Visualizing Pinch Flow Fractionation Using Python and LAMMPS Simulation

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Introduction

- **What is PFF:** Pinch Flow Fractionation (PFF) is a microfluidic technique that separates particles by size using fluid streamlines in narrow channels, eliminating the need for physical membranes.
- **Why It Matters:** PFF offers improved precision, reduced clogging, and better scalability, with applications in biomedicine, diagnostics, and nanotechnology.
- **Project Goal:** Simulate PFF using the LAMMPS molecular dynamics engine to model particle behavior in a controlled flow environment.
- **Research Question:** Do particles of different sizes migrate to distinct regions within the pinch channel?
- **Hypothesis:** Smaller particles will stay closer to the base wall, while larger particles will move toward the center of the channel due to their stronger interactions with the walls.

Objectives

- **Demonstrate PFF Effectiveness:** Show that spherical particles separate by size in a simulated microchannel environment.
- **Improve Device Design:** Analyze particle behavior to guide optimization of flow parameters and channel geometry.

Methods and Controls

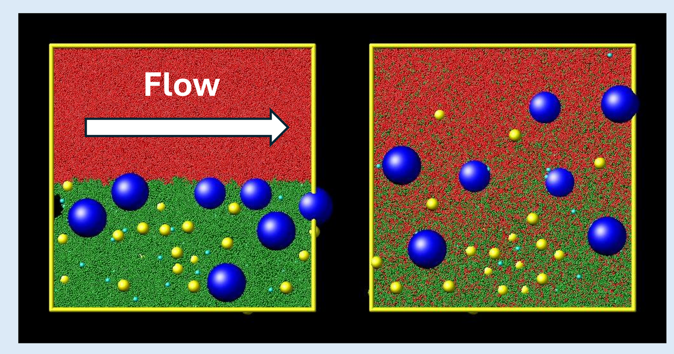
- **Simulation Engine:** Coarse-grained simulations using LAMMPS were performed to simulate a fluid channel containing spherical particles of different sizes, along with solvent and buffer fluids.
- **Simulation Setup:** Periodic boundary conditions replicated continuous flow; parameters like velocity and particle concentration were varied.
- **Parameter Control:** A Tkinter interface was developed to adjust particle size, velocities and densities.

Tools

Tkinter
Pandas
plotly | Dash

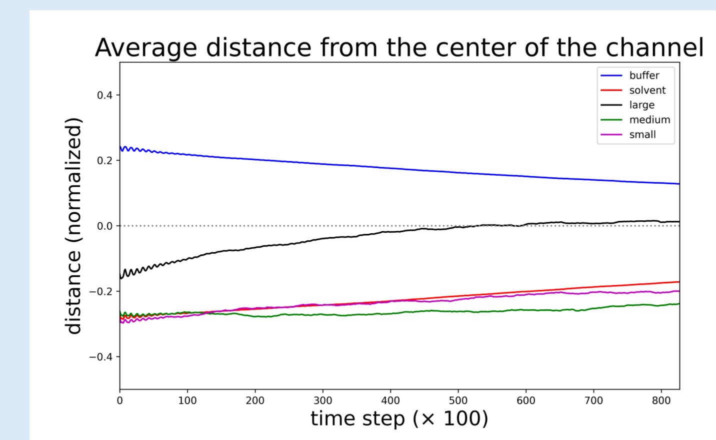
Results

Simulation

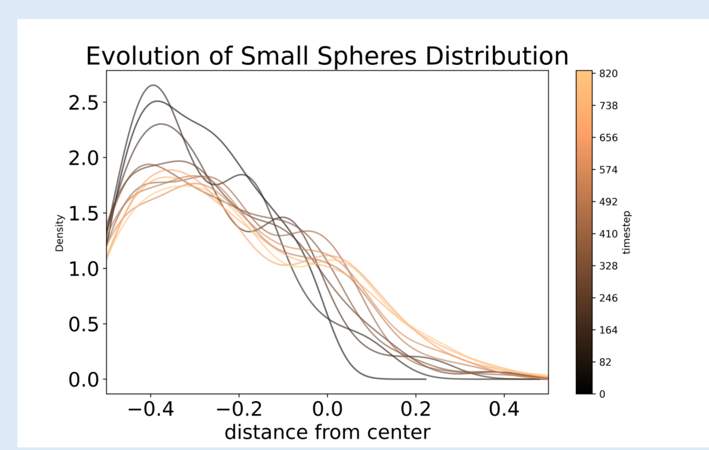


START END

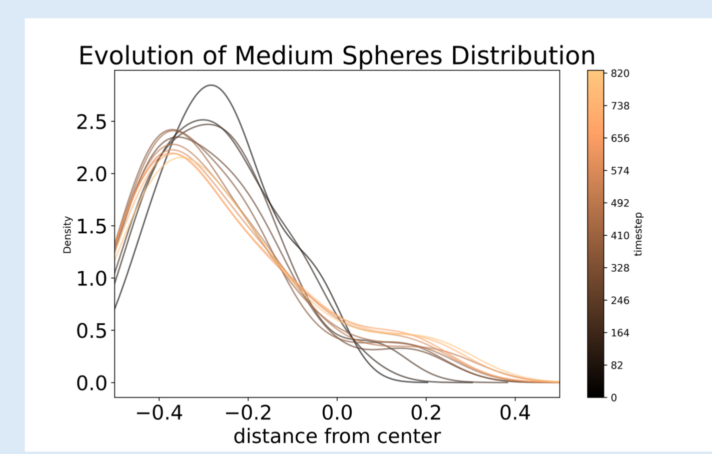
At the start, the channel is separated into two regions: buffer fluid at the top and solvent with particles at the bottom. As flow progresses, the particles begin to migrate in different directions based on their size, demonstrating separation over time.



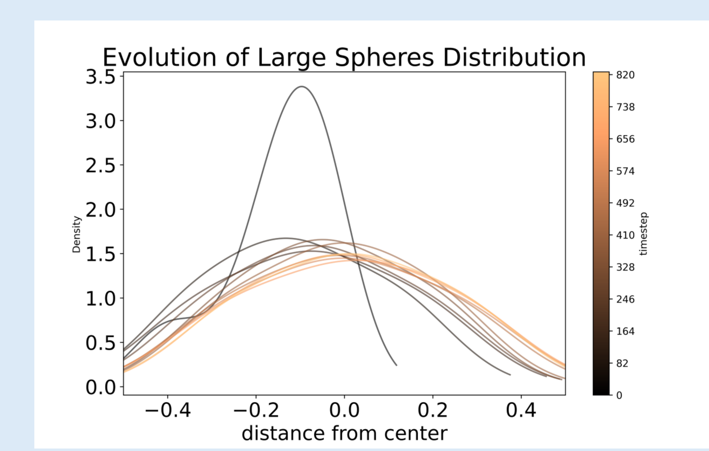
This graph shows how far particles migrate from the lower wall over time. Small and medium particles drift less, while large drift in average towards the center. **Average positions:** Large: 0.0125 above center, Medium: -0.2380 below center, Small: -0.2006 below center.



Small spheres show a low spread of their distribution away from the wall. **21.92%** ended above the centerline, confirming downward shift.

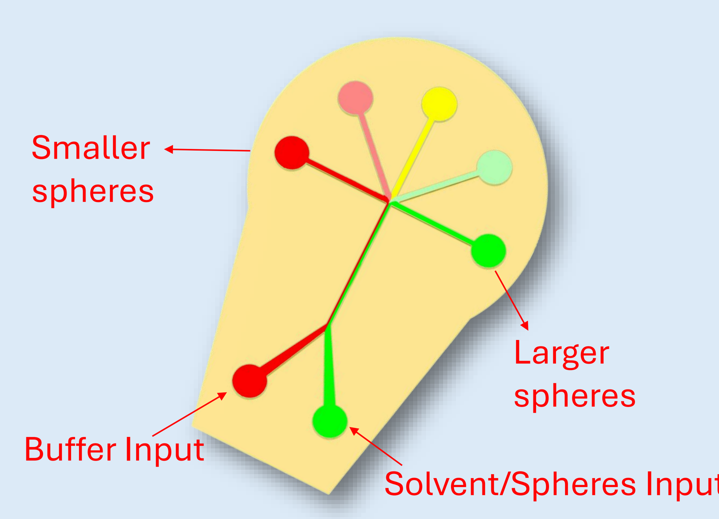


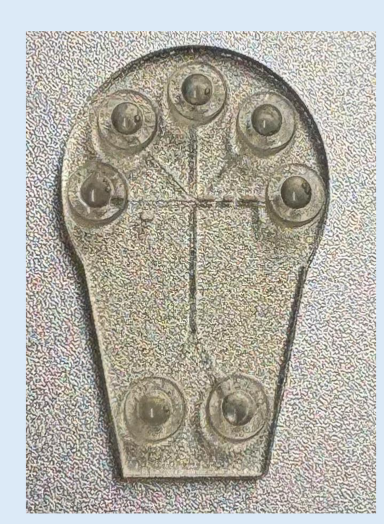
Medium spheres show a pattern similar to the smaller spheres. **16.07%** ended above the centerline.



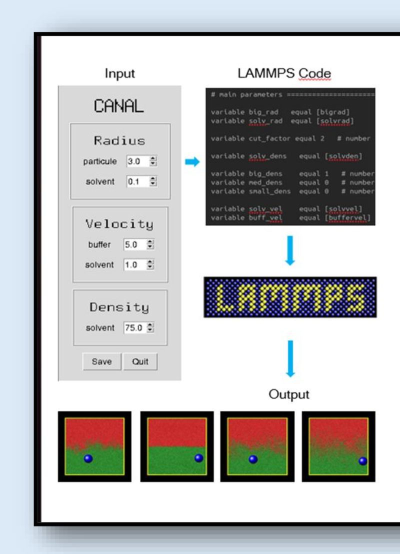
The average position of the larger spheres does not change much but their distribution spreads significantly. A much larger percentage of the larger particles, **57.14%**, ended up above the centerline.

Device





Interface



Conclusions

After running the simulations, we successfully visualized the dispersion of particles, providing clear evidence of pinch flow fractionation.

The results show distinct size-based migration patterns, supporting the separation behavior between larger spheres from the rest.

However, further validation is needed to confirm the consistency and reliability of these trends. To achieve more precise modeling of particle behavior, we are actively exploring additional simulation techniques and optimization methods.

Future Research

- **Automanted Optimization:** Implementing methods like Bayesian Optimization to better select flow parameters that enhance particle separation.
- **Interactive App Development:** Designing a tool that visualizes particle movement within the channel at each timestep. The current version is built using Plotly and Dash.
- **Finite Element Method (FEM):** Integrating FEM simulations to model velocity and pressure, improving fluid flow accuracy at the continuum level.

References

Takagi, Junya, et al. "Continuous particle separation in a microchannel having asymmetrically arranged multiple branches." Lab on a Chip, 5.7 (2005): 778-784.

Bayareh, Morteza. "An updated review on particle separation in passive microfluidic devices." Chemical Engineering and Processing-Process Intensification, 153 (2020): 107984.

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