Chemotaxis Simulator
Technical Summary

Purposes of This Activity

1. Demonstrates how the continuous application of simple rules for sensing and responding to the environment can generate useful (seemingly “purposeful”) behavior.
2. Provides a detailed functional example of an allosteric mechanism.
3. Provides an example of the principle that life achieves success by optimizing rather than maximizing.
4. Serves as a central component of a simulation module in Chapter 7 which demonstrates evolution by adding competition, selection, and random variation to the Chemotaxis Simulator.

Spatial Model

The bacterium moves within a two-dimensional square region in which food particles are distributed. Typical food distributions include gradients around maxima, with some maxima more concentrated than others. For the prototype simulator, the same fixed food distribution is used for all trials. The final design allows the user to generate endless new random food distributions of any of three different pattern types.

If the bacterium hits a wall during run mode, it “reflects” off the wall at an equal angle. This is expected to have no effect on the mathematics or the emergent behavior of the simulator.

The bacterium can move in any direction (any angle from 0 to 2π radians) during a run. Due to limitations in the prototype, the bacterium does not turn to face the exact direction it is moving, but it does face in whichever of its eight possible orientations most closely approximates its direction of movement.

Bacterium Behavior

The bacterium moves in two modes: “run” mode where the bacterium moves in a straight line in its chosen direction, and “tumble” mode where the bacterium tumbles randomly in place to establish a new direction. The velocity of the bacterium’s movement is constant during run mode and is not adjustable in the simulator (since, all other things being equal, a faster-moving bacterium will always perform better than a slower one). The tumble time is also fixed.

The behavior model has only one input from the environment, which is the local concentration of food in the bacterium’s current location, and only one responsive variable, which is the length of each “run” cycle.

The measure of success of the bacterium’s performance in the simulator is the integral of the food concentration at the bacterium’s location through the entire simulation. Better performance requires that the bacterium’s movements trend toward higher food concentrations and remain within high concentration areas once found. In some food dispersion patterns, the ability of the bacterium to avoid becoming trapped in sub-optimal local concentration maxima becomes a factor.

Model for Sensing and Responding

The model bacterium has a minimum “run” time which is set by the user with the first of the three slider controls. This is modeled as being controlled by a biochemical clock that counts down to the end of the run cycle. The clock can be slowed, but not speeded up, by signals from the environment, so the bacterium will always run at least the minimum set distance in each run cycle.

The response of the organism to the food concentration is modeled as a three-part process:

1. Receptors on the surface of the bacterium respond to changes in the food concentration at the bacterium’s location and trigger corresponding allosteric changes inside the organism. It takes time for the proportion of active receptors to reach equilibrium with the concentration, so this process is modeled as a low-pass filter:

$$\frac{ds}{dt} = \frac{c - r}{T}$$

where r is the level of the internally “sensed” raw signal
c is the external concentration of food
and T is a characteristic time constant

Because c is determined once per time step and remains constant through the time step, the change in r at each time step t_0 to t_1 is calculated exactly by

$$\Delta r_{t_0 \text{ to } t_1} = k_1(c_{t_0} - r_{t_0})$$

where

$$k_1 = 1 - e^{-\frac{\Delta t}{T_e}}$$

and Δt is the length of the time step
T_e is the time constant for the external receptors.

2. The sensed signal influences the “run” clock controlling the flagella. However, its influence diminishes when the value of r holds constant. The receptors of the clock become accustomed to a given signal strength over time, changing the baseline level b above which the raw signal r must rise to influence the clock. This is modeled as a high-pass filter, as follows:

$$s = k_3(r - b)$$

where s is the effective net signal driving on the clock
r is the raw level of sensed signal
b is the baseline level of raw signal that the clock's receptors are accustomed to
k_3 is the sensitivity of the clock to the effective signal's influence

The baseline drifts according to the equation

$$\frac{db}{dt} = \frac{r - b}{T_s}$$

where T_s is the characteristic time constant for the baseline drift

This is numerically approximated during each time step of the simulation, based on the average of the values of r at the beginning and end of the time step, by:

$$\Delta b_{t_0 \text{ to } t_1} = k_2 \textbf{Error!} - b_{t_0})$$

where

$$k_2 = 1 - e^{-\frac{\Delta t}{T_s}}$$

3. The signal s, if it is positive (which it is whenever the general trend of the external food signal level c is increasing), slows the clock for the duration of the time step by a factor of (1+s). If the clock normally decrements an amount Δt, it decrements by

$$\frac{\Delta t}{1 + s}$$

if s is positive. If s is zero or negative, there is no effect on the clock and the time remaining in the bacterium's current "run" decrements by Δt. When the clock reaches zero or below at the end of a time step, the "run" is over and a "tumble" episode begins.

The User-Adjustable Parameters

The first slider control is labeled "Run Time" and determines the minimum amount of real time the bacterium will "run" between "tumbles." This is the amount of time the bacterium will "run" if there is no increase in the food signal throughout the entire run cycle. Because the velocity of the bacterium is constant, the Run Time also determines the run distance. An adjustment leftward shortens the Run Time.

The second slider control is labeled "Response Time" and determines the two time constants T in the high and low frequency filter model described above. The same control adjusts both time constants, which retain a constant ratio to one another, the time constant for the external sensing being faster than the time constant for the internal baseline drift. At the start of a trial in the simulator, these time constants are used to determine the factors k1 andk2, which remain constant throughout the trial and are used in the numerical calculations that are performed each time step. An adjustment leftward decreases the Response Time time constants and thus increases the factors k1 and k2.

The third slider control is labeled “Response to Increasing Food” and determines the factor k3 defining the magnitude of the influence of an increasing food concentration on the bacterium’s run clock. The left extreme of the scale represents a drive of zero, which causes the bacterium to ignore the signals and to always “run” the minimum time/distance only. Adjustment rightward increases the effect of the signals on the run clock.

Effects and Tradeoffs of the User-Adjustable Parameters

The simulator is designed so that for any given food dispersion pattern and any given setting of any two of the sliders, the best setting of the third slider for best performance is rarely if ever at either extreme of the slider’s range. The optimum position for each slider is somewhere within its range, and that optimum position changes if the food distribution pattern type or any of the other sliders is changed.

Shorter run length settings cause the bacterium to track toward food maxima with greater certainty, and to remain within high concentration areas more easily. However, shorter settings also cost the organism more tumbling time due to more frequent tumbles, make it less able to detect shallow gradients during the course of a run, and make it less able to sustain a profitable run up a steep gradient when it finds one. Shorter run times may also allow the bacterium to remain trapped in sub-optimal local maxima for longer periods. Excessively long run times, however, will cause the organism to overshoot the maxima and to be less likely to successfully remain in high-concentration areas once found.

Faster time constants (“Response Times”) allow the organism to respond to short-term food increases more quickly, but make it impossible for the organism to detect long-term increasing trends and gradual gradients. A bacterium with fast time constants will not sustain a run up a steady but “noisy” gradient, in which an overall increasing trend is overlaid with random variations that include short-term decreases, for as long as a bacterium with slower time constants. Slower time constants also allow the organism to detect very gradual gradients. However, slower time constants also decrease the organism’s overall sensitivity to short-term changes in the food signal (which can be partially compensated for by increasing the Response setting) and increase the likelihood of overshoot by sustaining a positive internal signal for some time after the food concentration has begun to trend back downward.

Decreasing the Response setting reduces the lengths of the bacterium’s runs when running up a positive gradient. In fact, setting the response to zero will eliminate all chemotaxic behavior. Increasing the response setting produces longer runs up positive gradients, but also makes the runs more prone to be lengthened by spurious short-term changes or noise even when the organism is not moving in a profitable direction. Excessive responsiveness will increase problems with overshoot and make the organism less able to remain within a maximum once found.

Prototype vs. Final Design

The design presented here is the prototype for a simulator activity for the CD-ROM version of The Way Life Works, but does not have all the features designed for the actual product. Besides more polished artwork, additional sound effects, the ability to generate endless different food dispersal patterns at random, and the additional instructional sequences described in the story boards, the final version has several additional features planned:

- The bacterium in the prototype does not have cilia depicted and does not animate (change shape) while moving. The final design calls for the cilia to be visible and animated, and for the bacterium's "body" to wiggle and change shape while moving.

- In the prototype, although the bacterium can move at any angle, it always faces in one of eight discrete directions. The final design calls for a larger number of directions of facing to more closely match the direction of movement.

- The final design adds a fourth slider to the controls, labeled "Mistakes." The setting of the "Mistakes" slider determines how often and to what degree the organism randomly modifies its set parameters (Run Time, Response Time, and Response to Increasing Food) for the duration of a single "run." This demonstrates that breaking its own rules from time to time can be beneficial to the organism by, for example, increasing its ability to be successful in environments (food distribution patterns) other than the one it was optimized for. This adds additional realism to the bacterium's simulated behavior and connects conceptually to the "life creates with mistakes" principle.

- The final design adds additional capabilities for averaging and comparing results of multiple trials. This makes it easier to compare the performance of different bacterium "designs" against one another. It might also be used to demonstrate the importance of running multiple trials when experimenting, since individual trials are affected by chance.