B5.1: Examinable content

All material which was lectured (either in this course or one of its formal pre-requisite courses), or which appeared in any exercise sheet, is examinable.

If any material, including exercises and examples, appears in the additional lecture notes, you should assume it is examinable. You should assume that you may be asked to apply any techniques or tools we used to problems you have not seen before. The following is a rough list of topics covered.

- 1. Elementary theory of chemical reaction systems, including: deterministic (ODE) and stochastic (continuous-time Markov chain – CTMC) models; reaction intensities (propensities); deterministic and stochastic mass action kinetics.
- 2. The Gillespie algorithm and its theoretical underpinning: waiting times and transition probabilities.
- 3. The Kolmogorov forward and backward equations corresponding to CTMC models of reaction networks. The chemical master equation.
- 4. Solutions to the chemical master equation ("evolving measures") and the stationary chemical master equation ("stationary measures").
- 5. Differential equations for the evolution of moments and probability generating functions.
- 6. Basics of stochastic differential equations (SDEs), including the "computational version".
- 7. The forward (Fokker-Planck) and backward equations corresponding to SDEs.
- 8. The chemical Langevin equation and the chemical Fokker-Planck equation.
- 9. Diffusion modelled by SDEs, and compartment-based models of diffusion. Boundary conditions corresponding to adsorption and reflection.
- 10. Diffusion-advection SDE models, including basic models of chemotaxis.
- 11. Reaction-diffusion models. Derivation via compartmental models. The "reaction radius" and modelling of second order reactions.
- 12. First passage time (FPT). Mean FPT. The distribution of FPTs. The differential equations and natural initial/boundary conditions associated with these.
- 13. The use of auxiliary differential equations and fluxes to compute conditional probabilities.

This list of topics corresponds roughly to the following sections in the course text: 1.1–1.5, 2.1, 3.1–3.8, 4.1, 4.2, 4.4, 4.6 (techniques, but not all the detail), 6.1–6.3, 6.5, 6.6 (but not the part "SSA for larger time steps"), 7.1, 7.2, and the appendices.

There are other sections in the course text which you may find useful to read, although we did not cover much of the material in these sections. For example, Sections 2.2–2.4 are useful for helping you set up deterministic and stochastic versions of the same chemical system. We covered some techniques from Section 8.1, but not the particular model developed there.

Chapters 5 and 9 are *not* examinable, and the majority of Chapter 8 will not be examined (but see above). We discussed chemotaxis, but not the model in Section 7.3, so this is not examinable. The content in Sections 7.4–7.6 is also *not* examinable.