond, the non-covalent chemical bond that defines the immune pathways involving T-cells and antigen presenting cells (APC). Results from our model calculations show T to be of the order of seconds instead of minutes. Close to the linearly stable regime, we show that in between the two critical spatial thresholds dened by the integrin:ligand pair (X2 ~ 40-45 nm) and the T cell receptor (TCR):pMHC bond (X1 ~ 14-15 nm), T grows monotonically with increasing co-receptor bond length separation d (= X2-X1) while it decays with X1 for fixed X2. The non-universal d-dependent power-law structure of the probability density function (PDF) further explains why only the TCR:pMHC bond is a likely candidate to form a stable synapse. A similar analysis implemented in the spatial regime confirms the average size and density of thermally induced regions of close contact in cell : cell contact interfaces to be below one-tenth of a micron across. Our calculations indicate that as the distance between the close contact threshold depth and the mean membrane-membrane separation increases, the density of close contact patches decreases exponentially while there is only a minimal variation in their mean size.

Development of a Resource Secure City using the City Analysis Methodology: the Liveable Cities approach to addressing this challenge over the next 50 years

Susan Lee (University of Birmingham)

Resources such as food, water, metals and minerals are in ever-increasing demand by cities, particularly as populations grow and urban environments expand. Associated tensions include the effects of climate change and the need to be resilient – i.e. being able to generate / harvest our own resources in a move towards self-sufficiency, while being able to rely upon imports when our own supplies are compromised. Resource efficiency, resource reuse / recycling, resource substitution, the ‘circular economy’, industrial symbiosis, energy-from-waste, and the concept of ‘zero waste’ all feature in this complex equation.

The Liveable Cities research programme set out to understand how cities perform across all dimensions of their people, environment, economy and governance, and to establish how urban performance relates to the vision of low-carbon living, working, and playing while using resources responsibly (i.e. not compromising future generations in terms of resource use by consuming only what the planet can provide and replenish). This research aims to reveal the radical engineering in cities necessary to realise these visions while positively benefitting its citizens, rather than compromising their activities.

This paper describes the development of a City Analysis Methodology (CAM), including its philosophy and structure. The CAM aims to aid all those who shape cities in achieving low-carbon, resource-secure future cities which prioritise the well-being of their citizens. A material and energy flow analysis is being undertaken for Birmingham to establish the resources imported into the city, generated within it, consumed, and exported from it or leaving as waste. These flows include water, energy, food, carbon, people, carbon-intensive materials and waste, and their analysis will provide data to inform the CDF. Two examples of the current flows of water and energy resources for Birmingham are shown. They highlight the water-energy nexus and its importance to citizens' well-being, city resilience and the carbon footprint of the city.

Engineering Transparent Simulations for Science

Paul Andrews (University of York)

Computer simulation approaches are taking an increasingly important role in many areas of the physical and social sciences. Whilst there are many appealing reasons for their use, it can be a non-trivial task to interpret or justify simulation result with respect to the system of study in the real world. The construction of simulators necessitates making assumptions (simplifications, approximations, abstractions, etc) during both the modelling and implementation stages. I will present our ongoing efforts to engineer simulations in a transparent way in order that their results can be meaningfully analysed and challenged. I will highlight the need to understand the underlying model that the simulator implements, examine the importance of calibrating simulations, and discuss an approach to openly documenting simulator design and use.

Mr Darcy was good enough for me - pragmatism and prediction in groundwater science

Alan Herbert (University of Birmingham)

Our understanding of groundwater flow started with Henry Darcy's experiments on the flow of water through sand columns used to help design the water supply for the city of Dijon, presented in a paper from 1856. His empirical equation is still at the heart of almost all groundwater flow calculations. It is clearly an oversimplification of the real, complex and heterogeneous systems to which it is applied, but a complete description of the flow processes and heterogeneous properties would be unusable and incapable of characterisation. We apply Occam's razor to direct us to the simplest theory which will allow us to predict the quantities of interest, to as good a resolution and accuracy as we need. And because of the difficulty of direct measurement of the relevant properties underground, our models are always uncertain.

Darcy's law provides the simplest and most easily falsifiable starting point for our predictive models. Sometimes, it can be shown that the simplest theory is inadequate to answer the questions we need to address, and then we reluctantly add in complexity where empirical evidence compels us to. Nevertheless, Darcy's law is surprising accurate, it is often the deviations of our measurements from the oversimplified models we use that tell us most about the system.

Maybe, as Sheldon asserts, geology isn't a real science, but at least the equations are easy to solve!

A Data-Driven Approach for Blood Glucose Modelling

Yan Zhang (University of Warwick)

Diabetes is a lifelong condition in which the body cannot control blood glucose. Patients living with diabetes must learn to control blood glucose levels. Researchers have been working on establishing an effective dynamic model to describe and predict blood glucose concentration levels for more than 50 years. Many models have been developed to reflect the complex neuro-hormonal control system, but determine large amounts of parameters in these models while only the glucose concentration time series is provided remains as a big challenge.

To simplify the model structure without losing the generosity, we used a top-down data-driven approach to establish a stochastic nonlinear model with minimal order and minimal number of parameters tailored for each patient to describe and predict the response of blood glucose concentration to food intake. Various degrees of nonlinearities are considered for three groups of people (the control group, Type I diabetes and Type II diabetes group). Variational Bayesian method is applied to select the best model and infer the needed parameters. The parameters describe the dynamics and characteristics of the underlying physiological processes. Since the mechanisms of the glucose absorption are different for Type I, Type II diabetes and non-diabetic people, different distributions of parameters and noises for these groups are expected.

The results from fifteen profiles with 72 hour continuous glucose time series shows that the glucose concentration change during 2 hours after food intake can be modelled by second order linear or nonlinear system for all three groups. The value of the parameters and intensities of the noises vary from peak to peak for a single profile. The analysis of variance for parameters and noise intensities shows significant differences between the control group and both diabetes group. Further comparison with existing models is going to be investigated in the near future.

Microbiology's N-body Problem: Interspecies Metabolite Transfer in Spatially-Structured Populations

Robert Clegg (University of Birmingham)

No microbe is an island: exchange of metabolites between microbes is crucial to nutrient cycles in both natural and man-made environments. However, even when it is experimentally possible, directly measuring or modelling the rate of exchange within observed populations is difficult. In a sense, this is comparable to the N-body problem of planetary motion, where predicting the long- term effects of gravitational pull between heavenly bodies becomes increasingly difficult the more numerous they are.

As metabolites are often transported by diffusion, reducing the physical distance between partners can greatly increase the rate of exchange and so also increase the productivity of the population. For example, degradation of organic matter to methane in lake sediments and sewage treatment plants often requires rapid transfer of acetate or hydrogen from producers to consumers. Ecologists and engineers interested in this problem have estimated the rate of metabolite exchange between groups using the average distance between a cell of one type and its nearest neighbour of the other. This statistic is a valid estimator in the detection and classification of spatial patterns, but its reliability in estimation of exchange rate is untested.

The uncertainty in estimating rate of exchange is an issue affecting many topics in microbial ecology and biochemical engineering, and our computational approach seeks to correct this. The rate of exchange is both solved numerically, and estimated using spatial statistics such as the distance to nearest neighbour. These estimates can then be compared to the numerical solution. The overall aim of this project is to determine the most reliable statistical estimator in a scientifically rigorous manner, so that those studying these systems in the field can make predictions in confidence.

Modeling Complexity: A Case-Based, Mixed-Methods Density Approach

Brian Castellani (Kent State University, USA)

Over the past several years we have developed a case-based, mixed-methods, density approach to modeling the temporal and spatial complexities of big data. The platform for this approach is called the SACS Toolkit. In terms of simplifying assumptions, the Toolkit employs two novel solutions: (1) it conceptualizes the complex causal organization of a system as a set of microscopic cases (k-dimensional vectors spaces); and (2) it translates their high-dynamic microscopic trajectories into the linear movement of macroscopic, low-dynamic densities.

The strengths of this approach are several. It allows researchers to: (1) map the complex, nonlinear evolution of ensembles (or densities) of cases; (2) classify major and minor clusters and time-trends; (3) visually identify dynamical states, such as saddles and attractor points; (4) plot the speed of cases along different states; (5) detect the non-equilibrium clustering of case trajectories during key transient times; (6) construct multiple models to fit novel data; (7) predict future time-trends and dynamical states; and, finally, in terms of impact, (8) generate results that are visually and conceptually intuitive to private/public sector users and policy makers.

Discussion Panellists

Paul Andrews
University of York

Brian Castellani
Kent State University

Alan Herbert
University of Birmingham

Aaron Sloman
University of Birmingham

Organisers

All organisers are PhD students at the University of Birmingham.

Robert Clegg
School of Biosciences

Craig Holloway
School of Mathematics