

Problem set II: Simulation and modeling (choose any one program)

Please turn in one of these exercises on a floppy disk. Your exercise should be completed within three weeks (by Friday, October 31). Note that you need to sign up for one of the exercises on the distribution sheet circulated in class: no more than 3 can sign up for any one problem. These exercises involve creation of a mathematical model for a biological phenomenon. Please use any objects like message boxes, input boxes, menus, command buttons, list boxes, combo boxes, option buttons, etc. as appropriate for creating an effective graphical user interface for your model.

Each of the five exercises to be done in the course, including this one, is worth 25 points, based on the following values: Does the program follow the specifications and description provided in the statement of the problem? (5 points). Does the program run without crashing and provide the expected output? (10 points). Is the Graphical User Interface well designed and easy for the user to understand? (5 points). Are your documentation and comments adequate? (5 points) Was the exercise turned in on time? (5 bonus points) You are expected to work on these assignments independently - no clones of exercises written by others, please. The disk you turn in should be labeled clearly with your name, problem set number and exercise name (shown in parentheses below). Be sure to keep backups of all your work in case your disks are lost or damaged!

1. Simulate the mechanical behavior of an isolated muscle subjected to electrical stimulation. Plot muscle force vs. time curves for a single maximal stimulus, for low frequency (producing an incomplete tetanus) and for high frequency stimulation (fused response). Let maximum tetanic force = 2.5 x the twitch force.
2. Model the basic responses of the human respiratory system output as might be recorded on a spirometer. The curve of volume vs. time should show the following components: tidal volume, inspiratory and expiratory reserves, residual volume, vital and total lung capacities. All curves can be sinusoidal.
3. Simulate the diffusion of a substance between two compartments of a cell, where initially only one of the compartments contains a quantity of the diffusing material. The equation in this case is $(dQ_i/dt)_{\text{forward}} = -k Q_i / V_j$ where Q_i is the concentration of substance in compartment i diffusing into compartment j , V_j the volume of compartment i , and k the diffusion coefficient. Try sample values of $k = 0.75 \text{ ml min}^{-1}$, $V_i = 60 \text{ fl}$, and $V_j = 20 \text{ fl}$.
4. Simulate the "random walk" of a small molecule showing Brownian motion in a two-dimensional space of 10 by 10 cells. Place the particle at a starting location chosen at random within the 100 cell space. Calculate the number of time intervals required for the molecule to have 'visited' all 100 cells at least once. Do this for 10 trials. Show the movement of the molecule from one cell to another dynamically on the screen, and list the values for each of the trials.
5. Simulate the "random walk" of a small molecule showing Brownian motion in a three-dimensional space of 10 by 10 by 10 cells. Place the particle at a starting location chosen at random within the 1000 cell space. Calculate the number of time intervals required for the molecule to have 'visited' all 1000 cells at least once. Optional: show the movement of the molecule from one cell to another dynamically on the screen.
6. Search the DNA strand nucleotide sequence given below for the occurrence of a shorter sequence TATAAA. Search the sequence and its complement in both directions. Indicate graphically where on the original strand the shorter sequence is found.

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ATCCATTACAGGTCACCTTTATAAACACCCCCATTAGTACTATAAATCGACAAATATC
CAGTACTCAGGACGCATTATTATAAAGCATCGATCCAAACTAAGCGAGTACGCACG
ATCAGCATTTCGATCAGTCAGATGTATCCATTAGAGG
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7. Search the nucleotide sequence in the preceding problem for the occurrence of a shorter sequence ATCCATTACAGG, or for a similar sequence that differs only by one or two nucleotides (indicate which) from the original sequence.
8. Simulate the action potential firing pattern of a motor neuron which synapses with two excitatory and two inhibitory neurons. Allow the pre-synaptic neurons to fire at random times. Display the firing of the four input and one output neurons as discrete events, i.e., at each time interval each cell is either firing or not firing. To make this model interesting, introduce a feedback loop: let the output from the motor neuron stimulate the activity of one of the pre-synaptic neurons.)
9. Simulate hemoglobin's oxygen saturation (or dissociation) curve response to a specified increase in CO₂ or H⁺ concentration or temperature. Compare the control curve with the shifted curve by plotting both on the screen.
10. Model the growth of microorganisms under conditions where the population density is limited by available nutrient (e.g. in a closed environment like a Petri dish). Then subject the microorganisms to an antibiotic which kills off all but a small fraction of resistant cells. Hint: the inhibited growth equation can be written as $dN/dt = k*N*(LN)$, where L is the limit; the solution is $N_t = N_o * L [N_o + (L - N_o) * \exp(-L * k * t)]$; here N_o is the original population density.
11. Simulate a metabolic pathway with substrates A through E over 1,000 time intervals in which an inhibitor K of the forward reaction from B to C is applied at time t₁ and is removed at time t₂. Graph the concentrations of metabolites A through E.