REPORT

A Project Report Submitted

By

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PROJECT REPORT CERTIFICATE

This is to certify that the Research Project titled Simulation of Stokesian Dynamics , submitted by Muskan Yadav, to the Indian Institute of Technology, Ropar, I hereby declare that the work presented in this report entitled “Internship Report” in partial fulfilment of the requirements for the award of the degree of Bachelor of Technology in Chemical Engineering submitted in the department of Chemical Engineering.

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INTRODUCTION

1.1 Understanding Creeping Flow On a Sphere

Definition: The term "creeping force" is often used in the context of low Reynolds number fluid dynamics, where inertial forces are negligible compared to viscous forces. This is commonly referred to as Stokes flow or creeping flow. One of the classic problems in this regime is the flow around a sphere. The force exerted on the sphere by the fluid is called the Stokes drag or creeping force.

1.2 Derivation of Stokes Drag Force

For a sphere of radius a moving with a constant velocity U in a fluid with viscosity η, the creeping force F can be derived using Stokes' law. Here's the detailed derivation:

1. **Governing Equations**: The flow around the sphere is described by the Navier-Stokes equations. For creeping flow, the equations reduce to the Stokes equations:
    - Continuity equation: $\nabla \cdot u = 0$ (incompressible flow).
    - Momentum equation: $\rho(\partial u/\partial t + (u \cdot \nabla)\, u) = -\nabla p + \eta\, \nabla^2 u + f$

Where u is the fluid velocity, ρ is the fluid density, p is the pressure, μ is the dynamic viscosity, and f represents body forces

2. **Boundary Conditions**:
    - At the surface of the sphere (radius $r=a$): $u=U$
    - Far away from the sphere (as $r \to \infty$): $u \to 0$
    -
3. **Solution for Velocity Field**: The solution for the velocity field u in spherical coordinates can be expressed as:

    $$u(r,\theta)=(U(1-3a/4r+a^3/4r^3)\cos\theta, -U(1-3a/4r-a^3/8r^3)\sin\theta\ )$$

    where r is the radial distance from the center of the sphere, and θ is the polar angle.

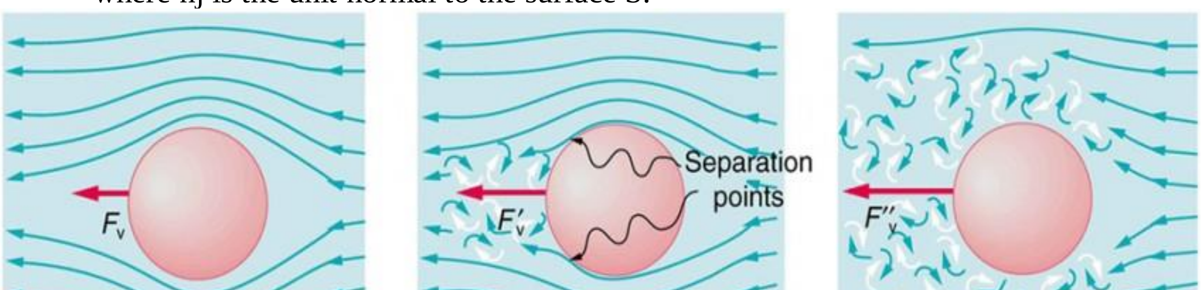
4. **Stress Tensor**: The stress tensor σ in the fluid is given by:

    $$\Sigma ij = -p\delta ij + \eta\ (\partial ui/\partial xj + \partial uj/\partial xi)$$

5. **Force on the Sphere**: The force F on the sphere is obtained by integrating the stress tensor over the surface of the sphere:

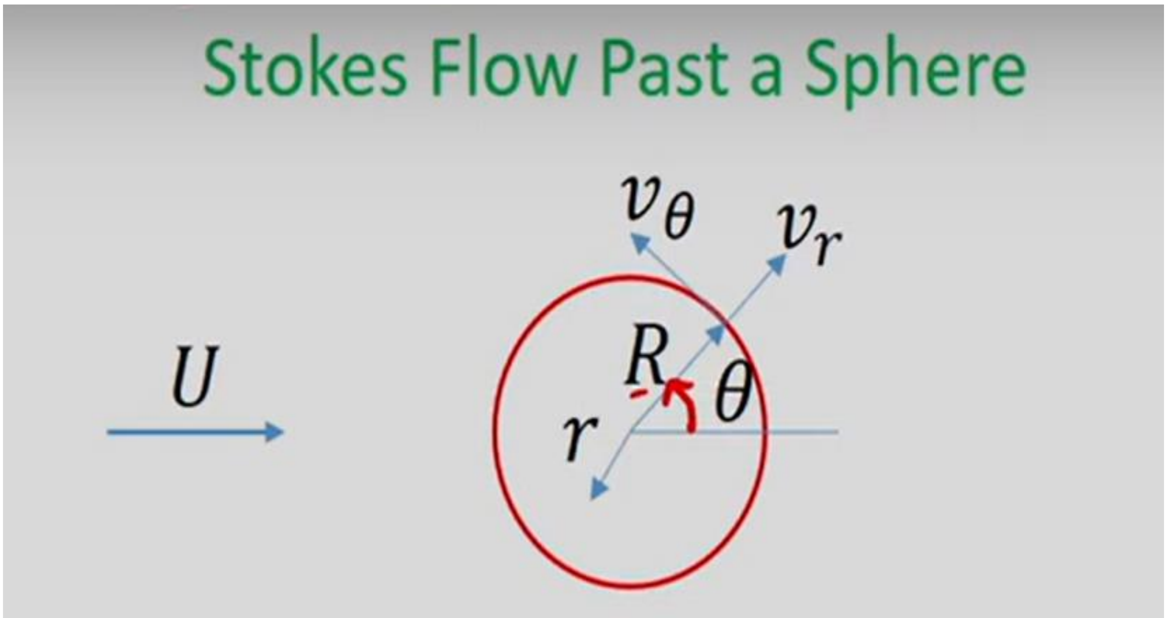
    $$F=\int \sigma_{ij} * n_j\, ds$$

    where nj is the unit normal to the surface S.



1.3 Derivation of Drag Force on a Sphere

- **Derivation Process:**
  - **Step 1:** Consider a sphere of radius r moving with velocity v a fluid with dynamic viscosity η.
  - **Step 2:** Apply the Navier-Stokes equations in the context of a low Reynolds number.
  - **Step 3:** Solve the simplified linear equations for the flow around the sphere.
  - **Step 4:** Integrate the shear stress over the surface of the sphere to obtain the drag force.
- **Resulting Formula:** $F_d=6\pi\eta rU$



1.4 Other Shapes Used for Measuring Creeping Forces

Shapes Used:

1. Spheres:

- Simplest and most common shape for deriving creeping forces.
- Provides isotropic properties for uniform interaction with the fluid.

2. Cylinders:

- Useful for studying flow past elongated objects.
- Drag force calculation: $F_d=2\pi\eta Lv$ (for an infinite cylinder)
- Where L is the length of the cylinder.

3. Ellipsoids:

- Used for understanding drag on elongated or flattened particles.

- Drag force depends on the axes' ratios.

4.Plates:

- Thin flat plates help study flow perpendicular to the surface.
- Drag force varies significantly with orientation.

Why These Shapes

- **Comparative Analysis:** Provides insights into how different geometries affect drag forces.

Application Specific: Different shapes are used to mimic real-world objects, such as microorganisms, debris, or engineered particles.

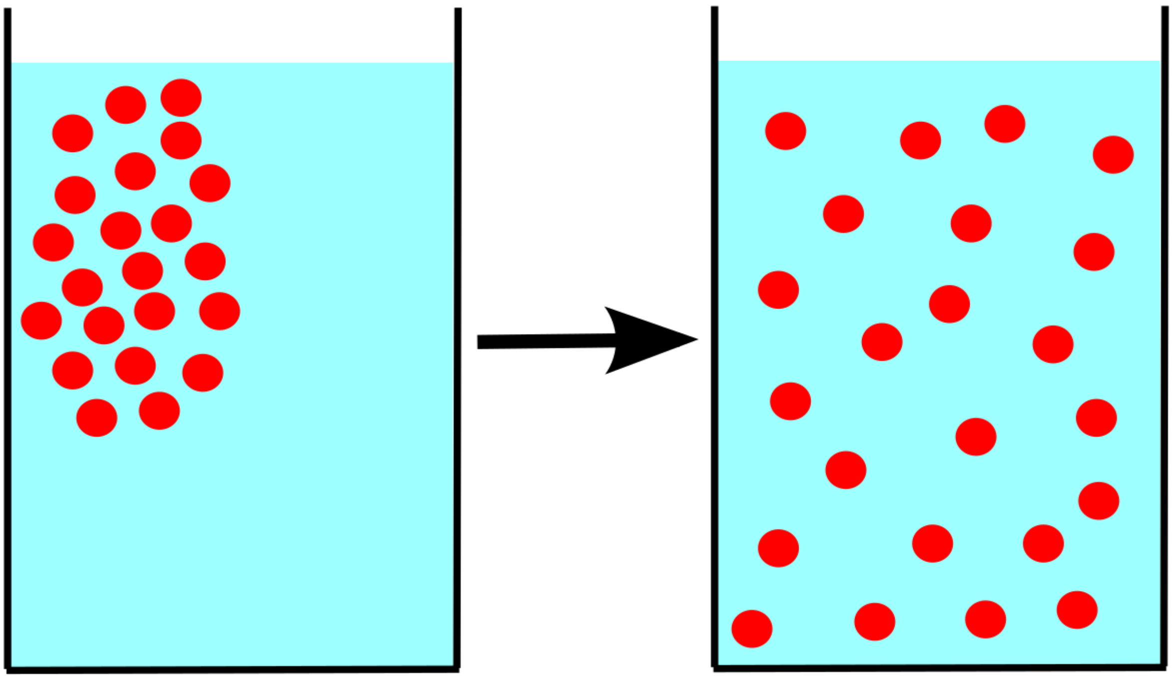
METHOD AND MATERIAL

2.1 The Benefits of Concise Study Methods

- The aim of this study is the prediction of suspension macroscopic properties from the microstructure - the temporal and spatial distribution of suspended particles.
- The macroscopic properties includes the shear viscosity, normal stress differences, short and long- time self-diffusivities. Suspension macroscopic properties and the microstructure are modeled as functions of two parameters: particle volume fraction and the Péclet number, which measures the relative importance of the imposed shear and Brownian forces.

2.2 Embrace Concise Study Techniques

- The method, which is very general and computationally efficient, imposes no restriction on the particle displacements and allows simulation of flowing suspension with particle volume fractions from infinite dilution to dense packing and a continuous range of the Péclet number from pure Brownian motion ($Pe \to 0$) to pure hydrodynamics ($Pe \to \infty$).



2.3 What is Stokesian Dynamics?

- **Definition:** Stokesian Dynamics is a computational approach used to simulate the behavior of particles in a fluid, particularly at low Reynolds numbers where viscous forces dominate. Stokesian Dynamics is a microhydrodynamic, low Reynolds number approach to modelling the movement of suspensions of particles in fluids which considers the interaction of particles with each other against a Newtonian background solvent. The fluid is modelled using the stokes equation . It is typically chosen for its suitability for three-dimensional simulation with low calculation and time penalty.
- **Key Features:**
    - Applicable in micro-scale fluid dynamics.
    - Accounts for hydrodynamic interactions and Brownian motion.

Applications: Colloidal suspensions, sedimentation, microfluidics

2.4 Equations Used for Simulating Stokesian Dynamics

The dynamic simulation starts with the N-body Langevin equation for the particle motion:

$$\mathbf{m * d/dt (U) = F^H + F^B + F^P}$$

Equation simply states the mass x acceleration equals the sum of the forces. Here, m is the generalized mass/moment of inertia matrix of dimension (6N * 6N) where N is the number of particles, U is the particle translational/rotational velocity vector of dimension (6N) and the force/torque vectors of dimension (6N) on the right hand side of describe three different types of forces. F^H is the hydrodynamic forces exerted on particles due to their motion relative to fluid. The stochastic force F^B gives rise to Brownian motion, the force which tends to restore the equilibrium structure from any deformation. F^P is the deterministic non-hydrodynamic forces, which may be of many forms.

The Langevin equation can be viewed as a coarse grain model of suspensions, a model which treats the suspending fluid as a continuum and gives rise to the hydrodynamic drag forces, F^H
, and the random thermal forces, F^B. For N rigid particles suspended in an incompressible Newtonian fluid of viscosity n and density p, the motion of the fluid is governed by the Navier-Stokes equations. When the motion on particle scale is such that the particle Reynolds number, Re, is small (Re = $p*a^2$ y/n «1, with the characteristic particle size and y the shear rate), the inertial terms can be neglected and we solve the simpler inertialess Stokes equation. For suspensions of spheres with a ~ lμm, in water, under a shear rate of y ~ $1*sec^{-1}$, we have Re ~ $0(10^{-5})$ while the Péclet number, Pe ~ $0(10^2)$. Here Pe= $y*a^2/Do = 6\pi*\eta*a^3/kT$ is the ratio of the shear and Brownian forces.

Neglecting inertia, equation becomes:

$$0 = F^H + F^B + F^P$$

Equation states that any deformation to the microstructure by the shear and/or by the interparticle/external forces is balanced by the Brownian motion which restores the structure to an isotropic random state.

- For Stokes' flow, the hydrodynamic force F^H exerted on the particles in suspension undergoing a bulk linear flow is :

$$\mathbf{F^H = -R_{FU} * (U - U^{\infty}) + R_{FE} : E^{\infty}.}$$

Here, U^{∞} is the imposed flow at infinity evaluated at the particle center x {alpha} , E^{∞} is the symmetric part of the velocity gradient tensor and is constant in space, although it may be an arbitrary function of time, for example in an oscillatory flow. The resistance tensors R_{FU} (x) of dimension (6N * 6N) and R_{FE} (x) of dimension (6N * 5N) depend only on the instantaneous particle configuration and the particle shapes and sizes. They are purely geometric quantities and independent of the flow field. R_{FU} (x) is the coupling between the hydrodynamic force/torque on the particles and their motion relative to the fluid. R_{FE} (x) is the coupling between the hydrodynamic force/torque on the particles and their motion due to an imposed shear flow. The vector x of dimension (6N) represents the generalized configuration vector specifying the location and orientation of all N particles. The inverse of the resistance tensor R_{FU} is known as the mobility matrix M ($=R_{FU}^{-1}$) and is the central element describing the hydrodynamic interactions among N particles. Stokesian dynamics, with its hydrodynamic origin, offers an accurate and efficient method for computing these hydrodynamic tensors.

The combination of the resistance matrices is denoted the grand resistance matrix:

$$R = \begin{bmatrix} R_{FU} & R_{FE} \\ R_{SU} & R_{SE} \end{bmatrix}$$

The invert of R, "the grand tensor" M, is expressed in the mobility formulation as:

$$\begin{pmatrix} U - U^{\infty} \\ -E^{\infty} \end{pmatrix} = -\begin{pmatrix} M_{UF} & M_{EF} \\ M_{US} & M_{ES} \end{pmatrix} . \begin{pmatrix} F \\ S \end{pmatrix}$$

For two spherical particles, R and M are known exactly for all sphere-sphere separations. For N particles, solving full N-body problem requires some approximations. The details of the methodology can be found in Brady and Bossis and Bossis and Brady. Here, we briefly summarize the procedure for obtaining M. Stokesian dynamics exploits the fact that the many-body hydrodynamic interactions are most easily computed in the mobility formulation, while the near-field lubrication interactions are more conveniently incorporated into the resistance formulation.

Stokesian Dynamics by Adam Townsend

Overview of the Simulation:

- Adam Townsend's work involves simulating the motion of particles in a fluid using Stokesian Dynamics.

- The simulation considers hydrodynamic interactions, Brownian motion, and external forces.

This software allows to place spherical particles in a fluid, apply some forces to them, and see how they move. We can also move the fluid in some way and see how the particles react to that. You can have a play with a simpler implementation of Stokesian Dynamics .

In particular, this software has the following features:

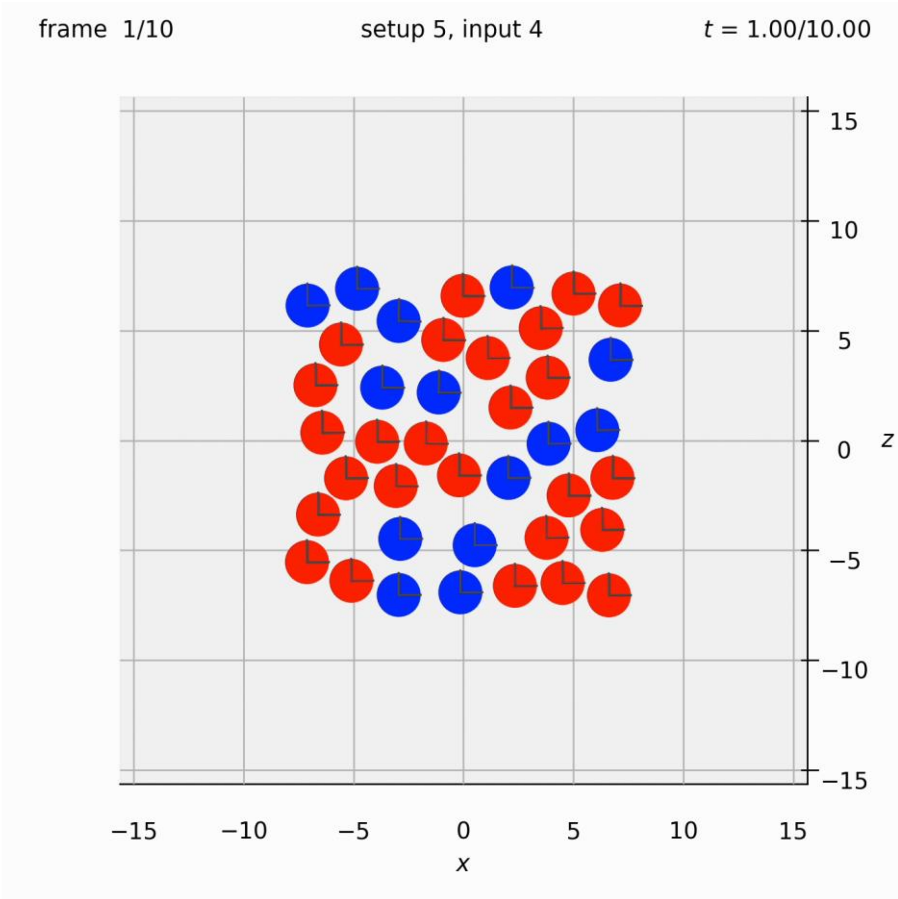
- Fully 3D simulation
- Free choice of number of particles
- Choice of simulating particles in an unbounded fluid ('non-periodic') or in a periodic domain
- Free choice of spherical particles sizes (up to *n* different sizes for low *n*)
- Choice to include bead-and-spring dumbbells, formed of pairs of (usually smaller) spherical particles, as a way to introduce viscoelasticity into the background fluid
- Free choice of particle interaction forces
- Choice of whether to include long-range hydrodynamic forces or not ($\boldsymbol{M}^{\infty}$)
- Choice of whether to include lubrication forces or not ($\boldsymbol{R}^{\text{2B,exact}}$)
- Choice of Euler, two-step Adams–Bashforth or RK4 timestepping
- Choice of how often to find $(\boldsymbol{M}^{\infty})^{-1}$, a matrix which varies slowly and takes a long time to compute, hence is typically computed every 10 timesteps.
- For each spherical, non-bead-and-spring particle in the system, the software takes the forces and torques you want to apply to it, as well as the background fluid shear rate ($\boldsymbol{F}$, $\boldsymbol{T}$ and $\boldsymbol{E}$), and gives you the particle velocities, angular velocities and stresslets ($\boldsymbol{U}$, $\boldsymbol{\Omega}$ and $\boldsymbol{S}$). It can also do $\boldsymbol{FTS}$ to $\boldsymbol{U\Omega E}$, for when you want to specify stresslets instead of the background shear rate; and $\boldsymbol{U_1F_2TE}$ to $\boldsymbol{F_1U_2\Omega S}$, for when there are some particles whose velocities you want to fix while letting some other particles move under specified forces (e.g. when you want to fix some particles as walls).
- Time-to-completion estimates
- Emails you on completion
- Output stored in convenient .npz format
- Video generation scripts to watch the particle behaviour

2.5 Key Components of the Code:

The SD method combines deterministic and stochastic components to capture the interactions and random motion of particles: –

- **Hydrodynamic Interactions**: The code calculates the forces and torques on particles due to the surrounding fluid using the Stokes equations.
- **Mobility Matrix**: This matrix links the forces and torques to the particle velocities. It accounts for near-field lubrication effects and far-field multi-body interactions.
- **Brownian Motion**: Thermal fluctuations are incorporated by adding random displacements to particles. These are drawn from a Gaussian distribution with variance dependent on temperature and the inverse mobility matrix.

- **Time Integration**: Particle positions and velocities are updated over time using numerical integration techniques .

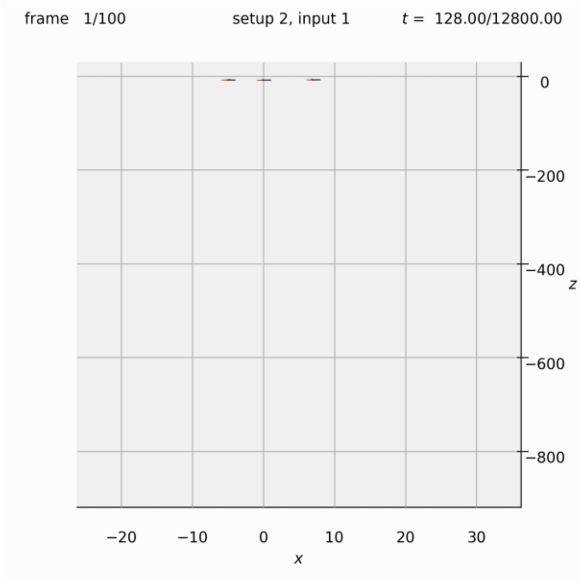


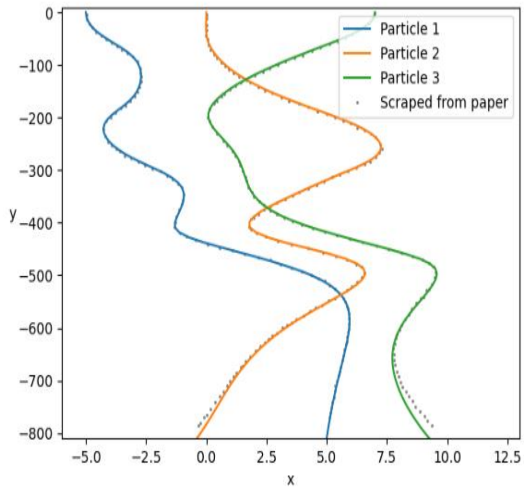
Results:

3.1 Result overview

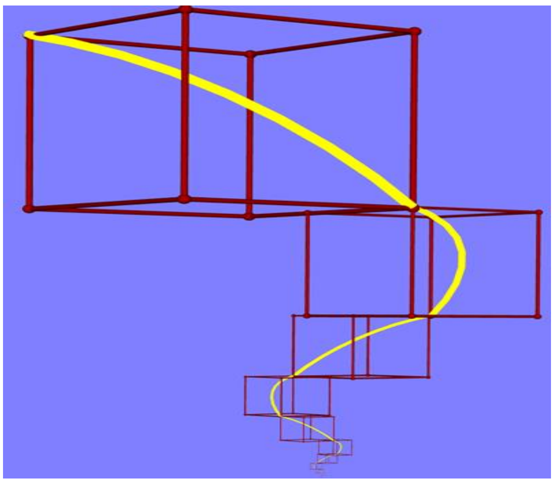
Result Obtained from Stokesian Dynamics Simulation

- This test case considers three horizontally-aligned particles sedimenting vertically, and looks at their interesting paths over a large number of timesteps

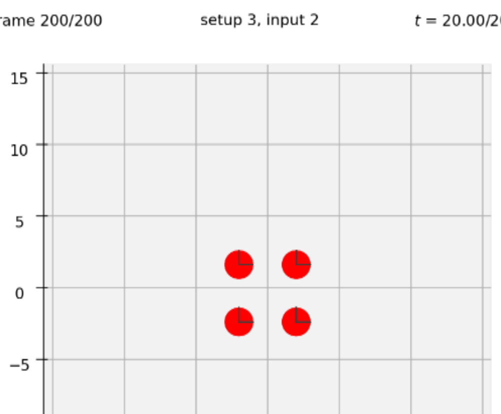


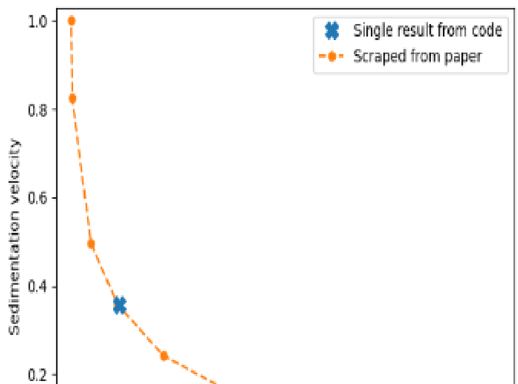


- A simple cubic array sediments vertically under a constant force. The velocity is measured for different particle concentrations. Vary the concentration by altering the cubic lattice size.



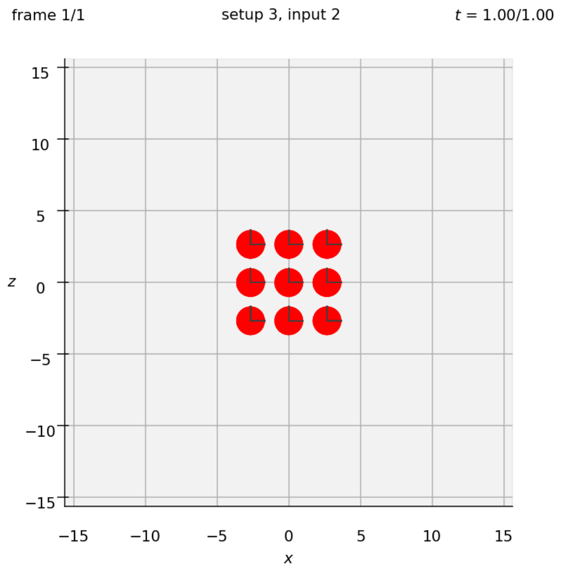
(a)

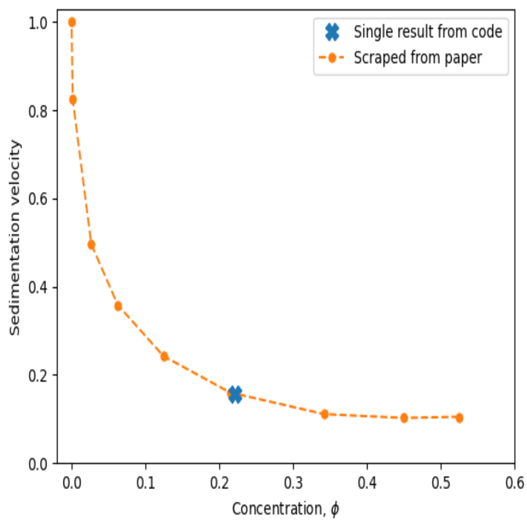




- ❑ Single result from code (blue "x"): The point is around a concentration of 0.1 and a sedimentation velocity of approximately 0.4.
- ❑ Scraped from paper (orange dots): The data shows a decreasing trend of sedimentation velocity with increasing concentration.

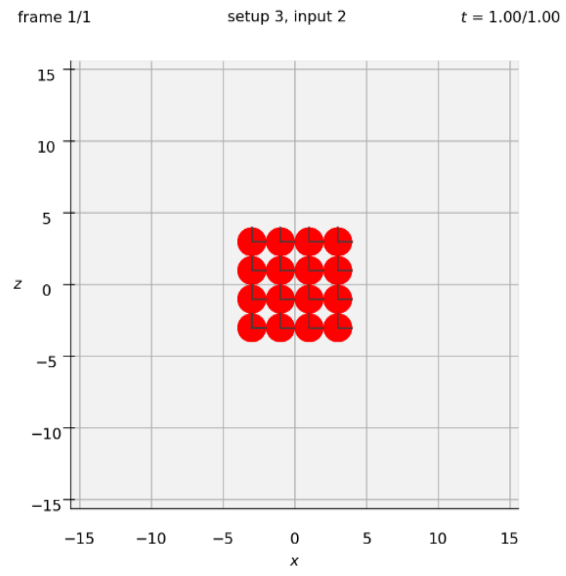
(b)

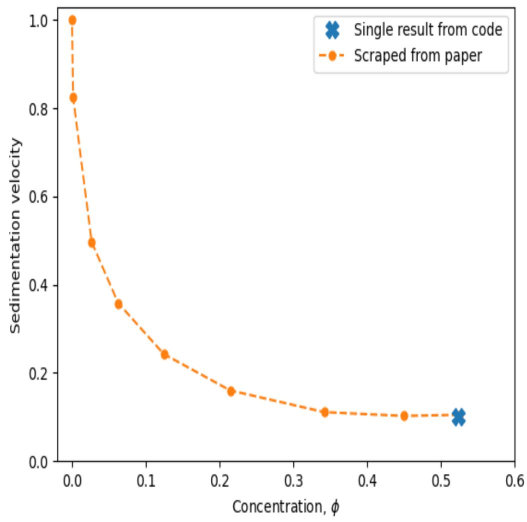




- ❑ Single result from code (blue "x"): The point is around a concentration of 0.2 and a sedimentation velocity of approximately 0.2.
- ❑ Scraped from paper (orange dots): The trend remains consistent, showing a decrease in sedimentation velocity with increasing concentration.

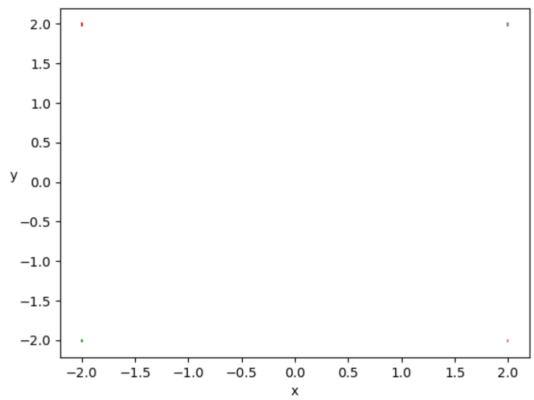
(c)





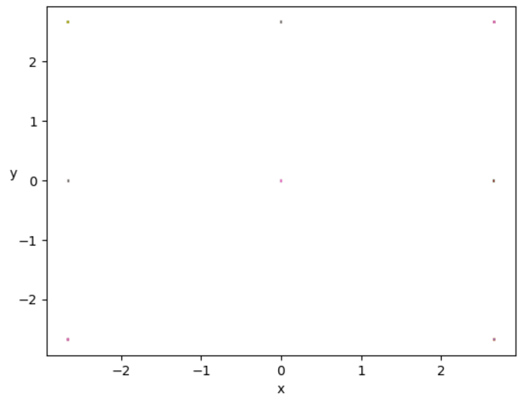
- Single result from code (blue "x"): The point is now at a concentration of around 0.5 and a sedimentation velocity of approximately 0.2.
- Scraped from paper (orange dots): The trend from the paper shows a similar decrease in sedimentation velocity, leveling off at higher concentrations.

Plot 1: Trajectory of 8 Particles



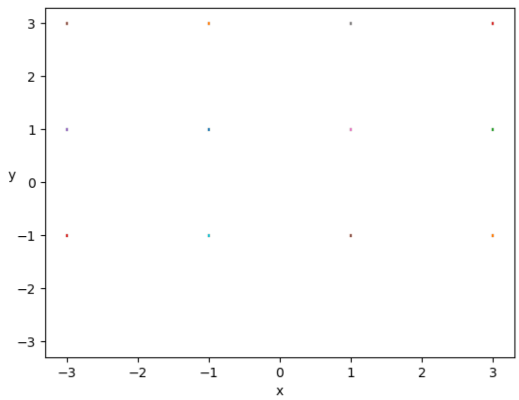
- **Description**: This plot displays the initial positions of 8 particles. Each particle is represented by a dot with different colors. The particles are scattered across the x and y axes, ranging from approximately -2 to 2.
- **Analysis**: With only 8 particles, the plot appears sparse. The positions seem to be randomly distributed, and the distinct colors make it easy to differentiate between individual particles.

Plot 2: Trajectory of 27 Particles



- **Description**: This plot shows the initial positions of 27 particles. The particles are again marked by dots of various colors, spread across the x and y axes from about -2 to 2.
- **Analysis**: With 27 particles, the plot is denser than the first one. The distribution of the particles is more even, and there are no obvious patterns or clusters. The variety of colors helps in identifying the individual particles.

Plot 3: Trajectory of 64 Particles



- **Description**: This plot illustrates the initial positions of 64 particles. The particles are represented as dots with a wider range of colors, and they are distributed across the x and y axes from about -3 to 3.
- **Analysis**: With 64 particles, the plot is significantly denser. The distribution appears more uniform, and the particles cover a larger area of the plot. The increased number of particles makes it challenging to distinguish individual ones, but the overall pattern indicates a more thorough sampling of the space.
- These plots likely represent the initial positions of particles in a simulation or experiment, and analyzing their trajectories over time could provide insights into their behavior and interactions.

4 Discussion

4.1 Discussion overview

The simulation of sedimentation dynamics using Stokesian dynamics provides valuable insights into the behaviour of particle suspensions under gravity. The results from the simulation, as plotted in the graphs, indicate a clear trend that aligns with theoretical expectations and empirical data. The following points summarize key observations and implications from the simulation:

1. **Sedimentation Velocity Trend**:
   - As the concentration of particles (ϕ) increases, the sedimentation velocity (Vs) decreases. This inverse relationship is consistent across all simulation data points and aligns well with the Richardson-Zaki equation.
   - The sedimentation velocity of particles in a fluid can be described by the Richardson-Zaki equation, which is commonly used to relate the sedimentation velocity to the concentration of particles. The formula is:

     $$\mathbf{Vs=V_0(1-\phi)^n}$$

     where:

     Vs is the sedimentation velocity at a given concentration.

     V_0 is the sedimentation velocity in a dilute suspension (when concentration $\phi \to 0$).

     ϕ is the concentration of particles.

     The Richardson-Zaki exponent (n) used in the model effectively captures the sedimentation behaviour observed in the simulations. The exponent value, typically between 4 and 5 for low Reynolds numbers, accurately describes the relationship between sedimentation velocity and particle concentration.

   - The decrease in sedimentation velocity with increasing concentration can be attributed to the increased hydrodynamic interactions and collisions between particles, which hinder their free settling.

2. **Validation with Empirical Data**:
   - The single result from the code (blue "x" points) shows good agreement with the empirical data (orange dots) scraped from the paper. This congruence validates the accuracy and reliability of the simulation model used in this study.
   - The slight deviations observed at higher concentrations could be due to assumptions and simplifications in the Stokesian dynamics model, such as

ignoring particle-particle interactions beyond a certain range or assuming a uniform particle size distribution.

3. **Effect of Concentration on Sedimentation Behaviour**:
    - At low concentrations ($\phi \approx 0.1$), particles settle relatively quickly with minimal hindrance, resulting in higher sedimentation velocities.
    - As the concentration increases ($\phi \approx 0.2$), the velocity decreases more rapidly due to more frequent particle interactions and increased resistance in the fluid.
    - At high concentrations ($\phi \approx 0.5$), the sedimentation velocity stabilizes at a lower value. This plateau effect suggests that the system reaches a dynamic equilibrium where the settling particles are sufficiently hindered by their neighbors , leading to a steady, reduced sedimentation rate
4. **Density and Coverage**: As the number of particles increases from 8 to 64, the plots become denser and the coverage of the x-y space becomes more uniform. This is expected as more particles provide a better representation of the space.
5. **Colour Differentiation**: The use of different colors for each particle helps in distinguishing them when the number is low (e.g., 8 particles). However, as the number increases, the colours become less effective for individual identification but still provide a visual cue of the particle distribution.

5 Conclusion

5.1 Conclusion overview

he simulation of sedimentation dynamics using Stokesian dynamics has successfully demonstrated the inverse relationship between particle concentration and sedimentation velocity. Key findings from this study include:

- **Consistency with Theory and Empirical Data**: The simulation results show a strong agreement with both theoretical predictions (Richardson-Zaki equation) and empirical data, reinforcing the validity of the Stokesian dynamics approach for modeling sedimentation in particle suspensions.
- **Impact of Particle Concentration**: The observed decrease in sedimentation velocity with increasing concentration highlights the significant role of hydrodynamic interactions and particle collisions in determining the settling behaviour of suspensions.
- **Practical Implications**: Understanding sedimentation dynamics is crucial for various industrial and environmental applications, including mineral processing, and the design of sedimentation tanks. The insights gained from this simulation can inform better design and optimization of such processes.

Overall, this study provides a comprehensive analysis of sedimentation dynamics in particle suspensions, offering valuable contributions to both theoretical understanding and practical applications. Future work could involve exploring the effects of different particle sizes, shapes, and fluid properties to further enhance the model's applicability and accuracy.

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