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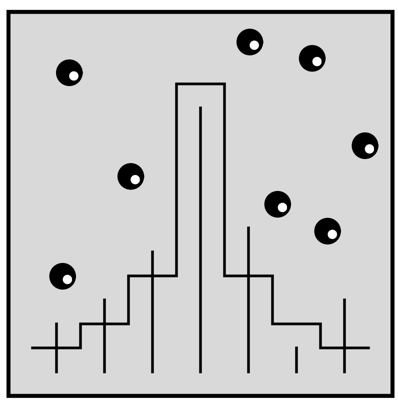
Chapter 2

RANDOM WALK MODEL OF DIFFUSION



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Equation	One Dimension	Three Dimensions
Fick's First Law	$\phi = -D\dfrac{\partial c}{\partial x}$	$\bar{\phi} = -D\overline{\nabla c}$
Continuity Equation	$\dfrac{\partial \phi}{\partial x} = -\dfrac{\partial c}{\partial t}$	$\nabla \cdot \bar{\phi} = -\dfrac{\partial c}{\partial t}$
Diffusion Equation	$\dfrac{\partial c}{\partial t} = D\dfrac{\partial^2 c}{\partial x^2}$	$\dfrac{\partial c}{\partial t} = D\nabla^2 c$

Table 2.1: The macroscopic laws of diffusion for a concentration of particles diffusing in a homogeneous region with a constant diffusion coefficient D, in the absence of a body force on the particles or convection of the medium, and where the particles are conserved.

2.1 INTRODUCTION

2.1.1 Historical Background

A bolus of soluble material will gradually spread out in its solvent, until a uniform solution results. This process has long been intuitively familiar. However, equations that descibe the change in solute concentration, the *macroscopic diffusion equations*, did not evolve until the 1850s, and a *microscopic* or particle-level model, not until the turn of this century. The macroscopic diffusion equations are named for Fick, who presented them (empirically) in 1855 [Fick, 1855]. They show that a concentration gradient causes a solute flux and a consequent concentration change; they may be solved to show the space-time evolution of solute concentration from an initial concentration. Fifty years later, Einstein considered ensembles of particles in Brownian (random) motion, and showed that statistical averages of the motion of these particles give rise to the macroscopic laws of diffusion [Einstein, 1956].

2.1.2 Microscopic and Macroscopic Models

Diffusion plays such an important role in physical as well as biological systems, that it is important for students of these disciplines to develop an understanding of the macroscopic laws of diffusion and their microscopic basis. These are described in a number of textbooks (e.g. Weiss, 1995). Here we will review some important characteristics of the macroscopic laws of diffusion and their relation to random-walk models.

Macroscopic laws of diffusion

The macroscopic laws of diffusion for the simple case when the particles are not subject to a body force, when the medium does not convect the particles, when the diffusion coefficient is a constant, and when the particles are conserved are summarized in one and three dimensions in Table 2.1. These equations relate the flux of particles (ϕ), which is the number of moles of particles transported through a unit area in a unit time, to the concentration of particles (c), which is the number of moles of particles per unit volume. Fick's First Law relates flux to particle concentration; it is analogous to other laws that relate a flow to a force such as Ohm's Law of electric conduction, Darcy's Law of convection, and Fourier's Law of heat flow. The Continuity Equation follows from conservation of particles, and the Diffusion Equation is obtained by combining Fick's First Law with the Continuity Equation.

Important characteristics of diffusion processes are revealed by examining the space-time evolution of concentration from a unit point source. Consider the one-dimensional Diffusion Equation with a unit point source located initially at $x = 0$; a spatial Dirac delta function of concentration having a strength (area) of 1 mole/cm^2. The solution is

$$c(x,t) = \frac{1}{\sqrt{4\pi Dt}}\, e^{-x^2/4Dt},$$

which is a Gaussian or Normal distribution in space whose maximum value is at $x = 0$ and whose width (standard deviation) is equal to $\sqrt{2Dt}$. Hence, an initial unit source of particles spreads out in space at a rate that is $\sqrt{2Dt}$ although the mean position of the particles remains at $x = 0$.

Microscopic basis of diffusion

In a one-dimensional random walk in a homogeneous region of space, we assume a particle moves along the x-axis in a series of statistically independent steps of length $+l$ or $-l$, where the time between steps is τ. In an unbiased walk, positive and negative steps are equally likely, i.e., each has probability 1/2. This simple model can be shown [Weiss, 1995] to yield Fick's First Law and consequently the Gaussian distribution of space-time evolution from a point source. Analysis also shows that the diffusion coefficient, which characterizes the macroscopic laws of diffusion, is related to length and duration of steps, which characterize the random walk, as follows:

$$D = \frac{l^2}{2\tau}.$$

2.1.3 Overview of Software

The software described here is intended to allow students to investigate the properties of the simplest microscopic model that captures the essence of diffusion: the discrete-time, discrete-space random-walk model.

In the discrete-time, discrete space random walk model described here, there is a population of particles which execute statistically-independent, but otherwise identical two-dimensional random walks in a rectangular field. The field can be divided into one, two, or three homogeneous regions whose widths are specifiable, and whose properties may differ. Each particle undergoes a random walk with parameters that include: the probability that the particle takes a step to the left or right, and the step size. These parameters can be set independently in the three regions. The particles can be set to have a specifiable lifetime.

One source and one sink of particles can be placed in the field and the initial concentration of particles can be specified in each of the three regions. Characteristics of the boundary conditions between regions can also be specified. With this software package it is possible: to visualize the spatial evolution of particle concentration from a variety of initial distributions selectable by the user; to examine the evolution of particle concentration from a source and in the presence of a sink; to examine diffusion in regions of differing diffusion coefficients; to simulate diffusion of particles subjected to a body force; to simulate diffusion between two compartments separated by a membrane; to investigate the effects of chemical reactions or recombination which consume particles at a fixed; and to investigate the effects of different boundary conditions between regions. Two diffusion regimes can be run and displayed simultaneously to allow direct comparison between the space-time evolution of two different diffusion processes. In addition, a variety of statistics of the spatial distribution of particles can also displayed.

By watching the particles move and by comparing simulation results to expectations, the user can develop an intuition for the way in which the random motions of particles lead to their diffusive spread.

2.2 DESCRIPTION OF THE RANDOM-WALK MODEL

In this simulation, the discrete-time, discrete-space random walk takes place on a finite two-dimensional grid of locations accessible to the particles and called the *field*. The location of each particle is specified by giving its coordinates on this grid (i, j) where i is the horizontal coordinate and ranges from 0 to 399 and j is the vertical coordinate and ranges from 0 to 99. The horizontal distance between adjacent grid locations is 1 unit of distance and all spatial dimensions of the random walk are expressed as multiples of this unit distance. The position of the particle in the grid can change probabilistically at each step of the random walk. Thus successive steps represent successive times that are separated by a unit time interval. All times are expressed in terms of the number of steps of the random walk.

The field can be divided into one, two or three homogeneous *regions* (Figure 2.1). Certain parameters of the simulation are defined for the entire field, others at boundaries between regions, and still others are defined independently for each region. The latter parameters will be described first and include: region size, particle step size, directional probabilities, and initial particle distribution.

2.2.1 Particle Parameters Within a Region

The parameters that define the random walk are identical at each location *within* a region — each region is homogeneous. These parameters are:

Region size

The width of each region can be specified, but the sum of the widths cannot exceed 400. This allows a variety of diffusion regimes to be defined. For example, if Region 1 has

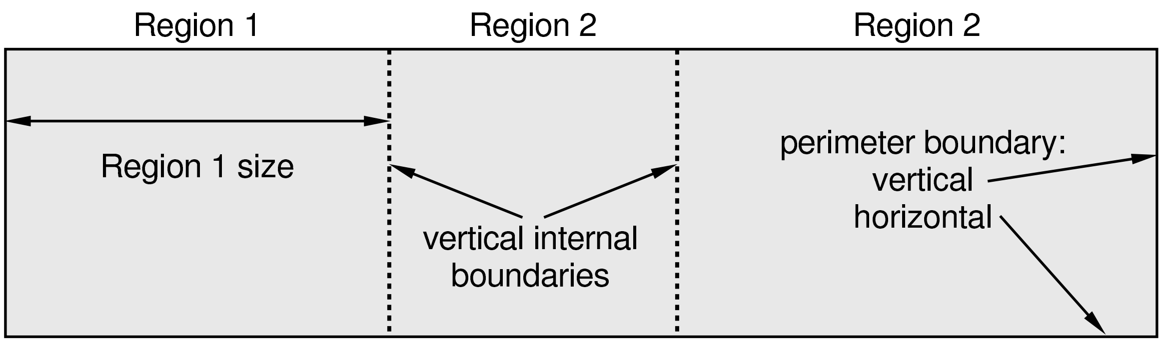

Figure 2.1: Definition of simulation field, regions, and boundaries. Solid lines delimit the perimeter boundaries of the field; dashed lines indicate the internal vertical boundaries that separate the regions.

width of 400 then the other two regions must have width 0 and the random walk is defined for one homogeneous region. By specifying two regions with non-zero widths, it is possible to define a diffusion process with different initial conditions in the two regions. This allows a rich variety of initial distributions to be defined. Three non-zero width regions allows simulation of diffusion between two regions separated by a third region with different properties. This might be used to investigate diffusion between two baths separated by a membrane.

Step size

The step size defines the distance, in multiples of unit distances, that particles may move in each step of time. Varying the step size simulates varying the diffusion coefficient. The size of a region is always set to a multiple of the step size in that region; all particles in a region are located at integer multiples of the step size starting from the left boundary of the region. This ensures that particles at a boundary fall on the boundary and simplifies the specification of particle motion at a boundary.

Particle motion — directional probabilities

At each instant in time, a particle is at some location in the region. The disposition of the particle at the next instant in time is determined by one of six mutually exclusive and collectively exhaustive possibilities as illustrated in Figure 2.2. The particle can move one step size to the upper left, upper right, lower left, or lower right; stay in the same location (center); or be eliminated (expire). The prbabilities for each of the six outcomes is as follows:

$$\begin{aligned}
\text{P[expired]} &= 1/L\,, \\
\text{P[center]} &= (1-1/L)\,(1-p-q)\,, \\
\text{P[upper left]} &= 0.5\,(1-1/L)\,q\,,
\end{aligned}$$

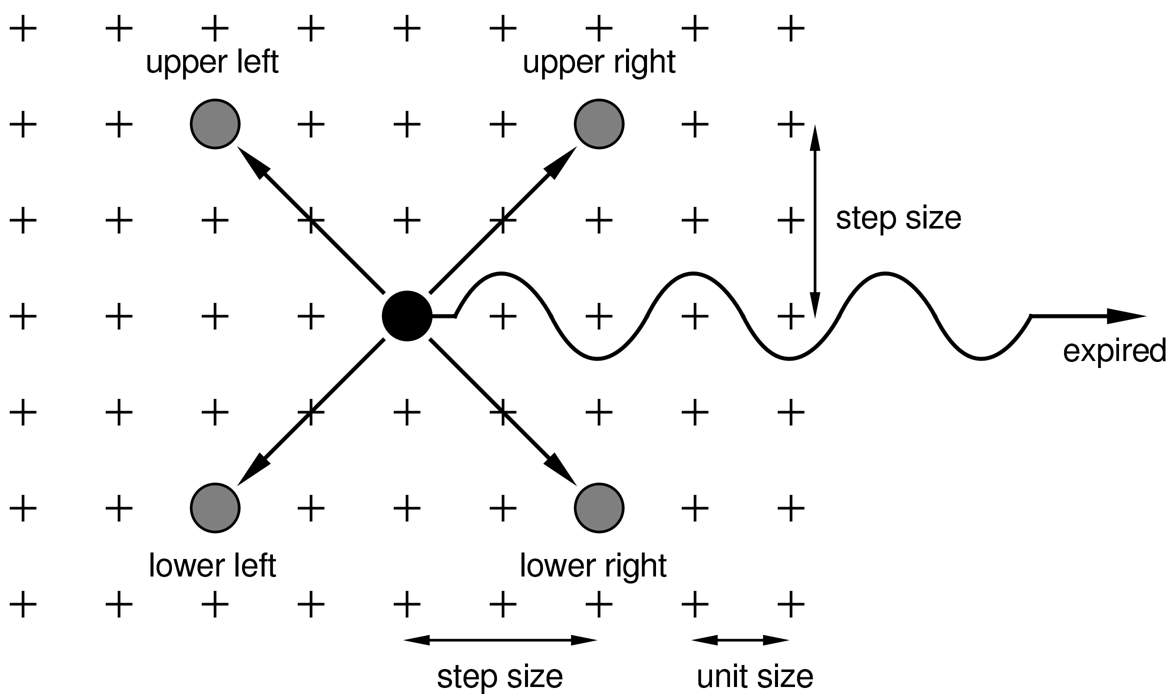

Figure 2.2: Schematic diagram of motion of a particle in a homogeneous region. The grid of possible particle locations, separated by unit distances, are indicated by + symbols. A particle is shown in the center of the figure at one instant in time. One time step later the particle either stays in the same location or moves to one of 4 possible locations (indicated by the shaded particle) or it expires (is removed from the field). If the particle moves it translates one step size (here shown as 2 units of distance) in both the vertical and the horizontal direction.

$$\begin{aligned}
\text{P[upper right]} &= 0.5\,(1-1/L)\,p\,, \\
\text{P[lower left]} &= 0.5\,(1-1/L)\,q\,, \\
\text{P[lower right]} &= 0.5\,(1-1/L)\,p\,,
\end{aligned} \tag{2.1}$$

where L is the average lifetime of the particle, i.e. the average number of time steps to expiration; p is the conditional probability that the particle moves to the right given that it has not expired; q is the conditional probability that the particle moves to the left given that it has not expired. Note that while the probability of moving to the left and to right can differ, the probability of moving up or down is always the same. Because the six probabilities define all the possible outcomes at each instant in time, they sum to unity.

Different types of random walks are described by changing the directional probabilities. The random walk defined by assuming $p = q = 1/2$ is the simple, unbiased random walk described in Section 2.1. In general, if $p = q$ the random walk is unbiased; there is no statistical tendency for particles to move preferentially in either horizontal direction. However, if $p \neq q$, the random walk is biased so that there is a tendency for particles to move in one horizontal direction. For a step size of S, the mean distance $E[m]$ that the particle moves to the right in n units of time is

$$E[m] = Sn(1-1/L)(p-q)\ .$$

Initial distribution of particles

The initial distribution of particles can be specified in each of the three regions. Particles must start at locations that are integral multiples of the step size in each region. The initial distribution of particles can be:

- **Empty** which implies that initially there are no particles in the region.
- **Impulse** which implies that a specified number of particles are placed at a specified horizontal position in the region and spaced randomly in the vertical direction.
- **Linear** which implies that a linear concentration profile is generated whose slope and number of particles are specified. Negative concentrations are not allowed: if the parameters are chosen such that the concentration would become negative at some point in the region, these putative negative concentrations are set to zero.
- **Sine** which implies that the spatial distribution is sinusoidal with a specified period and number of particles.

2.2.2 Boundary Conditions

The field contains three different types of boundaries (Figure 2.1) which are, in order of increasing complexity, horizontal perimeter boundaries at the top and bottom of the field, vertical perimeter boundaries at the left and right ends of the field, and vertical internal boundaries that separate regions.

Horizontal perimeter boundaries

Horizontal perimeter boundaries act as perfectly reflecting walls. If a particle is located within one step size of such a boundary and takes a step toward the boundary then the new vertical location of the particle is determined in the following manner: the vertical distance the particle travels to reach the wall plus the vertical distance the particle travels after reflecting from the wall must sum to the step size. This relation determines the new position given the old postion and the value of the step size.

Vertical perimeter boundaries

The vertical perimeter boundaries are also reflecting walls. Because the probabilities of stepping to the left and right need not be the same, we found that purely reflecting wall of the type described for the horizontal perimeter boundaries created undesirable artefacts especially when the conditional probabilities of moving to the left and right were not equal ($p \neq q$). Therefore, we modified the boundary condition so that a particle that would have crossed a vertical perimeter boundary at a given step was placed on the boundary and then subject to the following boundary condition which is illustrated for the left boundary in Figure 2.3 and whose directional probabilities are:

$$\begin{aligned}
\text{P[expired]} &= 1/L\,, \\
\text{P[center]} &= (1-1/L)\,(1-p)\,, \\
\text{P[upper right]} &= 0.5\,(1-1/L)\,p\,, \\
\text{P[lower right]} &= 0.5\,(1-1/L)\,p\,,
\end{aligned} \tag{2.2}$$

i.e. the particle cannot move to the left.

Vertical internal boundaries

The motion of particles at a vertical internal boundary is similar to that within a homogenous region. The differences are that: the step sizes in the two adjacent regions may differ; and special directional probabilities, specified by the user, apply at the boundary. These have been provided to allow users to explore the consequences of a rich variety of boundary conditions. To simplify boundary conditions, the software ensures that particles do not cross this boundary in one time step but rather they land on the boundary. This is guaranteed by forcing the width of boundaries, initial particle locations, locations of sources and sinks to be commensurate with the step size. Given this restriction, the possible outcomes for a particle on a boundary are shown schematically in Figure 2.4. The directional probabilities are identical to those in a homogeneous (region given above) except that the conditional probability of moving to the left and to the right given that the particle did not expire (p and q in the homogeneous region) are independently specified at each internal boundary. The step size to the left is equal to the step size in the region to the left of the boundary; the step size to the right is equal to the step in the region to the right of the boundary.

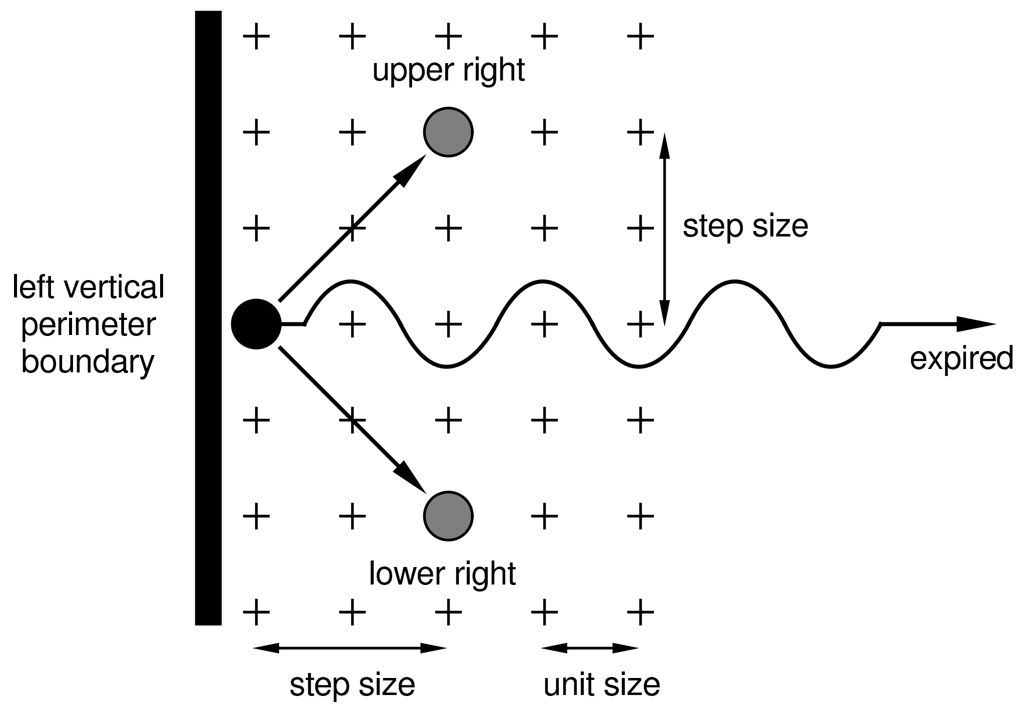

Figure 2.3: Schematic diagram of motion of a particle at a vertical perimeter boundary. For purposes of illustration, the particle motion at the left boundary is shown. Conditions at the right boundary are the mirror-image of those shown here.

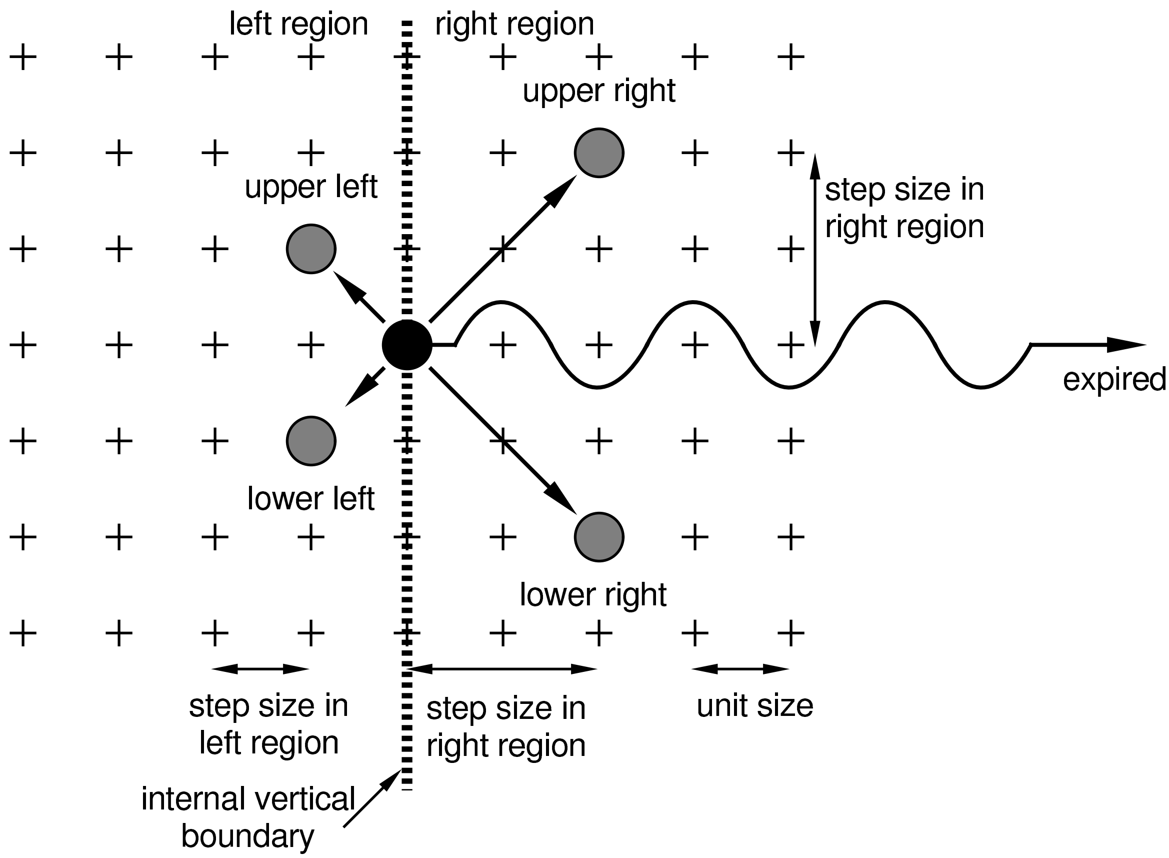

Figure 2.4: Schematic diagram of motion of a particle at an internal vertical boundary between two regions. The step size is 1 to the left of the boundary and 2 to the right of the boundary.

2.2.3 Parameters that Change the Number of Particles in the Field

After the simulation has been initiated with some initial distribution of particles, there are three ways in which the total number of particles in the field can change.

Particle lifetime

The average lifetime L of particles at any location in the field is specifiable. The effect of particle lifetime on the directional probabilities was described earlier.

Source

One source can be placed at a horizontal location in the field and covers the entire vertical height of the field. The source must be located at an integer multiple of the step size from the left boundary of each region in which it is located. The rate of generation of particles is specified by giving the number of particles (specified as a two-digit number) produced in some number of time steps (specified as a two-digit number). Thus the rate of generation of particles can be a rational number. The particles are generated at the horizontal position of the of the source and are distributed randomly along the vertical direction using a uniform distribution.

Sink

A sink can be placed at a horizontal location in the field and covers the entire vertical height of the field. The sink must be located at an integer multiple of the step size from the left boundary of each region in which it is located. Particles that land on the sink are absorbed; hence the number of particles at the sink is always zero.

2.2.4 Statistics

Two sets of computations are performed simultaneously during a simulation: statistics based on the actual locations of particle and statistics based on the expected locations of particles. Given a particle location at one step and a set of directional probabilities, a random number generator is used to determine which of the possible new locations occurs at the next step. These sequence of locations determines the positions of the particles on the screen and all the statistics labelled *actual*. However, given a particle location at one time and the same directional probabilities, it is possible to estimate the *expected* location of the particle in the next step. Thus during a simulation both the set of actual and expected locations for the particles are computed. Both the actual and expected statistics may be examined.

Histogram of horizontal particle locations

Histograms summarize the spatial distribution of particle locations. Each histogram consists of a set of bins that span the field; the number of bins depends upon the specification of the bin size. With a bin size of 10, there are 40 bins that span the entire field of 400 locations. The histogram shows the number of particles in each bin as a function of bin location. Choice of bin size is important. If the bin size is small then each bin will contain relatively few particles and the number of particles will fluctutate randomly from bin to bin. However, a small bin size depicts the particle distribution with a high spatial distribution. Conversely, a large bin size gives a histogram with poor spatial resolution but a larger amount of statistical averaging of the spatial distribution of particles.

The shape of the histogram is sensitive to the choice of bin size and can lead to confusing patterns. For example, suppose the bin size is five and the step size is two. Suppose further that particles are located uniformly in the field; one particle per accessible location. However, the step size constrains the possible locations that a particle may occupy to be separated by 2. Therefore, with a bin size of five, successive bins in the histogram alternate between 2 and 3 particles. Thus the histogram will not appear uniform, but oscillatory. This problem is cured if the bin size is an integral multiple of the step size. If the step size differ in the three regions, then the bin size should be set equal to the least common multiple of the three step sizes.

Statistics as a function of step number

A number of statistics (both *actual* and *expected*) can be plotted versus step number. These are:

- **Mean Position** is the mean position of the particles in the entire field.
- **Standard Deviation** is the standard deviation of particle location in the entire field.
- **#Generated** is the cumulative number of particles generated by the source since the beginning of the simulation.
- **#Absorbed** is the cumulative number of particles absorbed by the sink since the beginning of the simulation.
- **#Expired** is the cumulative number of particles lost due to the finite lifetime of particles since the beginning of the simulation.
- **Total #Particles** is the total number of particles in the entire field at each step number.
- **Region 1 #Particles** is the total number of particles in Region 1 at a given step number.
- **Region 2 #Particles** is the total number of particles in Region 2 at a given step number. For this total only, the particles located at the boundary between Region 1 and Region 2 are counted as belonging to Region 2.
- **Region 3 #Particles** is the total number of particles in Region 3 at a given step number. For this total only, the particles located at the boundary between Region 2 and Region 3 are counted as belonging to Region 3.

These statistics allow a quantitative evaluation of a simulation. A systematic change in the mean position of the particles as a function of step number demonstrates a drift or migration of the particles as can be achieved by a bias in the directional probabilities. A difference in the standard deviation of two distributions can be achieved by changing the step size. The dependence on step number of the number of particles in the field, in a region, generated, absorbed, or expired can be used to assess whether a particle distribution has reached steady state. The change in the total number of particles in each region can be used to estimate the rate of transport of particles between regions.

2.3 USER'S GUIDE TO THE SOFTWARE

The program has two environments: the *parameter* and the *simulation* environments. The *parameter* environment allows the user to change the characteristics of the random walk, the initial conditions, and the inter-region boundary conditions. The user may also load and save data files, and view the initial conditions, without leaving this environment. In the *simulation* environment, the user may watch the particles execute the random walk, while histograms display their actual and expected distribution along the horizontal axis. In both environments, the user may view statistics of the random walk and print the contents of the screen.

2.3.1 The Parameter Environment

When the program is initiated, it puts a *window* (bordered box for display of text and graphics) on the screen. At startup, the program is in the parameter environment, and the window is as shown in Figure 2.5.

The menu bar

The menu bar at the top of the window contains three commands: **Simulation**, **Files**, and **Statistics**. To select a command, the user highlights it by positioning the arrow cursor, and clicks any mouse button. Clicking on a highlighted command causes a *drop-down menu* to appear, as shown in Figure 2.6. Items in the drop-down menu are selected with the mouse as they were in the menu bar. In both the menu bar and the drop-down menu, if the command cannot be highlighted, it is not available for selection.

Simulation. Selection of Simulation allows five options:

- **Edit** allows modification of the random walk parameters by clicking on any highlighted value to modify it (detailed below). After selecting **Edit** and changing parameter values, the **Statistics** option is no longer available because the new parameters do not correspond to the computed statistics.

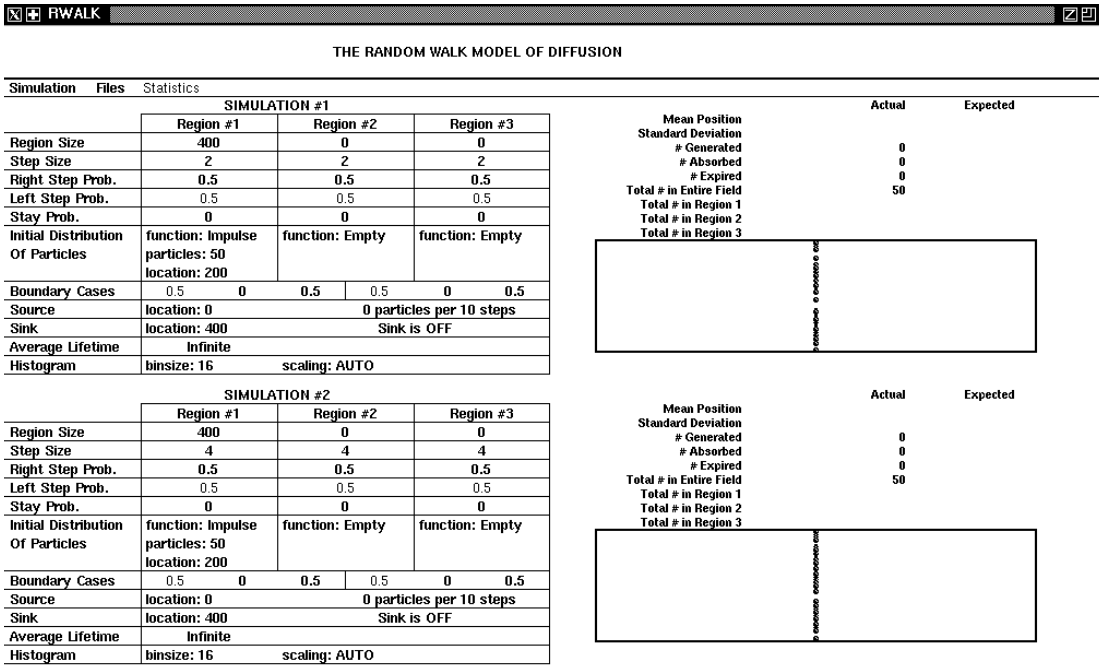

Figure 2.5: Window in the parameter environment after the **View** option has been selected to show the initial distribution of particles.

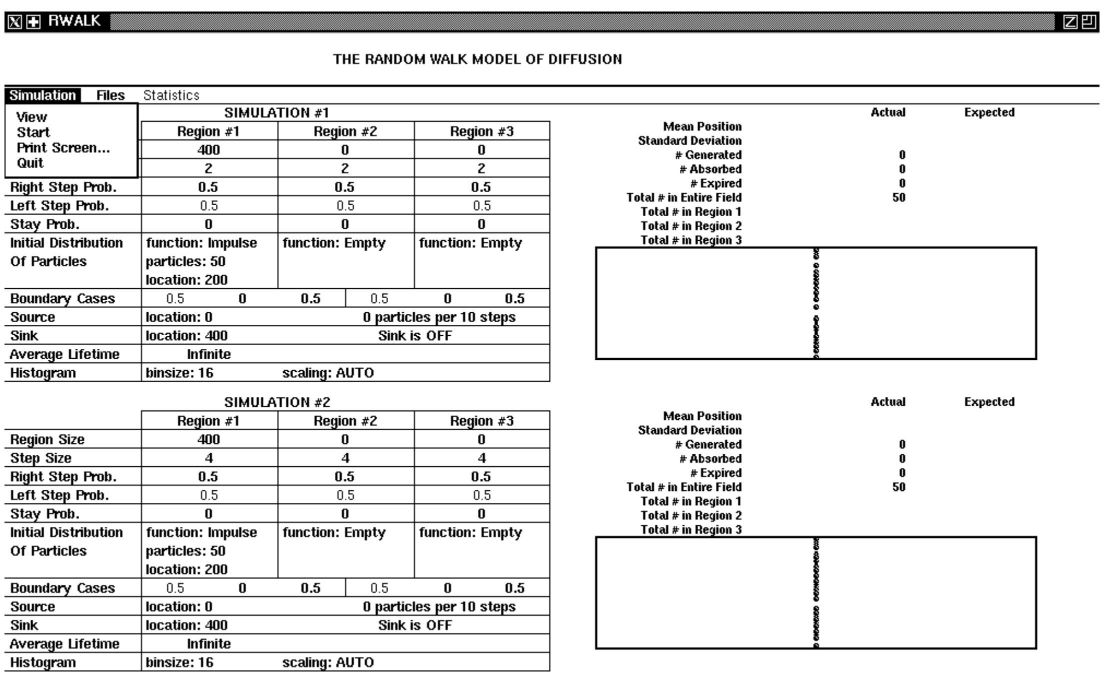

Figure 2.6: Window in the parameter environment showing the drop-down menu for the **Simulation** command.

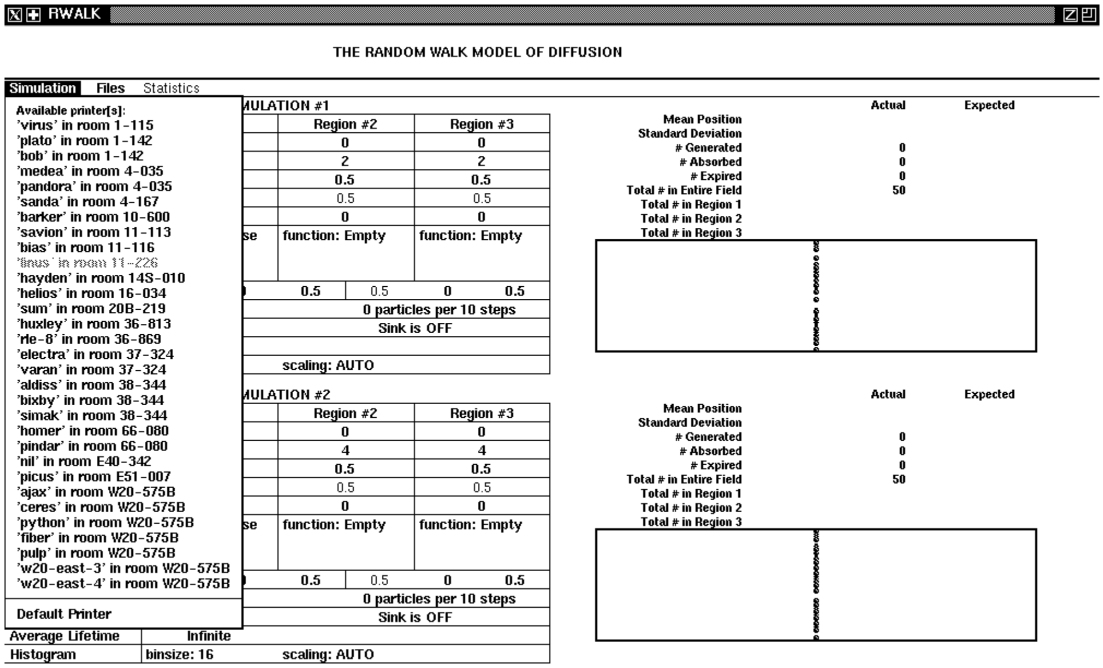

Figure 2.7: Window in the parameter environment showing the drop-down menu used to select the printer.

- **View** allows viewing the initial conditions of the random walk for the chosen parameters (Figure 2.5) without exiting the Parameter environment. (**View** always shows initial conditions, even after a simulation has been run.)

- **Start** transfers control to the Simulation environment.

- **Print Screen** allows selection of a printer for printing the contents of the screen (Figure 2.7).[1]

- **Quit** transfers control out of the random walk software and to the main menu that allows access to other software.

Files. Selection of **Files** allows several options (Figure 2.8):

- Clicking on **Simulation** allows selection of the simulation that will be read or written. Each click changes the selection between #1 and #2.

- Clicking on **Read in data from file...** allows reading the results of a previous simulation *into* simulation #1 (top) or #2 (bottom) as selected previously.

- Clicking on **Write data to file...** allows writing the results of a simulation *to* a file.

- Clicking on **Delete file...** allows files to be deleted.

[1] *Printing the screen is VERY slow! Do not overuse it!*

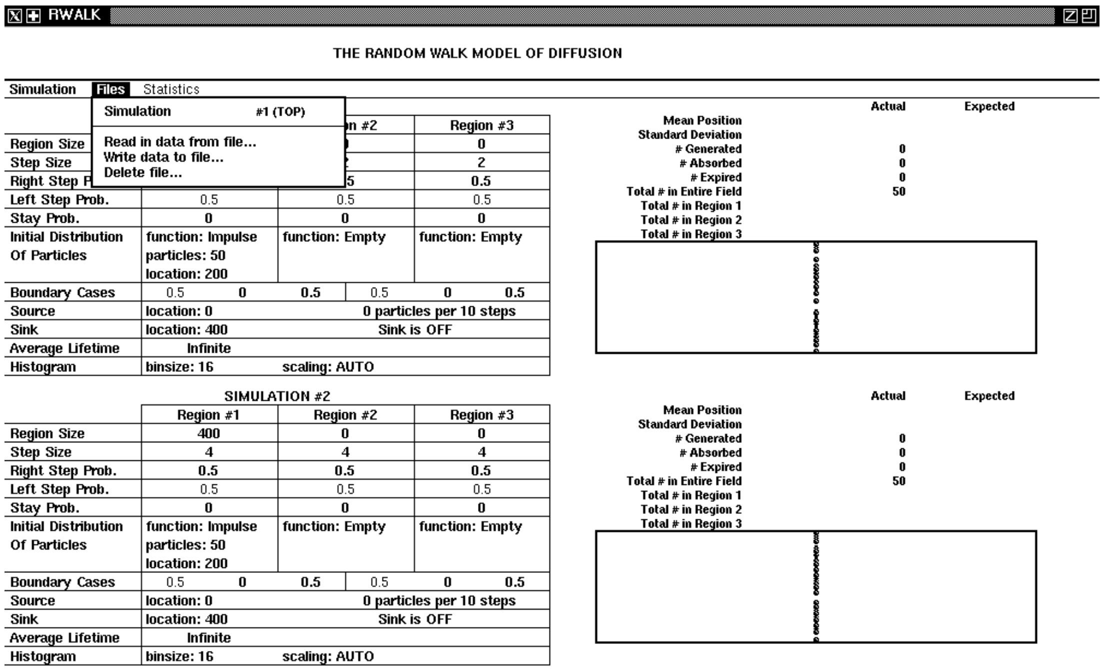

Figure 2.8: Window in the parameter environment showing the associated menu when **Files** is selected.

When any of the file handling options are selected, a new menu appears that allows selection of files and directories (Figure 2.9). The contents of the current directory is shown. The current directory can be changed to a subdirectory either by clicking on the name of the subdirectory or by typing its name into the rectangular window. In either case, click on set directory after selecting the directory. (Recall that two dots .. means back up one level in directory hierarchy.) Clicking on a filename selects that file for subsequent action. Clicking on **Read** reads the file. Typing into the rectangular window allows naming a file for purpose of writing to disk. Filenames must end in **.rw**.

Statistics. Selection of **Statistics** allows graphic display of the latest statistics. This command is available only after a simulation has been run for 1 or more steps or has been loaded from a data file. Statistics allows the user to display statistics of the simulation as well as the expected statistics for the simulation plotted versus step number. However, only 400 entries can be saved in a file. If the step number exceeds 400, then the sequence of entries is decimated by a factor of two (the data for every other step are discarded); each entry corresponds to the data from every other step. As the simulation proceeds, the decimation process is continued to maintain a number of entries less than or equal to 400.

The simulation parameters

- **Region Size.** The user may define up to three regions, whose combined width may not exceed 400.

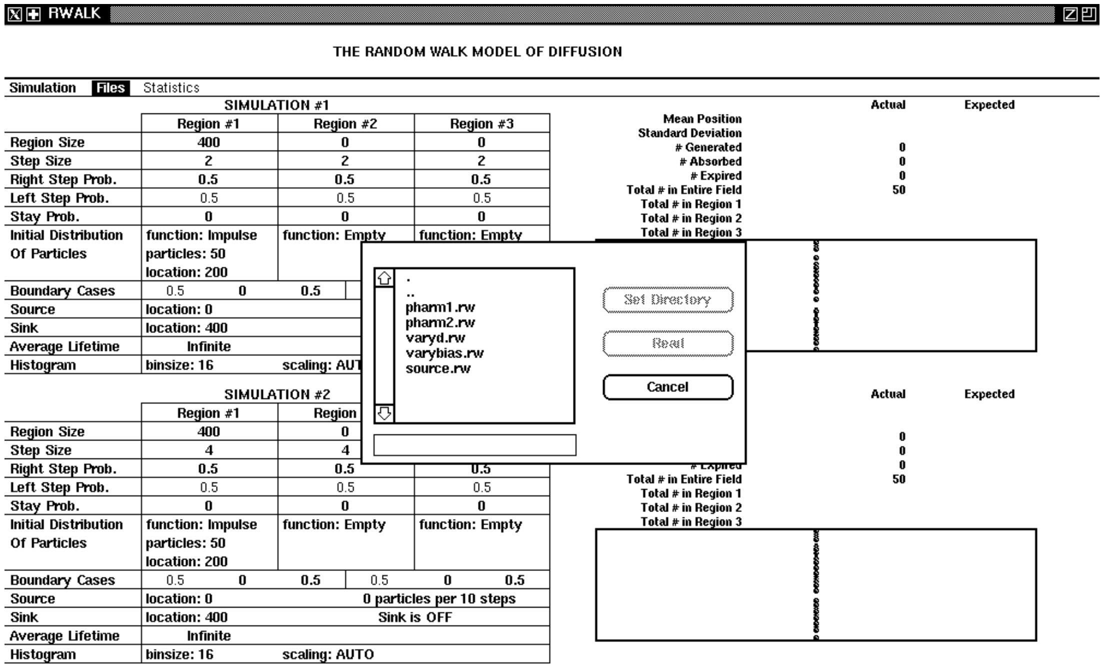

Figure 2.9: Window in the parameter environment showing the associated menu when **Read in data from file...** has been selected from the **Files** menu.

- **Step Size.** The step size can be specified independently in each region.

- **Right Step Prob.** The conditional probability of a step to the right given that the particle has not expired can be specified independently in each region.

- **Left Step Prob.** The conditional probability of a step to the right given that the particle has not expired *cannot* be specified but is set so that in each region the sum of the conditional probabilities of stepping to the left and right and staying in the same place all sum to one.

- **Stay Prob.** The conditional probability that the particle stays in the same location given that the particle has not expired can be specified independently in each region.

- **Initial Distribution Of Particles.** The initial distribution of particles can be specified independently in the three regions. Selection of a different function allows selection of the parameters for that function.

- **Boundary Cases.** The perimeter boundaries of the field act as reflecting boundaries; the boundaries between regions are characterized by user-defined boundary conditions or **Boundary Cases**. Boundary conditions are defined as shown in Figure 2.5: left-step-probability q_{ij}, stay probability s_{ij} , and right-step-probability p_{ij} at the boundary between Region i and Region j (Region #1-#2, Region #2-#3). For example, if the Region #1-#2 has the set of probabilities $(q_{12}, s_{12}, p_{12}) = (0, 0, 1)$ then particles at the boundary may only step to the right. Therefore, to a particle from

Region #2, this looks like a reflecting boundary, whereas all particles reaching the boundary from Region #1 will cross into Region #2. As with the directional probabilities within a region, the user selects the probability of a step to the right and the probability of no step; the probability of a step to the left is then computed so that the three probabilities sum to one.

- **Source.** The location of the source can be specified as well as the number of particles generated in a specified number of steps.

- **Sink.** The particle sink may be turned ON and its location specified.

- **Average Lifetime.** The user may define the average particle lifetime in steps. There is one quirk to this — in order to set the lifetime to infinity (particles do not expire), type zero for the average lifetime. The display will indicate that the lifetime is now infinite.

- **Histogram.** The histogram **binsize** determines the resolution of the histogram. Small bin sizes produce histograms of particle locations with high spatial resolution but a great deal of statistical variation. Large bin sizes result in histograms with poorer spatial resolution but less statistical variation in the histogram. The binsize should be a multiple of the particle step size. Selecting **scaling** allows the ordinate scale of the histogram to be selected manually or automatically.

2.3.2 The Simulation Environment

When **Start** is selected in the parameter environment, control passes to the simulation environment. Initially, the screen might look like the one shown in Figure 2.10. There is no single Menu Bar; instead, the top of the screen shows Display Controls and Simulation Controls.

Display Controls

- **Expected Histogram** ON or OFF. Click on ON or OFF at any time *while the simulation is running*. The simulation runs faster with the expected histogram OFF.

- **Particle Display** ON or OFF. Click on ON or OFF at any time *while the simulation is running*. The simulation runs much faster with the particle display OFF. When the simulation is PAUSED, the particle display automatically reappears.

Simulation Controls

Available commands are in boldface type; they are selected by pointing to them with the mouse and clicking. (Unlike other menus, pointing and clicking does not highlight Simulation Controls.)

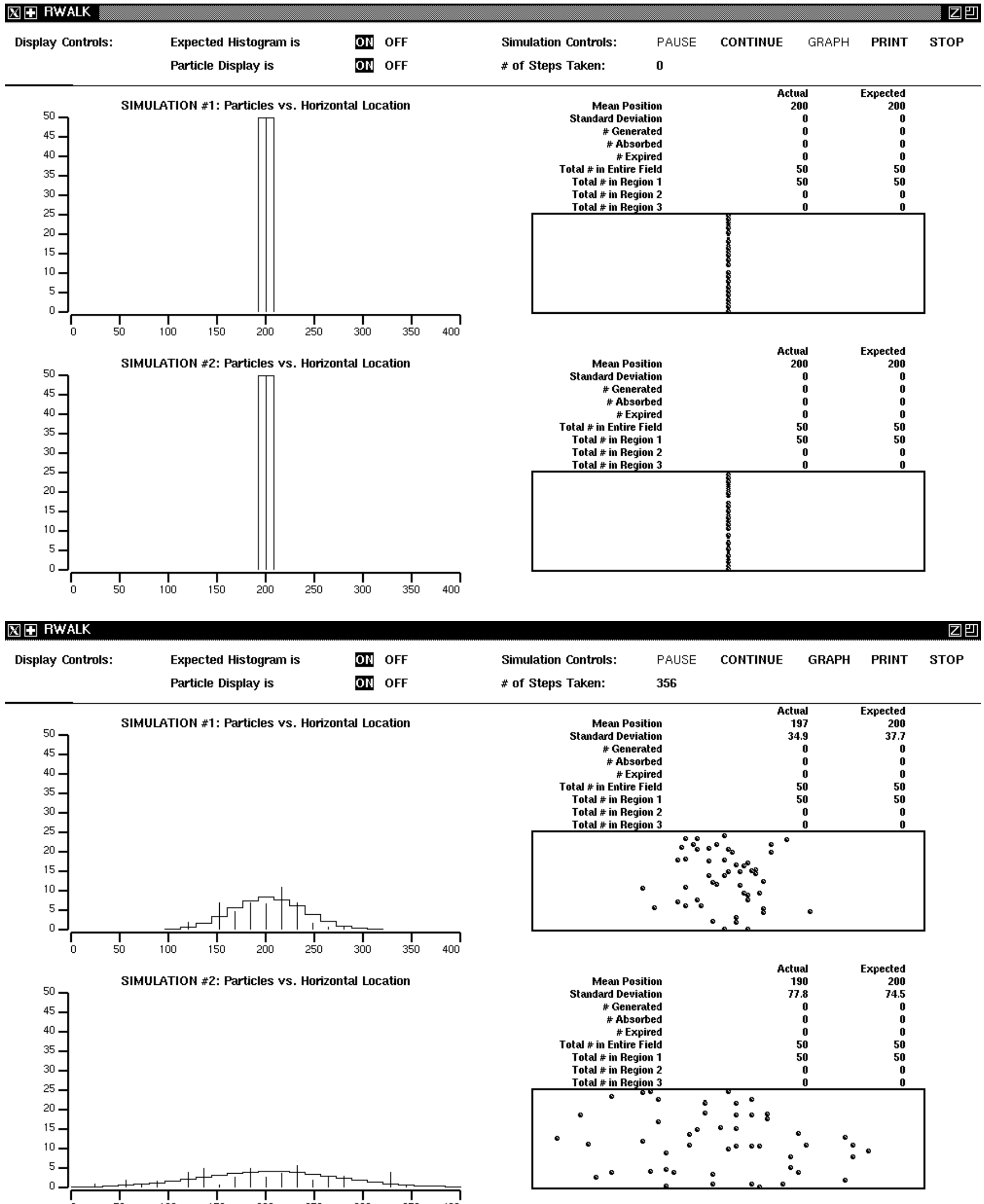

Figure 2.10: Window in the simulation environment before (upper) and after (lower) running the simulation for 356 steps using the the parameters shown in Figure 2.5.

- **PAUSE.** Halt particle motion, and calculate actual and expected values. A running simulation must be PAUSED before any other choices are available.
- **CONTINUE.** Resume particle motion, *i.e.*, run the simulation. The simulation must be CONTINUING if Display Controls are to be changed.
- **GRAPH.** Graph statistics, just as in the Parameter environment (**Statistics** item in Menu Bar). An example of the display is shown in Figure 2.11.
- **PRINT.** Print contents of screen on a designated printer, just as in the Parameter environment (**Print Screen** option, **Simulation** item in Menu Bar).
- **STOP.** Return to Parameter environment.

2.4 PROBLEMS

Problem 2.1 This problem deals with random walks for particles that all begin from the same location at an initial time, i.e. the initial distributions are impulses.

a) Use the default simulation parameters, run the simulation for about 100 steps, and then pause the simulation. Note that the parameters of Simulation #1 and #2 differ only in step size. Examine graphs of the average and the standard deviation of the horizontal locations of the particles versus step number.

   i) Explain quantitatively the differences in the graphs in terms of the difference in step size of the two simulations.

   ii) Why does the slope of the standard deviation decrease with step number? What type of dependence on step number do you expect?

b) Now set the step size to 2 for both simulations and decrease the number of particles in the impulse for one of the simulations to 25. Rerun the simulation. How does the number of particles affect the dependence of average position and standard deviation on step number?

c) Set all the parameters at their default values and then set the step size for both Simulation #1 and #2 to 2. For simulation #1 set the right step probability to 0.75, the left step probability to 0.25, place an impulse of 50 particles at location 100. For simulation #2 set the right step probability to 0.25, the left step probability to 0.75, place an impulse of 50 particles at location 300. Run the simulation for at least 100 steps. Examine graphs of the average and the standard deviation of the horizontal locations of the particles versus step number. Explain these results quantitatively.

Problem 2.2 This problem deals with the steady-state distribution of particles in the presence of a source and sink for both unbiased and biased random walks. For all parts of this problem set the parameters for both Simulation #1 and #2 as follows: make the size of

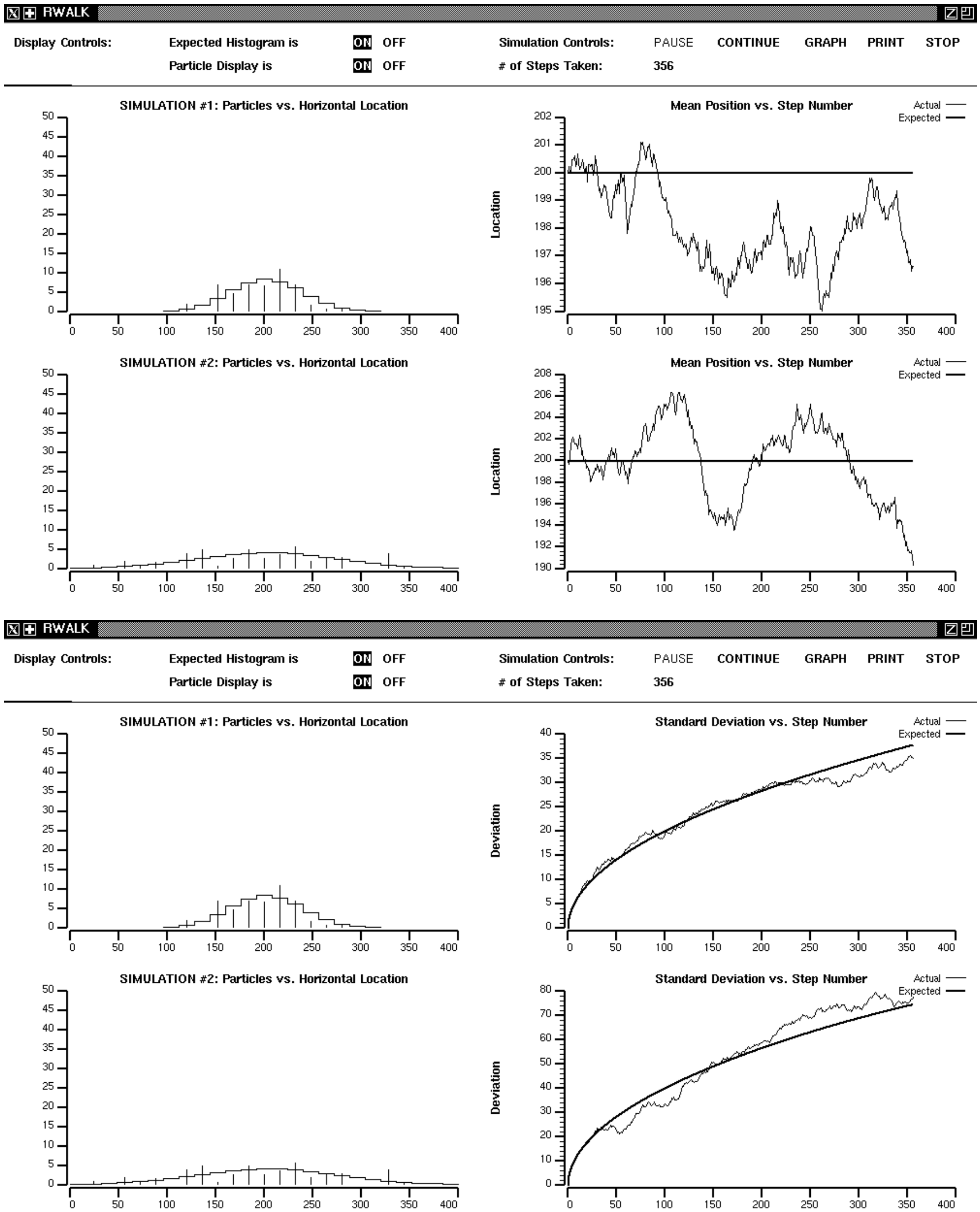

Figure 2.11: Example of statistics option. The displays show the mean (upper) and standard deviation (lower) of the distributions of horizontal particle locations plotted versus step number for the simulations shown in Figures 2.5 and 2.10.

Region #1 400; the step size 20; and make the initial distribution of particles empty. Also place a source at location 0 and a sink at location 400 and make the histogram bin size 20.

a) Make the random walks for both Simulation #1 and #2 unbiased with a right step probability of 0.5. For simulation #1 make a source that generates 1 particle every 2 steps and for Simulation #2 make a source that generates 1 particle every 1 step. Make the particle lifetime infinite for both simulations. Now run the simulation. In the steady-state, by definition the particle distribution will not depend upon step number.

   i) Before you run the simulation, estimate the form of the steady-state particle distribution. Is it uniform, exponential, an impulse, linear, Gaussian, or none of these?

   ii) Using the statistics available, determine a criterion for estimating when the particle distribution is in steady state.

   iii) Now run the simulation until your criterion for steady state is met. What is the steady-state particle distribution? Does it fit with your initial expectation?

   iv) How can you explain the difference in steady-state distribution for the two simulations?

   v) Show that the steady-state particle distribution you have found for the random walks is consistent with Fick's Laws.

b) Use the same parameters for Simulation #2 as in a), but change those of Simulation #1 so that the source rate is also 1 particle every 1 step; and so that the probability of a right step is 0.55. Run the simulation until it has reached a steady state.

   i) Compare the steady-state distributions for the biased and unbiased random walks. How do they differ?

   ii) What is the shape of the steady-state distribution for the biased walk?

   iii) How would you modify Fick's First Law to account for not only diffusion of particles but a steady drift of particles of velocity v? What steady-state distribution of particles is predicted from Fick's Laws and the Continuity Equation in the presence of this steady drift of particles? Is this consistent with the simulation results you obtained?

c) Keep the parameters of Simulation #1 and #2 the same as in b), but change the right step probability of Simulation #2 to 0.48. Explain the differences in the shapes of the steady-state distributions for the two simulations.

Problem 2.3 This problem deals with the effect of a finite particle lifetime on the statistics of random walks.

a) Define a simulation with an initial particle distribution that is a uniform distribution of particles in space, but with a finite average particle lifetime. Run the simulation until all the particles have expired. Examine a graph of # particles versus step number. Explain the shape of this function.

b) Define another simulation that is identical with the one in a), but this time with a source of particles. Do you expect a steady state to be reached between the the source and expirations? Determine a criterion for steady state and check out your intuition.

c) Design a combination of source rate and lifetime such that the distribution reaches a steady state. This might correspond, for example, to a drug concentration reaching steady state in the body, as it is both infused and eliminated.

d) Design a combination of source rate and lifetime such that most particles in the region have expired by the time the source injects the next batch. This might correspond to the drug concentration when the dosing interval is longer than the elimination half-life of the drug.

Problem 2.4 This problem deals with a random walk in three regions. Set up the parameters as shown in Figure 2.12. For both simulations, the two end regions contain uniform concentrations of particles; but the number of particles differ. There is a concentration difference between the end regions. The center region can be regarded as a membrane that separates the two end regions. The random walk in the membrane region is unbiased in one simulation and biased in the other. Run the simulation for several hundred steps.

a) Explain the differences between the distributions of particles for the two simulations.

b) Quantitatively describe the flux of particles between the two end compartments — both the magnitude and sign of the flux.

c) What physical process might this simulation represent?

Problem 2.5 Design a three region diffusion regime where the center region is considered to be a membrane. Design membrane characteristics such that the membrane is transparent for particles moving from left to right but purely reflecting for particles moving from right to left. Test your design by running the simulation.

Problem 2.6 Start with two identical simulations with Regions #1 and #2 that have: a region size of 400; a step size of 2; unbiased random walks; no sources or sinks; infinite particle lifetimes; and sinusoidal initial particle distributions. Choose one simulation with a period of 200 and the other with a period of 50. Choose an appropriate bin size for the histograms. Run the simulation.

a) What is the shape of the equilibrium distribution of particles?

b) Which particle distribution approaches this equilibrium faster?

c) Experiment with different frequencies and generalize your conclusion from b).

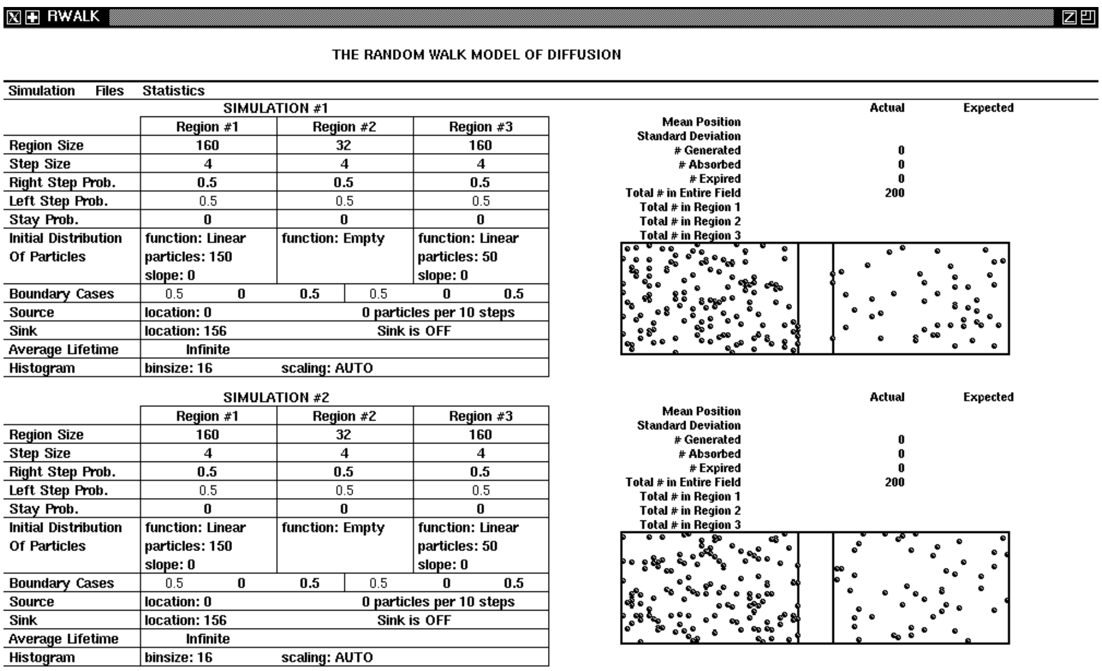

Figure 2.12: Random walk in 3 regions.

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