Simulation of Particle Interactions in DNA-laden Flows

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Microfluidic devices are becoming state-of-the-art in many significant applications including pathogen detection, continuous monitoring, and drug delivery. Particle interactions are introduced into a developing framework for simulation of DNA-laden flows in such devices. A screened Coulomb potential efficiently models electrostatic interactions while also accounting for excluded volume effects.

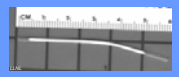
Introduction

•Microfluidic devices are becoming state-of-the-art in many significant applications including pathogen detection, continuous monitoring, and drug delivery.

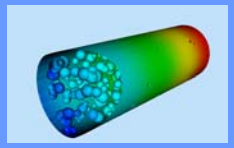
•Numerical algorithms which can simulate flows of complex fluids within these devices are needed for their development and optimization.

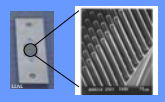
•A method is being developed at LLNL for simulations of DNA-laden flows in complex microscale geometries such as packed beds and pillar chips.

•**Objective:** introduce particle interactions into this method.

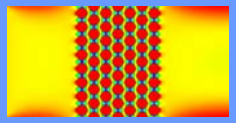


Packed bed





Pillar chip



Methods

•**Fluid**: Newtonian, incompressible, subject to body force

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}\right)=-\nabla p+\mu\nabla^2\boldsymbol{u}+\boldsymbol{F} \qquad \nabla\cdot\boldsymbol{u}=0$$

Navier-Stokes

•**DNA**: bead-rod polymer model

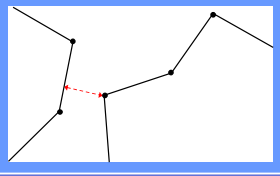
$$m\frac{\partial^2\boldsymbol{x}}{\partial t^2}=\boldsymbol{F}_{drag}+\boldsymbol{F}_{Brownian}+\boldsymbol{F}_{constraint}+\boldsymbol{F}_{particle}$$

Langevin

•**Particle Interactions**: screened Coulomb potential between rods

$$U_{particle}=A\frac{e^{-\kappa r}}{r}$$

Debye-Hückel



Forces applied to beads via inverse lever-rule

Discussion

•DNA is charged--use screened Coulomb interaction via Debye-Hückel approximation

•Debye-Hückel potential is much less steep than Lennard-Jones repulsive potential (r^{-12}) allowing a larger time-step

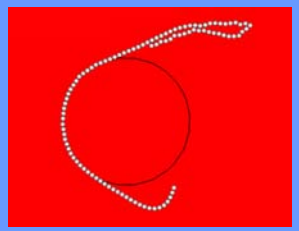
•Rod-rod potential required instead of bead-bead potential to ensure rods do not cross thus accounting for excluded volume

•Singularity of rod-rod potential also required to ensure rods do not cross

Future Work

•Introduce attractive particle-surface interactions to simulate DNA capture

•Experimental validation of parameters for interaction potentials



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