Mesoscopic Simulations of Microfluidic Flow in Irregular Geometries

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Stochastic Rotation Dynamics, a particle-based model for mesoscopic fluid dynamics, is used to study two and three-dimensional flow in a variety of complex boundaries and for a range of low Reynolds numbers (between 10 and 250). The systems considered consist of irregular geometries such as etched channels to be used as conduits for transporting small particles. We apply our techniques to microfluidic devices with complex channel walls such as those used for slalom chromatography and surface patterned chromatography. Preliminary numerical results show solute motion through such microfluidic devices and offer a mesoscopic method to study such systems.

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Motivation

Microfabricated structures present potential for controlled research into polymer dynamics problems by allowing specific and reproducable environments.

Hydrodynamic chromatography applies laminar flow within small spaces to transport particles leading to size-fractionation. Micromachining the boundaries allows for the fabrication of specific flow conditions and suggests increased control over the separation process.

Slalom separation constitutes a viable chromotgraphy method where the fabricated structures flows which in turn hinders the elution of polymers moving through the channel[1,2,3].

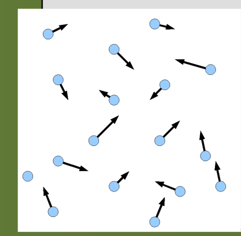
Alternatively, one can imagine hydrodynamic traps where in solute could statically reside for long periods of time.

Stochastic Rotation Dynamics

Stochastic rotation dynamics (SRD), also called multi-particle collision dynamics, is a particle-based, Navier-Stokes solver[4,5].

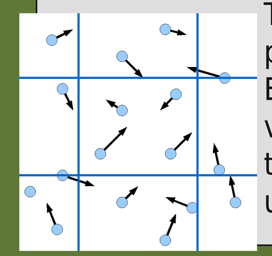
Collisions between particles constituting the fluid are manner by omitting all molecular details but are defined to conserve mass, momentum, and energy such that the thermo-hydrodynamic equations of motion are obeyed on long length and time scales.

SRD simulations occur in two steps:
i) The first step is a streaming step,
ii) the second a collision step.

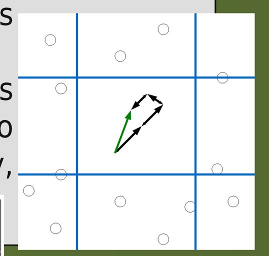


i) During the streaming step, the particles of mass m_i move ballistically with continuous positions $r_i(t)$ and velocities $v_i(t)$ but are simultaneously updated in discrete time intervals δt:

$$\mathbf{r}_i(t+\delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\delta t$$

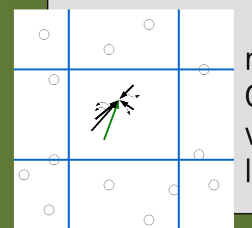


The simulation domain is paritioned into cells.
Each cell has a centre of mass velocity, which corresponds to the local macroscopic velocity, u_{CM}.



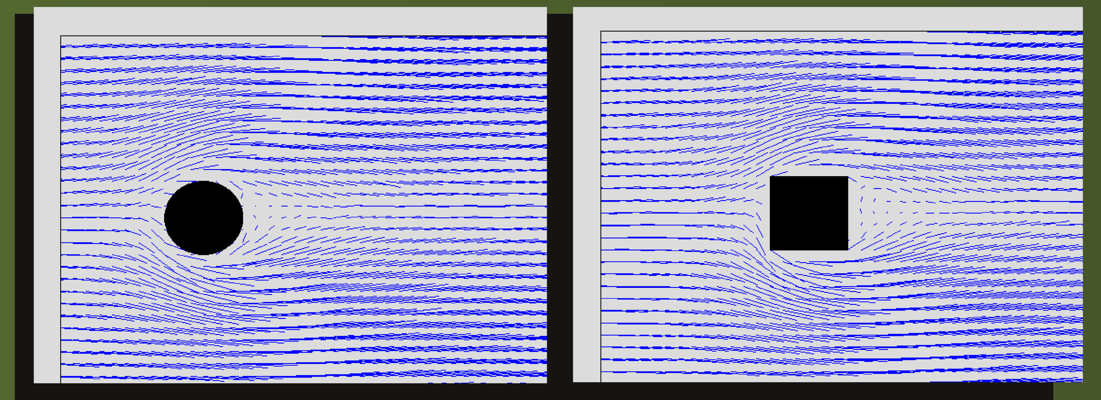
$$\mathbf{u}_{CM}(t) = \left[\sum_{i=1}^{N} m_i \mathbf{v}_i\right] / \left[\sum_{i=1}^{N} m_i\right]$$

$$\mathbf{v}_i(t+\delta t) = \mathbf{u}_{CM}(t) + \mathbf{R}\left(\mathbf{v}_i(t) - \mathbf{u}_{CM}(t)\right)$$



represents multiparticle collisions within each cell. Conservation of energy, isotropy and a MB velocity distribution are met in the continuum limit by rotating about an arbitrary axis.

Simple Flows



Low Reynolds number (Re=13) flows around a cylindrical and rectangular obstruction in 2D. Flow developes in the 50x162 simulation box with periodic boundaries because the 40500 fluid particles feel an external body force.

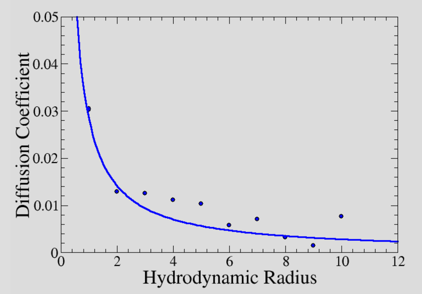
The dynamic viscosity of the fluid is determined from the Green-Kubo relations of the fluid and have two terms, a kinetic contribution and a collisional contribution[6]. The viscosity for these simulations is 0.47 which corresponds to a number density of 5 fluid particles per SRD cell, an SRD rotation angle of 90° and a temperature of $k_bT=0.05$.

Particles collide with the obstical through a bounce-back boundary condition. As is expected with this kind of boundary condition, the effects of slip can be observed[7].

Diffusion

Stokes flow occurs when viscous forces dominate over neglible inertia force. Stokes flow can arises from confined fluid conditions such as in microfluidic devices and has the consequence that the drag force felt by a particle is simply a friction coefficient, ζ, times the velocity difference between the particle and the fluid.

Simulations of beads in stagnant SRD fluid indicate that their random walk follows the Einstein relation which relates the diffusion coefficient to the thermal energy and the friction coefficient. The graph to the right shows that the measured diffusion coefficient is inversely proportional to the radius of the particle.



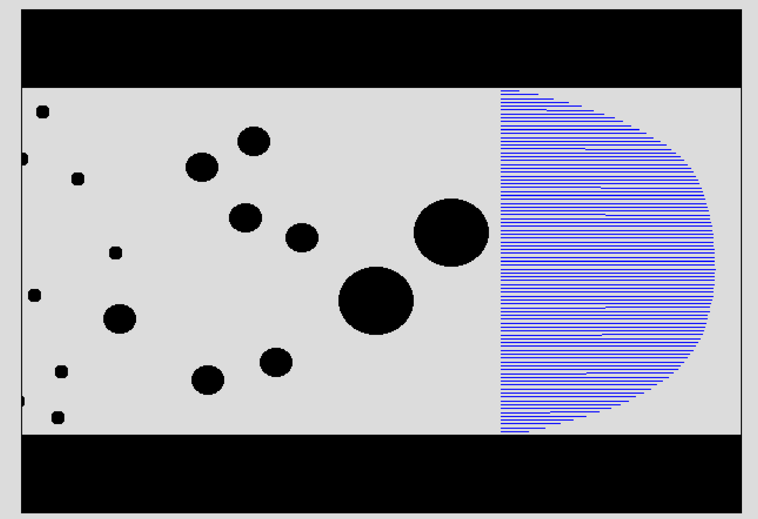
This test of the SRD shows that the algorithm acts as an heat bath for large particles in the system

Advection

The solvent acts on the particle through drag causing advection. The Péclet number weighs the importance of advection to diffusion - the higher Pe the more the flow dominates over diffusion processes.

$$Pe = \frac{U\ell}{D}$$

Hydrodynamic Chromatography



The diagram above shows a simulation of flow through a channel with Reynolds number of 220. The profile agrees well with the expected parabolic shape of laminar flow.

When particles travel through a microchannel, larger particles tend to elute before smaller ones. This occurs because the drag force acting on them is greater and because they tend to travel closer to the centre line of the canal due to steric repulsion.

We run preliminar investigations on micro-scale beads. Since separation occurs when the ratio between the radius and the channel dimension is between 0.01 and 0.35 [8], our beads are between 0.02 and 0.31.

Hele-Shaw Cells

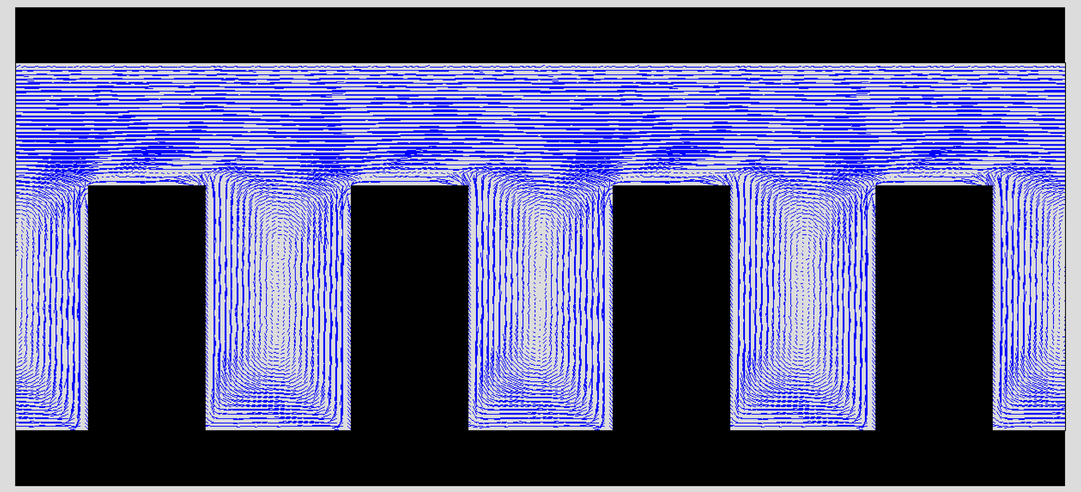
Perhaps more complex boundaries can amplify the hydrodynamic separation.

Hele-Shaw flow occurs between two parallel plates separated by such a narrow gap that the vorticity is neglible.

When a small cavity is cut in one of the bounding plates, a Hele-Shaw cell is formed in the limiting case that the flow remains irrotational.

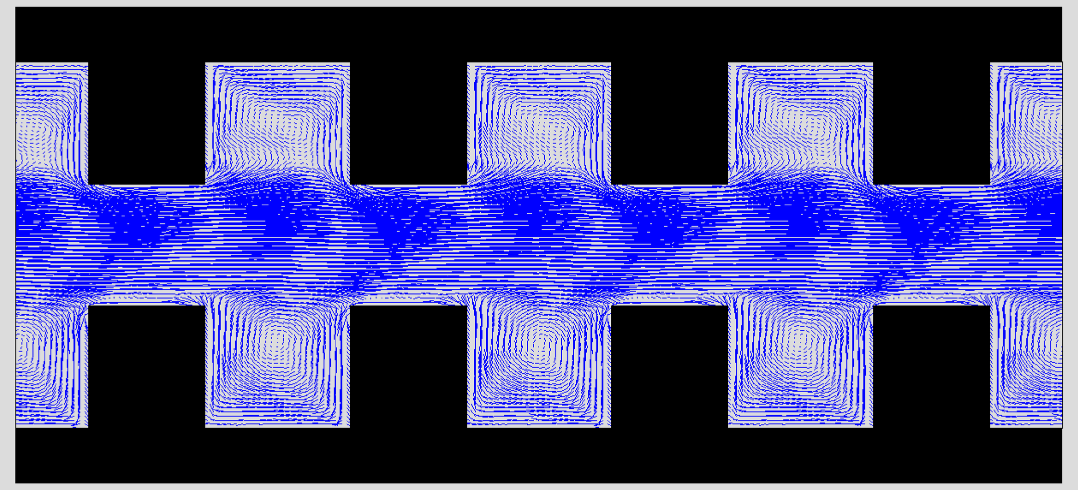
Cells further increase the elution time of smaller particles because any particle that diffuses deep into the cavity must lose advection.

Micro-well Structures Cavity Flow



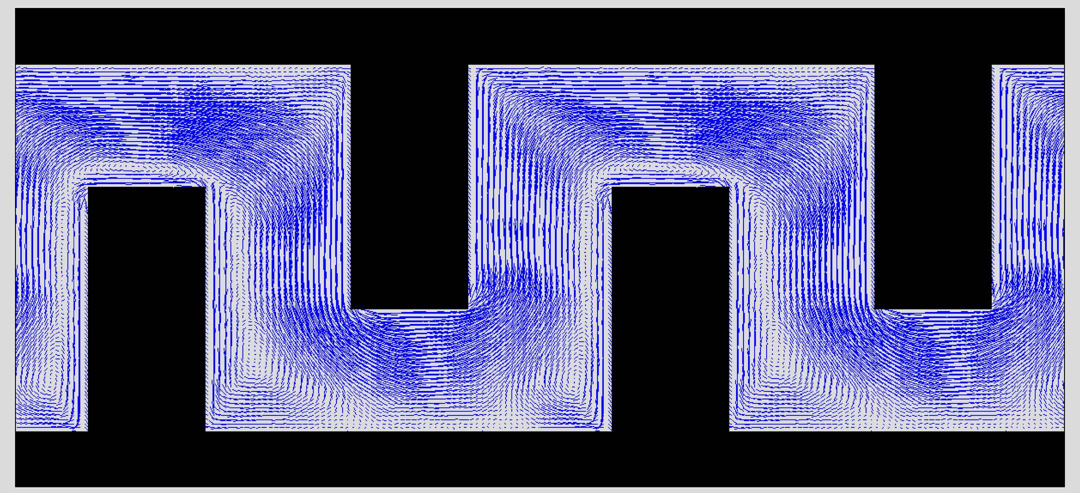
If the cells extend deep enough then vorticity is able to form in the cavity. In this case, the circulation produced would provide further trapping for small Pe particles.

Cogged Microchannel



The same volume can be excluded from microchannel by fabricating obsticles on both sides. The well depth between teeth is shallower but the probability that a solute particle enters a well is greater.

Slalom Flow



In slalom chromatography the particles do not enter wells but rather explore corner regions of higher vorticity. This circulation leads to the extension of the small particles elution time.

Conclusion

As a mesoscopic method, SRD is useful for simulations of microfluidic flows. We have shown that SRD acts as a heat bath to particles suspended in fluid while preserving the momentum transfer needed for simulating flows. To check the operation of the SRD algorithm we have verified that the diffusion of large particles is inversely proportional to their radius as expected and have reproduced classical flow configurations like laminar flow around a cylinder and Poiseuille flow.

This method is particularily useful for simulations of microfluidic devices designed for hydrodynamic chromatography. The separation process depends on the Péclet number. Because they can get closer to the wall, smaller particles being carried by the fluid spend less time near the quick flowing centre line and so advect slower.

Hele-Shaw flow is common in microfluidics but neglects any vorticity in the system. Particles advecting past a Hele-Shaw cell may diffuse into the cavity and thus the elution time will be further retarded with respect to the larger colloids.

We have simulated systems in which vorticity can not be neglected. By enlarging the cells it is possible to obtain more complex microfluidic systems whose circulation may constitute hydrodynamic traps. The ability to fabricate microstructures presents the opportunity to specifically engineer flow profiles. We have demonstrated a handfull of systems and plan to extend this study to a wide variety of structures and alternative hydrodynamic separation techniques such as field flow fractionation.

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