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PHYS 129L

Milestone Report 3

Methodology

Diffusion Coefficient Calibration The diffusion coefficient of a fluorescently labeled particle is extracted by simulating the 1D diffusion and then matching the slope around the center of then intensity curve to the slope of the real data. Using this, one can obtain a correspondence between real time and simulated time and get a real diffusion coefficient from the data.

Progress Summary

This week, I developed a method to fit my data to a diffusion coefficient by matching slopes and using a linear fit.

Challenges and Solutions

I was able to fix the bug I was having last week by changing my choices of D and dt. It turns out if D * dt is <= ½ in my simulation then things break. [1] I found this reference to be interesting since it went deeper than the previous reference that I used into the different boundary conditions and types of simulations that one can use for PDEs. This also gave me a lot of insight into the math behind simulations like this.

Since simulating the PDE using a finite differences method doesn't give you a function to fit, I had to get creative in how I was going to extract a diffusion coefficient and uncertainty. I ended up settling on the current method that I did since it gave me nice linear data to fit.

Future Work

The last few things I want to do before my presentation / archive post is (1) to simulate 2-D diffusion and use a diffusion-reaction model to try to get insight on the DNA nanostar condensation (will probably be wrong), (2) to try to find correspondence to theory or maybe a simple back-of-the-envelope calculation to see how feasible my diffusion coefficient is, and (3) add animation to my plots.

References

[1] Diffusion equations¶ [Internet]. Diffusion equations. [cited 2023 Dec 1]. Available from: https://hplgit.github.io/fdm-book/doc/pub/book/sphinx/._book011.html