Electrokinetic Flow Simulations with a Widely Applicable Lattice Boltzmann Solver

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waLBerla

- Widely applicable Lattice Boltzmann solver
- Suited for various flow applications
- Easily adaptable to further extensions
- Flexibly parametrizable via input file
- Large-scale, MPI-based parallelization
- Dynamic application switches for heterogeneous architectures

Electrokinetic Flows

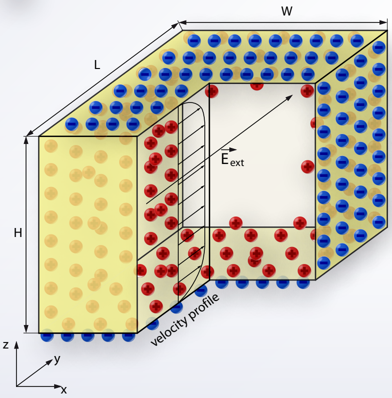
- Electroosmosis: Flow of dilute solution due to electric field
- Electrophoresis: Movement of charged particles relative to fluid due to electric field
- Dielectrophoresis: Movement of particles in non-uniform electric field due to polarization effects
- Aim: Simulation of electrokinetically driven particle-laden micro-fluid flows in Lab-on-a-Chip systems

Electro-Osmotic Flow

Mechanism

- Charged surface causes formation of electric double layer (EDL)
- External electric field causes migration of EDL due to Coulomb force
- Fluid viscosity causes movement of surrounding fluid

Physical Setup



Mathematical Model

Poisson-Boltzmann Equation (binary symmetric electrolyte):

$$-\Delta\Phi(\overline{x}) = \frac{\rho_e(\overline{x})}{\epsilon_r\,\epsilon_0} = -\frac{2\,z\,e\,c^\infty}{\epsilon_r\,\epsilon_0}\sinh\left(\frac{z\,e}{k_B\,T}\Phi(\overline{x})\right)$$

Debye-Hückel approximation: $-\Delta\Phi(\overline{x}) \approx -\kappa^2\Phi(\overline{x})$

Electrical Double Layer thickness: $\lambda_D = \frac{1}{\kappa} = \sqrt{\frac{\epsilon_r\,\epsilon_0\,k_B T}{2\,z^2\,e^2\,c^\infty}}$

Net charge density: $\rho_e(\overline{x}) = -2\,z\,e\,c^\infty \sinh\left(\frac{z\,e}{k_B\,T}\Phi(\overline{x})\right)$

External force: $\overrightarrow{F} = \rho_e \cdot \overrightarrow{E}_{ext} - \nabla P$

Lattice Boltzmann Equation with external force:

$$f_i(\overline{x}+\overrightarrow{c_i}\delta t, t+\delta t) - f_i(\overline{x},t) = -\frac{\delta t}{\tau}\left[f_i(\overline{x},t) - f_i^{eq}(\overline{x},t)\right] + \delta t \cdot F_i$$

Equilibrium probability distribution function (PDF):

$$f_i^{eq} = f_i^{eq}(\rho,\overrightarrow{u}) = t_i\left[\rho + \frac{1}{c_s^2}\overrightarrow{c_i}\cdot\overrightarrow{u} + \frac{1}{2c_s^4}(\overrightarrow{c_i}\cdot\overrightarrow{u})^2 - \frac{\overrightarrow{u}^2}{2c_s^2}\right]$$

External force term:

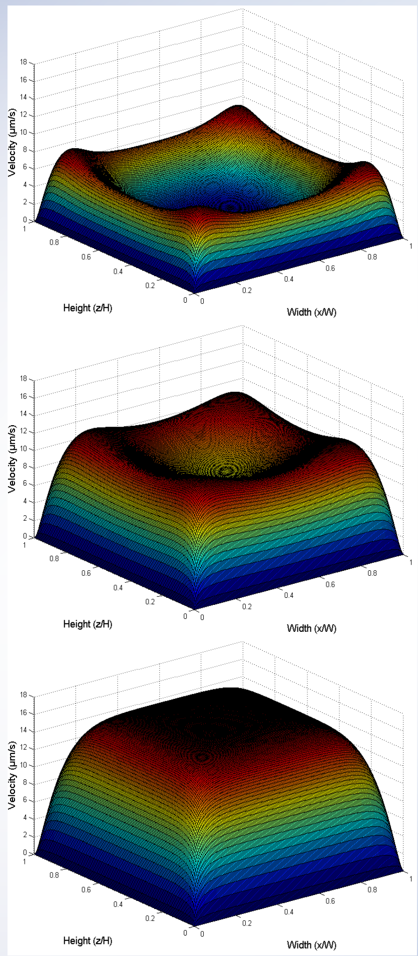
$$F_i = \left(1-\frac{1}{2\tau}\right)t_i\left[\frac{(\overrightarrow{c_i}-\overrightarrow{u})}{c_s^2} + \frac{(\overrightarrow{c_i}\cdot\overrightarrow{u})}{c_s^4}\overrightarrow{c_i}\right]\cdot\left[\overrightarrow{F}\right]_{Lattice}$$

Macroscopic velocity: $\left[\overrightarrow{u}\right]_{Lattice} = \frac{1}{\rho}\sum_i f_i\overrightarrow{c_i} + \frac{\left[\overrightarrow{F}\right]_{Lattice}}{2}$

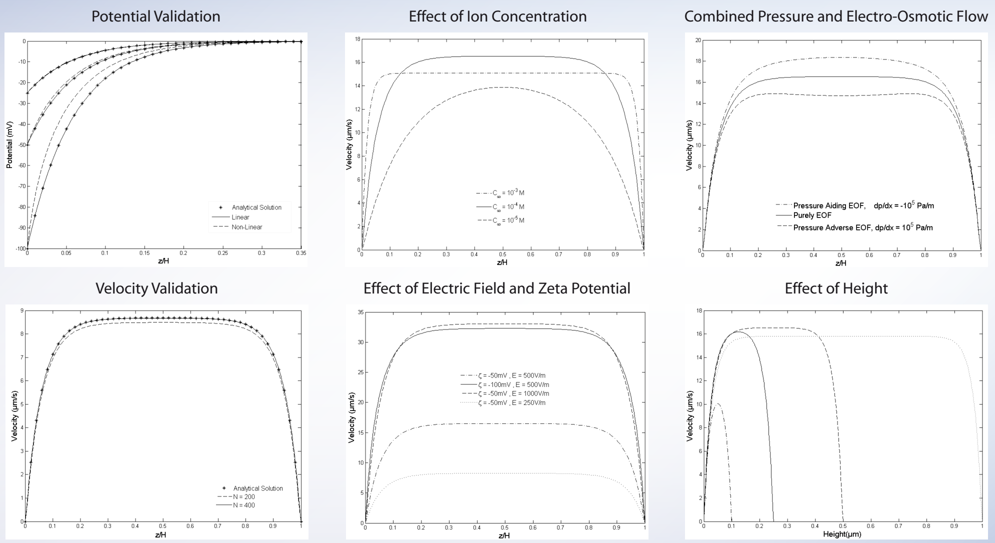
EOF Algorithm

```
for each time step do
  // solve Poisson-Boltzmann equation (PBE)
  while residual too high do
    set RHS of PBE
    apply iterative solver to PBE (SOR, MG, ...)
    MPI-communicate electric potential
  end
  calculate external force
  // solve Lattice Boltzmann equation
    stream PDFs (stream step)
    calculate macroscopic variables considering forcing
    relax towards equilibrium PDF (collide step)
end
```

Flow Formation

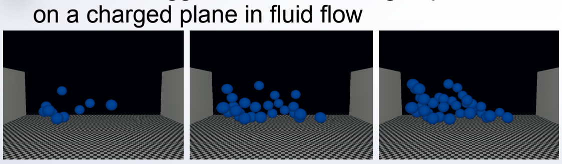


Validation and Results



Charged Particles in Non-Electrolyte Solution

- Charge density determined by particle charge
- Fluid-particle interaction by hydrodynamic force
- Simulation: Agglomeration of charged particles on a charged plane in fluid flow



Algorithm:

```
for each time step do
  // solve Poisson equation with particle charge density
  while residual too high do
    set RHS of poisson equation
    apply iterative solver to poisson equation
  end
  calculate and add hydrodynamic force on particles
  calculate and add electrostatice force on particles
  // solve Lattice Boltzmann equation
    stream PDFs (stream step)
    calculate macroscopic variables considering forcing
    relax towards equilibrium PDF (collide step)
  update particle positions
end
```

Current and Future Work

- Development of solver module for linear systems of equations, including Geometric Multigrid solver
- Solution of Poisson-Nernst-Planck equation for simulating transient behavior of EDL and electrophoresis
- Finite Difference discretization for elliptic PDEs with jumping coefficients required for dielectrophoresis