Project 1: diffusion and the harmonic oscillator

KEM 342 project assignments

The teams!

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1 Get the Mersenne Twister up and running

1. Write or otherwise aquire a Mersenne twister script in the language you chose to use, get it spitting out sequence of integers
2. Write code around it so you have 5 functions that produce:
   a) Sequence of pseudorandom integers
   b) Sequence of only positive integers (**HINT**: binary operation set register 1 to 0)
   c) Seqence of pseudorandom real numbers [0,1)
   d) Sequence of pseudorandom real numbers (-1,1)
   e) 50% probability -1, 50% probability +1 (**HINT**: inverse of b))
3. Use histograms to show these work:
   - Divide up between [0,1) and (-1,1) into bins of width 0.01 or something like that and increment the bins each time a random number falls in it, do for long time , each bin should have same number in, maybe normalize for neatness to get P(bin)
   - Do same for the random number generator e) showing equal chance of 1 and -1

2: 1D diffusion

- Starting with particle at $x = 0$, let it hop -1/+1 with 50/50% probability
- Average together multiple runs or consider many particles and show that you get a result that matches the analytical solution:

$$P(x|D,t) = \frac{1}{\sqrt{2\pi\sigma_t^2}} e^{-\frac{x^2}{2\sigma_t^2}} \qquad \sigma_t^2 = 2Dt \qquad D = \frac{l^2}{2\tau} \rightarrow \langle r^2 \rangle = \frac{l^2 t}{\tau}$$

- Hint: histogram mechanism you made in part 1…
- Hint: make hop between boxes distance $l = 1$ and each hop takes time $\tau = 1$
- Hint: I have done this it really works, if you use enough statistics it should fall right on the probability distrubution and I never ran my laptop for more than 5 mins…
- Hint: in your final calculation I want you to use the mersenne twister PRND BUT one person can be working on the Mersenne twister while another codes and debugs this using the coding languages canned PRND

3: 2D diffusion

- Perform 2D diffusion, using the algorithm described in my notes
- Show this relationship, the 2D case, holds:

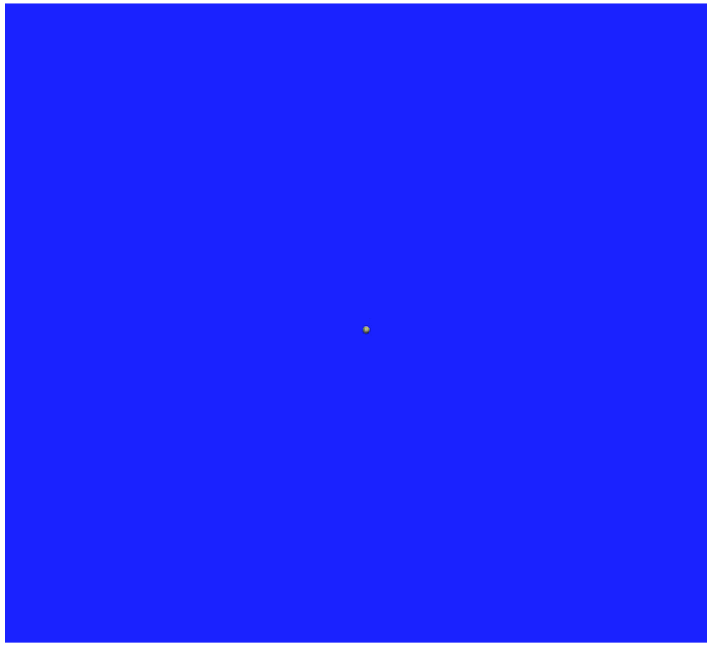
$$P(\vec{r}|\mu,\sigma^2,t) = \frac{1}{2\pi\sigma_t^2}e^{-\frac{\vec{r}^2}{2\sigma_t^2}} \qquad \sigma_t^2 = 2Dt \qquad D = \frac{l^2}{2\tau} \rightarrow \langle r^2 \rangle = \frac{l^2 t}{\tau}$$

- Hint: this result for the probability distribution is in cartesian coordinates, when you make histogram of distances travelled you have made a coordinate transformation without realizing it, figure out how to deal with this (some math here…, you can also google random walks and diffusion for some further hints here)
- **Bonus:** in the algorithm that selects the new position of the particle $\sin\theta$ and $\cos\theta$ are used, try replacing these with first few terms of their respective Taylor series expansions, does it work? How many terms do you need?

4: Visualizing 2D diffusion

- Right a code that outputs the position of many (here for example 10,000) particles diffusion from single point
- Visualize their motion using VMD
- HINT: create dummy z coordinate = 0 of all particles and write script that outputs in VMD readable format (bit of bookkeeping and looking up formats needed)
- Basically I want to see this:
- Hint: when you visualize a trajectory

You do not have to show every frame



5: 3 and 4 dimensional cases

- Simulate diffusion in 3 and 4 dimensions show the general relation

$$P(\vec{r}|D,t) = \frac{1}{(2\pi\sigma_t^2)^{d/2}} e^{-\frac{r^2}{2\sigma_t^2}} \qquad \sigma_t^2 = 2Dt \qquad D = \frac{l^2}{2d\tau} \rightarrow \langle r^2 \rangle = \frac{l^2 t}{\tau}$$

- Hint: just as in part 3 you use fact that $2\pi r$ is circumference of circle, $4\pi r^2$ is the surface area of a sphere and $2\pi^2 r^3$ is the hypersurface volume of a glome, you need this for coordinate transformation like you did in part 3 (you can google what a glome is ☺)
- Hint: on the web you can find info on how to make a random point on a sphere in 3D or the surface of a hypersphere in higher volumes.
- **BONUS points**: can you do this in even higher dimensions than 4?
- I have done 3D and 4D it works perfectly… I have not done higher D so you are on your own there ☺

6: Harmonic oscillator

1. Write a program that numerically solves a one dimensional harmonic oscillator and compare the result to the analytical solution. This is two particles governed by the potential $U = (x_1 - x_2 - 1)$. Allow initial velocity and position of the two particles to be input parameters set particle masses = 1
2. Try different time steps, see how small the timestep needs to be for the results to match the analytical result. Play around with the input parameters, see what happens.
3. Once you have gotten this to work, find the largest timestep where the analytical result is matched for a reasonable range of input parameters (obviously starting particles very far from the equilibrium or moving very fast will be unstable),
4. Put this in 2 dimensions and visualize it with VMD looking from above, start with each particle having a random velocity in random direction in xy plane $U = (|\vec{r}_1 - \vec{r}_2| - 1)$
5. Show that both angular and linear momentum are conserved and that the total energy is conserved while energy moves back and forth between potential and kinetic energy

- HINT: calculate linear momentum and remove that, then the two balls will be spinning around their center of mass, a coordinate transformation at this point may be helpful, nudge nudge wink wink… write subroutines to calculate total kinetic and potential energy, these will come in handy later…

Due date

- Beginning of class, 21st of February
- This is a hard deadline, there will be four projects each with three weeks time to do them
- Hand it in like a research paper: main text that references supplementary material
- Code and VMD visualizations are to be handed in with the main text as supplementary material, data files are also permitted but not recommended
- Data is to be shown predominantly as plots in the main text.
- While the structure will not be like paper, it is questions you are answering, I expect publication quality format and look, proper text with figures embedded professionally, looking like journal publication