Modelling of electrokinetic flow using the lattice-Boltzmann method

Master's thesis presentation

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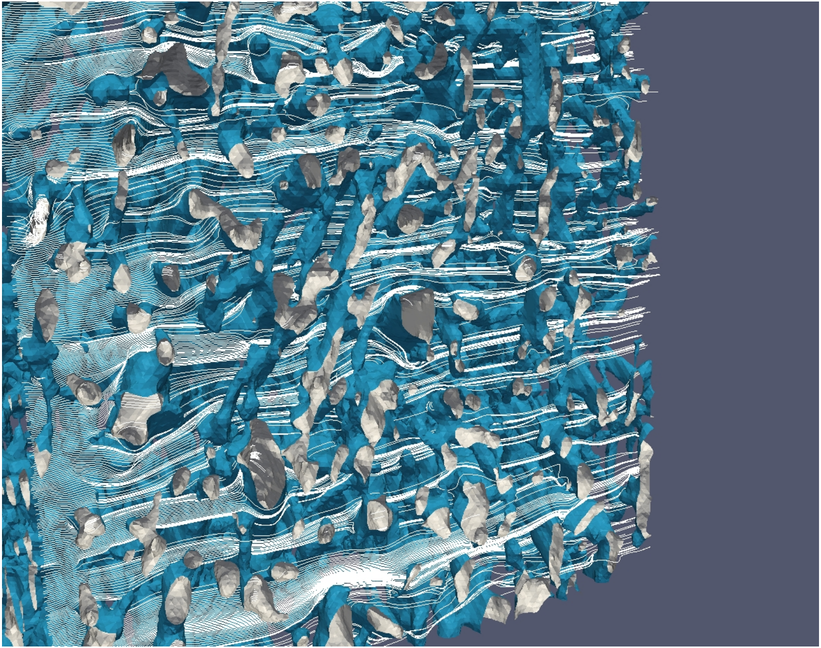
Outline

Background

Background

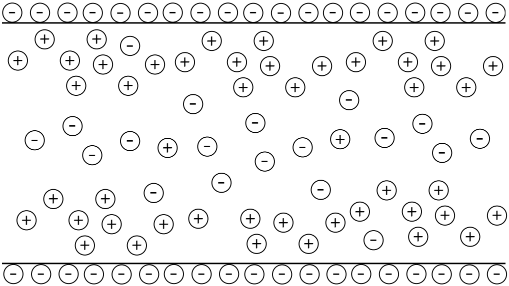
- Demand from both industry and academy on accurate modelling of electrokinetic systems.
- Example of applications: drugs, biological chips, fuel cells...
- A lattice-Boltzmann code is developed at Chalmers to deal with transport through complicated structures.
- This work aims to investigate how electric effects may be integrated.



Electrokinetics

Sample system - a 2D channel

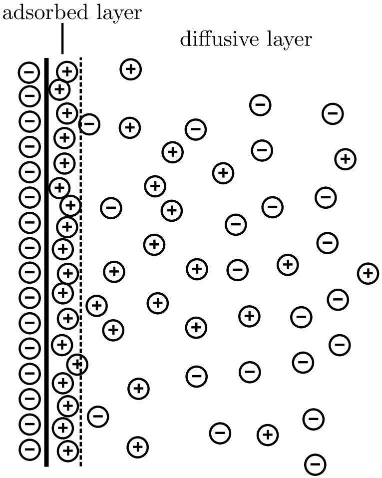
Example of a “simple” electrokinetic system:



The solution contains charges, the walls are charged, external electric/force fields may be present...

Electrical double layers (EDLs)

Ionic solution in contact with a charged object $\Longrightarrow$ EDL



Involved equations

- The electric potential from the charge presence. Poisson's equation for electrostatics:

$$\nabla^2 \psi = -\frac{\rho_e}{\epsilon_r \epsilon_0} \tag{1}$$

- The transport of charges due to diffusion, advection and the presence of electric fields. The Nernst-Planck equation:

$$\frac{\partial \mathrm{c}}{\partial t} = \nabla \cdot \left[D \nabla \mathrm{c} - \mathrm{c}\mathbf{u} + \frac{z q_e D}{k_B T} \mathrm{c} \nabla \psi \right] \tag{2}$$

- The flow field, affected by electrokinetic effects. (Incompressible) Navier-Stokes equations:

$$\nabla \cdot \mathbf{u} = 0 \tag{3}$$

and

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla \mathrm{P} + \mu \nabla^2 \mathbf{u} + \mathbf{F} \tag{4}$$

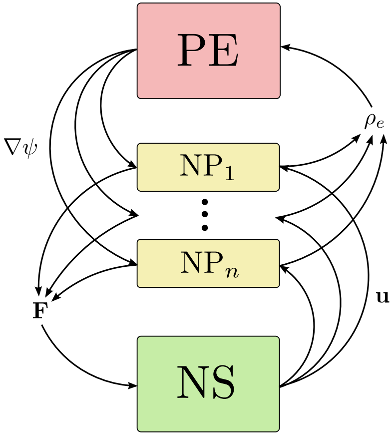
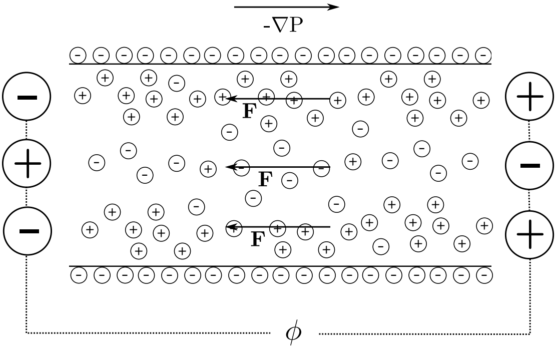


Figure: Visualisation of the coupling between the three equations present in the model. Poisson's equation (PE), The set of Nernst-Planck equations (NP$_1$ ... NP$_n$) for the different ion species and the Navier-Stokes equations (NS). The dependencies have also be marked with arrows indicating what quantities for a certain equation that are needed from an other.

The electroviscous effect

$$\mathbf{J} = -\sigma_c \nabla \phi \tag{5}$$

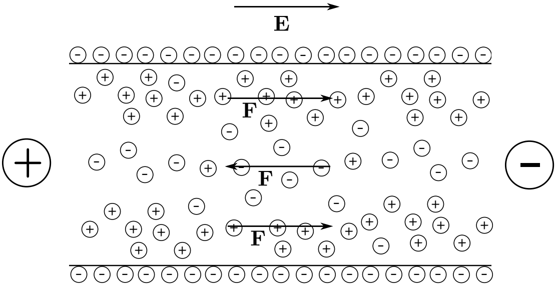
$$\mathbf{F} = -\rho_e \nabla \phi \tag{6}$$



Streaming potential

Electroosmosis

$$\mathbf{F} = \rho_e \mathbf{E} \quad (7)$$



Boundary conditions

Boundary conditions at (charged) walls, Γ

- Poisson's equation: fixed surface charge, σ_s

$$\nabla\psi(\mathbf{x})\cdot\mathbf{n} = -\frac{\sigma_s(\mathbf{x})}{\epsilon_0\epsilon_r}\ , \quad \mathbf{x}\in\Gamma \tag{8}$$

- Nernst-Planck: zero flux through wall

$$\mathbf{J}(\mathbf{x})\cdot\mathbf{n} = 0\ , \quad \mathbf{x}\in\Gamma \tag{9}$$

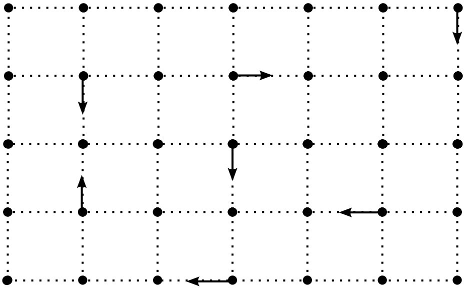
- Navier-Stokes: no-slip

$$\mathbf{u}(\mathbf{x}) = 0\ , \quad \mathbf{x}\in\Gamma \tag{10}$$

The lattice-Boltzmann method

Historical overview

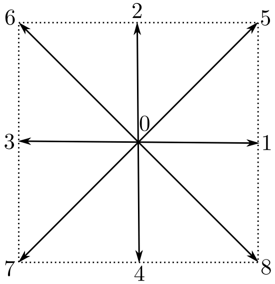
- Lattice gas automata (LGA) methods 70's, 80's



- Several flaws of the LGA cured: continuous distributions, higher symmetry in lattices... $\Longrightarrow$ LBM late 80's, 90's, 00's

Basic idea

- Discretisation of phase space $\implies$ the lattice, example D2Q9:



- The distribution function $f_i(\mathbf{x}, t)$ - probability of finding a particle at $\mathbf{x}$, t with velocity $\mathbf{c}_i$.

Basic idea

- Evolution of f_i, the lattice-Boltzmann equation:

$$f_i(\mathbf{x} + \mathbf{c}_i\delta_t, t + \delta_t) - f_i(\mathbf{x}, t) = \Omega_{ij}(\mathbf{x}, t) \tag{11}$$

- A popular choice is the BGK collision operator:

$$\Omega_{ij} = \Omega_i = -\omega \left[f_i(\mathbf{x}, t) - f_i^{(eq)}(\mathbf{x}, t) \right] \tag{12}$$

Basic idea

In the case with Navier-Stokes we have:

$$f_i^{(eq)} = w_i \rho \left[1 + \frac{\mathbf{c}_i \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{c}_i \cdot \mathbf{u})^2}{2c_s^4} - \frac{\mathbf{u}^2}{2c_s^2} \right] \tag{13}$$

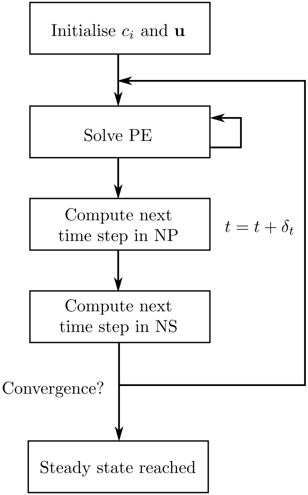
The macroscopic quantities ρ and $\mathbf{u}$ are obtained from f_i through:

$$\rho = \sum_i f_i \tag{14}$$

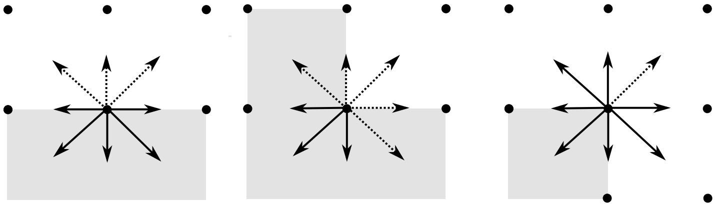
and

$$\rho \mathbf{u} = \sum_i f_i \mathbf{c}_i. \tag{15}$$

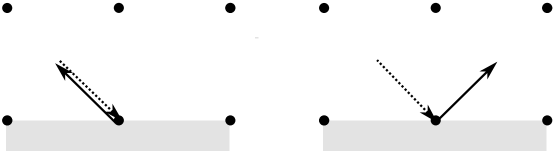
Coupled scheme



Boundary conditions



- Bounce back $(\mathbf{u} = 0)$
- Mirror reflection $(\mathbf{J}_{ion} \cdot \mathbf{n} = 0$ and $\nabla\psi \cdot \mathbf{n} = -\sigma_s/\epsilon_0\epsilon_r)$



Some results

Charge distribution in 2D channel

Thin channel, no flow, steady state:

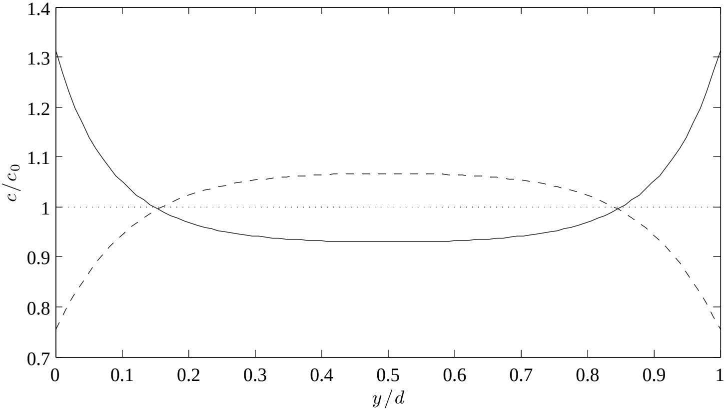


Figure: Computed positive (solid) and negative (dashed) charge distribution across a channel of width $d = 10\mu$m. The solution in the channel is a KCl solution defined by parameters in table **??**. The channel walls are negatively charged.

Electroviscous effect in 2D channel

Flow driven by a pressure gradient, walls of channel charged.

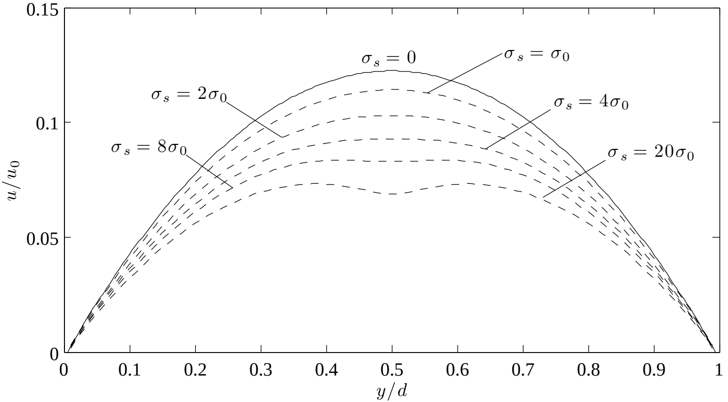


Figure: Computed velocity profiles across a 2D channel of width $d = 1\mu$m. The flow is driven by a pressure gradient and the flow is slowed down due to the electroviscouos effect, this effects dependence on the surface charge σ_s is here illustrated. The solution in the channel is a KCl solution defined by parameters in table **??**. In this simulation, $\sigma_0 = 0.89\mu\text{C/m}^2$, $\partial_x P = 1$ kPa/m and $u_0 = 10$ mm/s.

Comparison with "traditional" approach

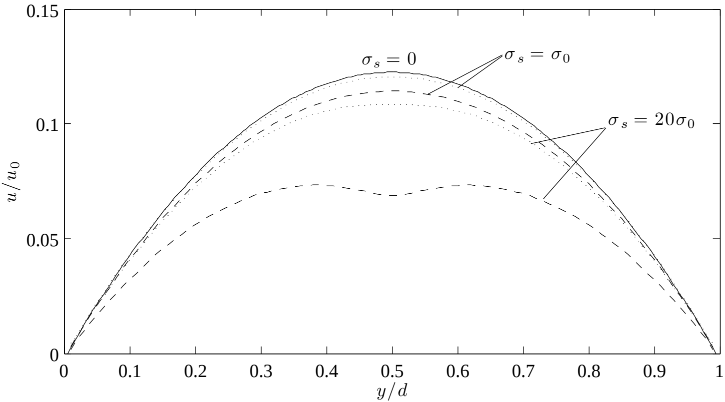
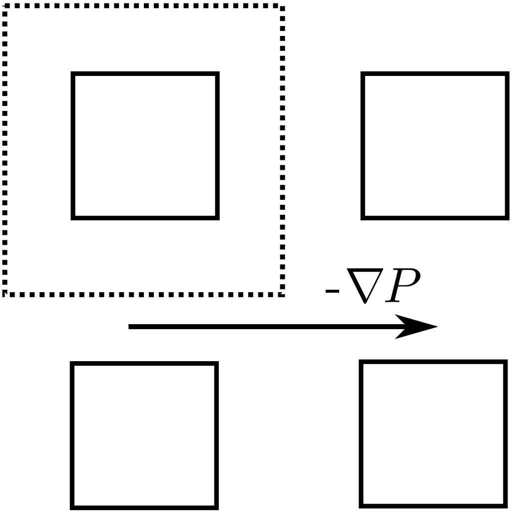
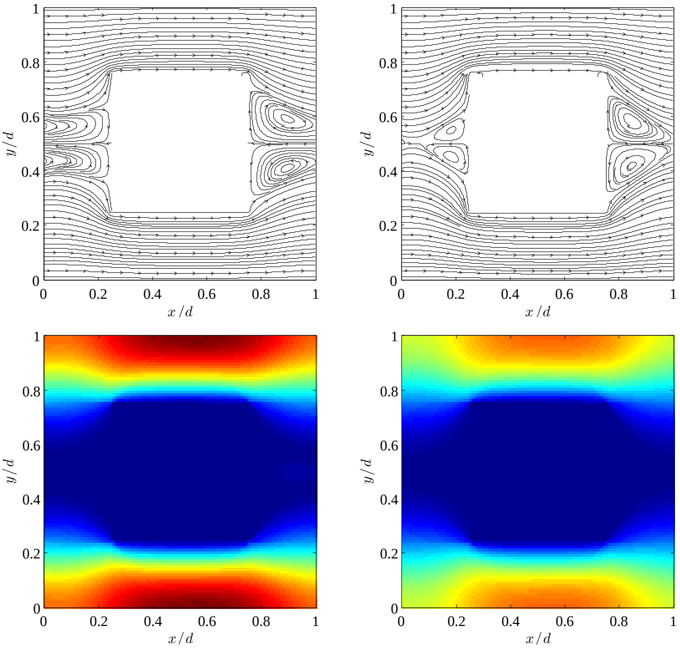


Figure: Comparison between velocity profiles computed using a mean current (dotted) and by using the actual local current (dashed) for the streaming potential. The solution in the channel is a KCl solution defined by parameters in table **??**. In this simulation, $\sigma_0 = 0.89\mu$C/m^2, $\partial_x P = 1$ kPa/m and $u_0 = 10$ mm/s.

Flow through square array





Uncharged

Charged

Flow through square array

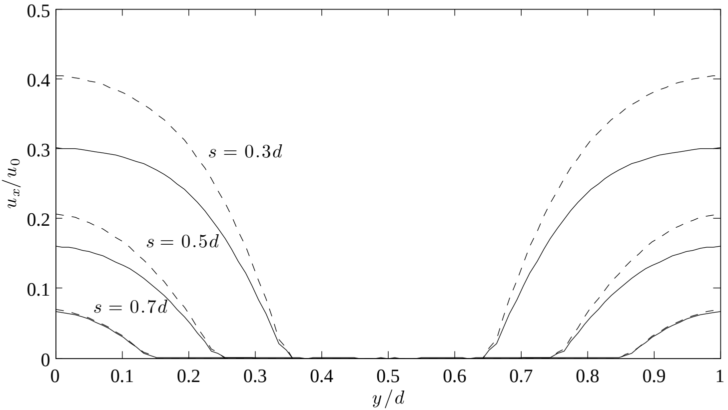


Figure: Velocity profiles across the square array at $x = d/2$ in the cell. The sides of the squares are varied between $0.3d$, $0.5d$ and $0.7d$ where $d = 10\mu$m is the length of the cell. The flow is driven by a pressure gradient and the uncharged (dashed) and charged (solid) squares are compared. In this simulation, $\sigma_s = 1.78\mu$C/m^2 (solid), $\partial_x P = 0.5$ kPa/m and $u_0 = 1$ mm/s.

Conclusions

Main conclusions

- The LBM is a computational alternative in the modelling of electrokinetics.
- The traditional way of computing the streaming potential does not give accurate results in thin channels.
- Due to the electrovicous effect, the permeability of charged structures is decreased.

Thanks for listening!

Questions?