Simulations: Diffusion, mixing and stirring.

1. **1-Dimensional random walk –analogue simulation.**

Have the student stand in a row on a tiled floor (position 0). Each student has a coin. A step consists of throwing the coin and moving right (head) or left (tail) on tile.

1) Line up (t=0)  2) Start flipping          3) Diffusion at work.

One student monitors the position of the student as function of time (the tiles should be numbered -6, -5,…-1,0,1,…5,6) and input it into a computer like so:

<table>
<thead>
<tr>
<th>Position at t=0</th>
<th>Participant 1</th>
<th>Participant 2</th>
<th>Participant 3</th>
<th>Participant 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position at t=1</td>
<td>0</td>
<td>-1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Position at t=2</td>
<td>0</td>
<td>-2</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>Position at t=15</td>
<td>6</td>
<td>-2</td>
<td>-5</td>
<td>0</td>
</tr>
</tbody>
</table>

Stop the simulation after 16 steps.
Restart until you obtain 20 independent realizations.

Get back to class with the spreadsheet projected on the screen. Add two columns on the right hand side of the table for the mean and standard deviation.

1. How does the mean position of the participants change as a function of time? How does one calculate that with the given data? Put the results in the first column to the right of the data.

2. What mathematical construct can be used to describe the dispersion of particles away from their mean position? How is the standard deviation changing as function of time? Put the results in the 2nd column to the right of the data. Plot it...
as a function of the number of steps. Is there a relationship between the standard deviation and the number of steps (time step)?

2. **1-Dimensional biased random walk –analogue simulation.**

Have the student stand in a row on a tiled floor (position 0). Each student has a coin. A step consists of throwing the coin and moving one tile right (head) or two tiles left (tail). One student monitors the position of the student as function of time (the tiles should be numbered -10, -5, -1, 0, 1, 5, 10) and input it into a computer like so:

<table>
<thead>
<tr>
<th>Position at t=0</th>
<th>Participant 1</th>
<th>Participant 2</th>
<th>Participant 3</th>
<th>Participant 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position at t=1</td>
<td>0</td>
<td>-2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Position at t=2</td>
<td>-1</td>
<td>-4</td>
<td>2</td>
<td>-1</td>
</tr>
</tbody>
</table>

Stop the simulation after 16 steps.
Restart until you obtain 20 independent realizations.

3. Get back to class with the spreadsheet projected on the screen and add the columns for mean position and standard deviation as function of time step.

4. How are these exercises related to diffusion?

3. **2-Dimensional random walk –computer aided simulation.**

Compare and contrast:

http://www.jhu.edu/~virtlab/diffus/diff_txt.htm
http://nerve.bsd.uchicago.edu/diffusion.html
http://opencourse.org/Collaboratories/harveyproject/DiffusionSimulation
http://www.scienceisart.com/A_Diffus/Jav2_2.html

4. **Environmental relevance: Oil spill simulation tool GNOME.**

Links references and resources:

Papers:

Books:

Selected web sites:
http://www.seas.harvard.edu/brenner/taylor/
http://www.seas.harvard.edu/brenner/taylor/handouts/diffu.htm
http://www.scienceisart.com/A_Diffus/DiffusMain_1.html#anchor1414680

 GNOME

http://response.restoration.noaa.gov/software/gnome/gnome.html
Download using the links on that page.

Get data from the Gulf of Maine at:
http://rocky.umeoce.maine.edu/GoMPOM/cdfs/gnome/web/

On our page, you select the first and last date of the range that you want and then hit the submit button. This will bring you a page with links to two files that you need to download, as well as a set of instructions on how to bring it into GNOME.
Appendix 1: A little bit of physics:

**Fick’s and Fourier’s laws** – gradient flux of material (Fick) and heat (Fourier). Down gradient means from where it is high to where it is low). Friction – cause gradient flux of momentum (from high to low).

Flux = -diffusion coefficient (D) x gradient {e.g. concentration (C) gradient [moles/s/m²]}

In 1-dimension: F=-Dd[C]/dx, where D is the diffusion coefficient.

What are the units of the diffusion coefficient? Same units (not value) for heat, momentum, and scalars (e.g. nitrogen).

Diffusivity of a given material depends on: Temperature, size of molecules, and viscosity of media.

Einstein: Diffusion is the macro scale realization of random motions (called Brownian motion) in the molecular scale.

The diffusion coefficient D=constant x Temperature/{radius of molecules x medium’s viscosity}

To make the connection between our simulation and diffusion we have to define a time interval over which a step of magnitude L is taken (in our case L is one tile). Let that be T. It turns out that we can recast the exercise we did above as a diffusion problem with a diffusion coefficient for the simulation above is simply D=L²/(2T).

A biased random walk, our second exercise, emphasizes how organisms may drift toward favorable condition even if they cannot control their motion. Some motile bacteria, for example, move using flagella. Due to their propulsion mechanism every given amount of time they have to unwind their flagella, tumble which causes a change in direction. It has been observed that they tumble more often when swimming to unfavorable conditions resulting in a net drift towards the attractor.

Appendix 2: A related oceanographic problem:

Oceanographer are interested in understanding how fast is the oceans are being mixed. This problem has profound implications with respect to the fate of material which sinks to the oceans depth but is needed for phytoplankton growth at the surface, the formation of dead zones, where oxygen is depleted due to respiration and degradation of organic material and where fish and cannot live.

How can one quantify the diffusion of material in the environment?

Answer: spill a chemical and observe how it disperses in the environment.
The following figures are from: Ledwell et al., 1993 and 1998, who injected SF₆ at 300m depth and observed (over 30 months!) how the dye dispersed as function of time.

They were able to show that the diffusion in the ocean is rather small, 0.11-0.17cm²/s, still much higher than molecular diffusion, which is 0.00001cm²/s. Why?

Note, however, that near small cells such as bacteria and phytoplankton a diffusion boundary layer exists and the transfer of molecule across it occurs due to molecular diffusion.

The values the obtain, however, are very low suggesting mid-ocean mixing processes are not effective in fluxing material and heat suggesting much of the mixing of ocean properties occur at boundaries and areas with steep topography.

Note how Gaussian the profile they observe is. What does it tells us about the environment?

![Figure 1: Evolution of the lateral distribution of the tracer](image_url)

**FIG. 1** Evolution of the lateral distribution of the tracer. The injection streaks are shown as short heavy lines near 26° N, 28° W. The contours just to the west show the patch later in May 1992. Heavy lines (further to the west) show tracks for the October survey, where the concentration C at the target surface was >500 fm; light solid lines, C was between 100 and 500 fm; dashed lines, C~0. Solid triangles indicate bottle stations occupied at the end of the October cruise, with C> 300 fm. Station symbols for the November survey are: plus signs, C<30 fm; open circles, C=30-300 fm; filled circles, C>300 fm. A fine curve has been drawn to envelop the high C regions for the two surveys. OM marks the location of the central mooring for the Subduction experiment.
**Figure 22.** Mean tracer profile for spring 1993 (solid curve), and the best fit Gaussian (dashed curve).

**Figure 25.** Mean tracer profile for November 1994 (solid curve), and best fit Gaussian (dashed curve). An ad hoc background correction of less than 0.1 m has been applied to bring the upper tail close to zero (see text).

**Figure 17.** Mean vertical profile for November 1992 (solid curve) and the best fit Gaussian (dashed curve).

**FIG. 2.** Evolution of the vertical distribution of the tracer. The mean profiles have been scaled so that the widths can be compared.
Figure 23. Tracer found in November 1994 viewed from the northeast. The height of the “fence” indicates the column integral, in nmol/m², with “posts” at the stations.