

Workshop on Modeling Biological Systems

Debraj Ghose

Contents

1	About the workshop	1
2	Programming prerequisites	2
3	Well-mixed biochemical reactions	3
4	A single diffusing molecule	3
5	Macroscopic diffusion	4
6	Reaction-diffusion systems	4

1 About the workshop

Biological systems often have many interacting components, and describing them mathematically allows us to formalize our (often pathetic) description of a given system. The mathematical model can then be used to make predictions or develop a better intuition about the biological system's behavior. This workshop will teach you to utilize simple numerical tools from computational physics and chemistry to mechanistically model processes seen in biological systems. The material covered will include modelling well-mixed biochemical reactions, microscopic diffusion, macroscopic diffusion, and reaction-diffusion systems. There will be a total of two sessions and each session will last between 2 to 3 hours. We will use the programming language MATLAB to execute all simulations, but

if you feel confident about replicating MATLAB's matrix and rendering capabilities on another platform that you are more comfortable with, feel free to do so. Prerequisites: Some familiarity with differential equations, matrix algebra, molecular biology, and programming. You will need to bring your own laptop to run simulations (you can get a licensed version through Duke). If you are new to programming with MATLAB, the MATLAB onRamp course is an excellent resource: <https://matlabacademy.mathworks.com>.

2 Programming prerequisites

The following exercises are meant to illustrate or help you acquire programming prerequisites necessary for this workshop. If these exercises look easy to you, skip them – you already possess the programming prerequisites for this course.

1. Generate 10 overlapping plots of the function $f(n, x) = \sin(nx)$ where n assumes integer values from 1 to 10.
2. Create a 100x100 matrix called A such that there is a linear gradient going from 1 to 100 along one of the dimensions of the matrix. For example:

$$A = \begin{bmatrix} 1 & 2 & \dots & 100 \\ 1 & 2 & \dots & 100 \\ & & \ddots & \\ & & & \ddots & \\ 1 & 2 & \dots & 100 \end{bmatrix}$$

Now, create $B = A^T$, where B is the transpose of A . Obtain $C = A \times B$ and visualize C using the `surf()` (or similar) function.

3. Generate 100 particles that are randomly distributed in two-dimensional space. Do not allow any particle to form further than 10 microns away from your origin. Visualize the positions of these particles using the `scatter` (or an equivalent) function.