

Guidelines for Model Implementation Assignments

<p><i>tr.v.</i> im·ple·ment·ed, im·ple·ment·ing, im·ple·ments (-m nt) To put into practical effect; carry out: <i>implement the new procedures.</i></p>

The purpose of these exercises is twofold:

- 1) to gain experience in quickly implementing numerical simulations of simple kinetic models; and
- 2) to examine biomolecular kinetic phenomena by computational experimentation.

You should implement a MATLAB version of the mathematical model in the indicated paper, and validate that your implementation is correct by reproducing some of the results presented in that paper. *Note that we do not expect you to reproduce every single data point in the paper; rather, it is left to your judgment to identify the key, most discriminating tests to assure that you've correctly implemented the model.*

You should then examine the behavior of the system by computational experiments. For example, alter, add, or subtract a particular step in the underlying mechanism and determine the consequences. Or, perform a sensitivity analysis on the parameters of the model to determine which are most critical for the underlying behavior. Explore ideas and issues that were raised during classroom discussion of the paper. Creativity is encouraged!

Turn in:

A) A 3 pp. executive summary describing the exercise, any difficulties with it, and the primary conclusions. Should you feel it is necessary to include extra pages of calculations or derivations, you may include them in an appendix. Such material is not expected and will only be read if the TAs cannot follow the logic of your report.

B) Email the TAs an executable copy of your MATLAB source code, including any additional files (m-files). Please name all your files according to the following convention:

Implementation code: yourusername_firstauthor.m (e.g., cookb_huang.m)

All function m-files: yourusername_fxname.m (e.g., cookb_dxdt.m)

<Note that you can name your function m-files however you like>

C) A small number of plots (i.e. < 10), each with a substantive figure caption (i.e. a self-contained description of the figure) describing the results presented. Please remember to label all your figures properly (title, legend, and axes with UNITS).