ANSC*6030 Modelling Metabolic Processes

After completion of the course, you should be able to:

knowledgeably discuss simulation modelling of any nature
build and test complex mathematical models
use the simulation language ACSL
understand the processes of numerical and analytical integration
think of biological problems in terms of mathematical constructs
more fully understand your area of experimental research, no matter the subject

Following is the outline of the course. The emphasis is really on teaching you to be able to build and test complex models of the systems you will study in your future research careers. All aspects of model development will be taught in lectures with weekly assignments on a common exemplary dynamic system. However, each of you will obtain independence in model construction and analysis with a term project to produce your own model from equations presented in the scientific literature. Once the basics of modelling have been taught, we will examine several different types of more advanced models considering such phenomena as distribution in space and chaos. The orientation of the models selected is towards an improvement in understanding of biological systems currently being studied by experimentation. A previous knowledge of animal biochemistry and physiology is required for the course.

You will learn the process of model development by conducting all the steps yourselves on a simple example model. The lectures will be used to discuss the results of the previous assignment(s) and introduce the methods for the subsequent piece of work. I will lead the discussion and lecture on modelling methodology. Weekly assignments will involve short write-ups and overheads or data files on disk prepared for discussion of results in class.

marks:	weekly assignments	55
	participation in discussion	15
	term project (written and oral presentation)	30

week 1 - introduction to modelling philosophies
- assignment:
  - find a simulation model on the web
  - download and run shark/fish WATORW.EXE model

week 2 - introduction to modelling procedure and ACSL using simple model as example
- demonstrate ACSL coding for one pool
- assignment:
  - finish ACSL code for model
  - examine effect of integration interval and initial values on outputs
  - produce figure(s) in manuscript

week 3 - variables and constants
- explain response/behaviour analysis
- assignment:
  - what else should be in model or model code?
  - conduct behaviour analysis of model

week 4 - variables and constants (cont'd)
- explain sensitivity analysis
- assignment:
  - make initial estimate of parameter values

conduct sensitivity analysis of model

<u>week 5</u> - parameter estimation

- least squares and maximum log likelihood
- assignment:

  each student assigned part of a grid of parameter values to input for comparison of example model predictions against observation data set handed out

<u>week 6</u> - collate prediction *vs.* observation analysis and identify best fits

- Monte Carlo analysis
- assignment:

  develop a proposal for the term project

<u>week 7</u> - project proposals

- short oral presentation of what you propose to do for the term project which is to:

  reconstruct a mathematical model from a scientific paper or develop your own model, produce outputs and simulate conditions of interest to test and critique model

- assignment:

  biological phenomenon chosen - how would you model it?

<u>week 8</u> - prediction *vs.* observation testing

- mean square prediction error decomposition
- assignment:

  determine goodness-of-fit of model to independent data set

<u>week 9</u> - kinetics

- derivation of first-order, Michaelis-Menten and sigmoidal equations
- assignment:

  identify which equation best describes a set of observations handed out

<u>week 10</u> - integral calculus

- intro to MAPLE
- assignment:

  find analytical solutions to example model pool sizes at time t

  check answers with ACSL

<u>week 11</u> - distributed-in-space models

<u>week 12</u> - chaotic models

<u>useful textbooks</u>:

Baldwin, R.L. 1995. Modeling Ruminant Digestion and Metabolism. Chapman & Hall, London, UK. QL 737.U5 B155

Close, C.M. and D.K. Frederick. 2002. Modeling and analysis of dynamic systems. 3rd ed. John Wiley & Sons, New York, USA. QA 402.C53 2002

France, J. and J.H.M. Thornley. 2007. Mathematical models in agriculture: quantitative methods for the plant, animal and ecological sciences . CABI Publ, Wallingford, UK. S 494.5.M3 F72 2007

Gentry, R.D. 1978. Introduction to calculus for the biological and health sciences. Addison-Wesley, Reading, USA. QH323.5.G46 1978

Lassen, N.A. and W. Perl. 1979. Tracer kinetic methods in medical physiology. Raven Press, New York, USA. QP43.L37

Shipley, R.A. and R.E. Clark. 1972. Tracer methods for in-vivo kinetics: theory and applications. Academic Press, New York, USA QP 521.S47