CHALMERS

Modelling of electrokinetic flows through charged structures using the lattice-Boltzmann method

SuMo Cluster Meeting

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Outline

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Electrokinetics
- Basic concepts
- Modelling approach
- Some electrokinetic phenomena

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The lattice-Boltzmann method

- A brief introduction

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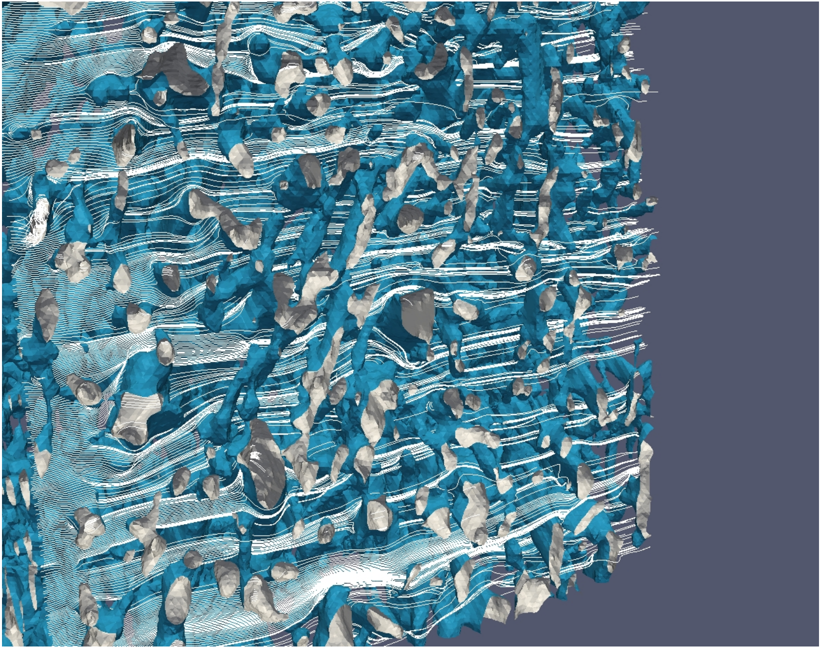
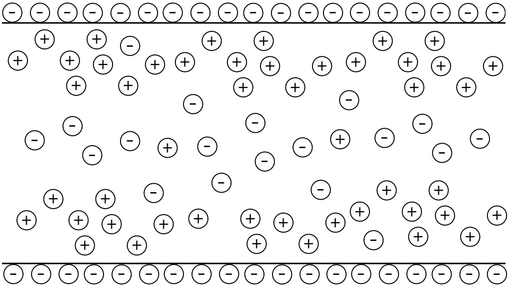
- A lattice-Boltzmann code is developed at Chalmers to deal with transport/flow through complicated structures.
- This work aims to investigate how electric effects may be integrated.



Electrokinetics

Sample system - a 2D channel

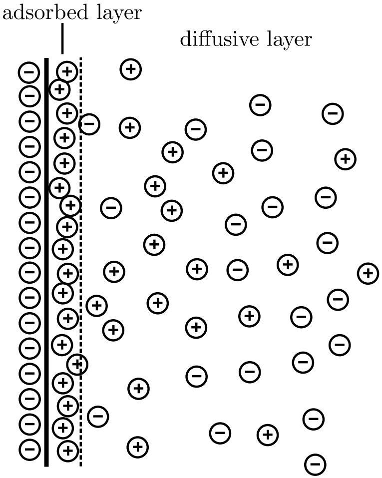
Example of a "simple" electrokinetic system:



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:

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

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

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

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

and

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

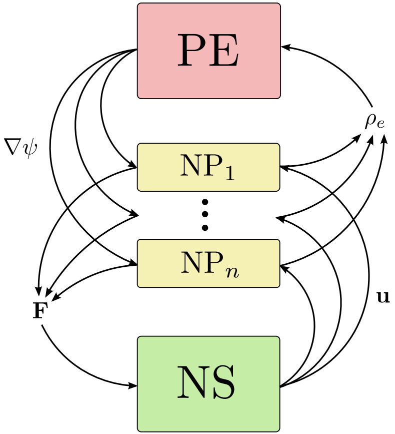
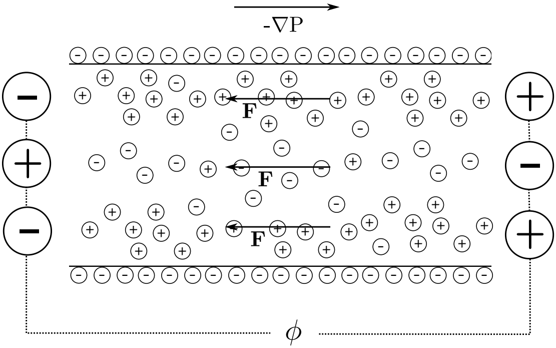


Figure: Visualisation of the coupling between the three equations present in the model. Poisson's equation (PE), The set of Nernst-Planck equations (NP$_1$ ... NP$_n$) for the different ion species and the Navier-Stokes equations (NS). The dependencies have also be marked with arrows indicating what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

The electroviscous effect

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

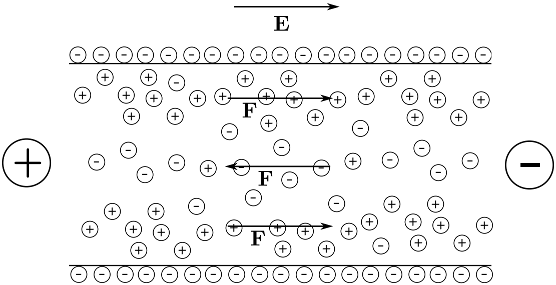
$$\mathbf{F} = -\rho_e \nabla \phi \tag{6}$$



Streaming potential

Electroosmosis

$$\mathbf{F} = \rho_e \mathbf{E} \tag{7}$$



Boundary conditions

Boundary conditions at (charged) walls, Γ

- Poisson's equation: fixed surface charge, σ_s

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

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

- Navier-Stokes: no-slip

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

The lattice-Boltzmann method

A few words about the LBM

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- Strengths: complex boundaries, straight-forward implementation, highly prallelisable algorithm
- Weaknesses: New method $\implies$ lack of theoretical work, uniform lattice required - Kn $\ll 1$,

Some results

Charge distribution in 2D channel

Thin channel, no flow, steady state:

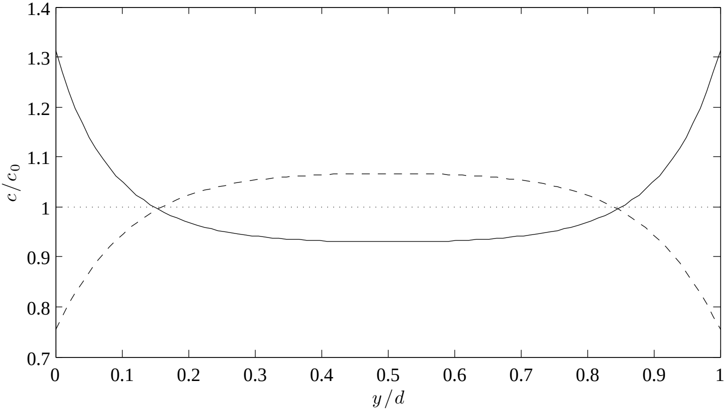


Figure: Computed positive (solid) and negative (dashed) charge distribution across a channel of width $d = 10\mu$m. The solution in the channel is a KCl solution defined by parameters in table **??**. The channel walls are negatively charged.

Electroviscous effect in 2D channel

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

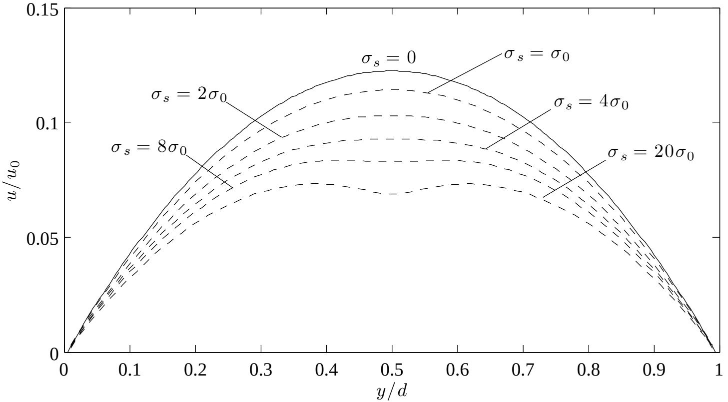


Figure: Computed velocity profiles across a 2D channel of width $d = 1\mu$m. The flow is driven by a pressure gradient and the flow is slowed down due to the electroviscouos effect, this effects dependence on the surface charge σ_s is here illustrated. The solution in the channel is a KCl solution defined 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

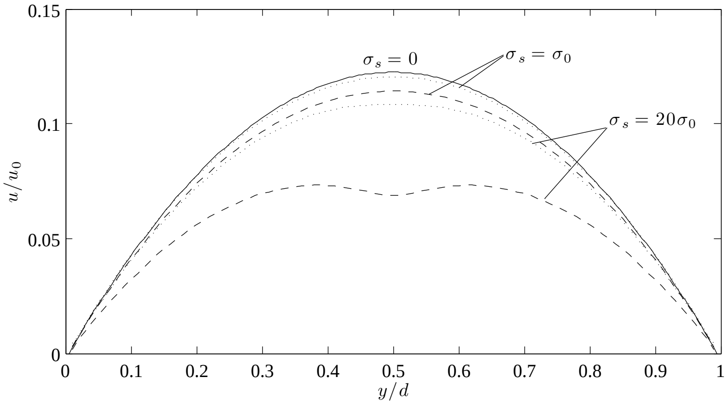
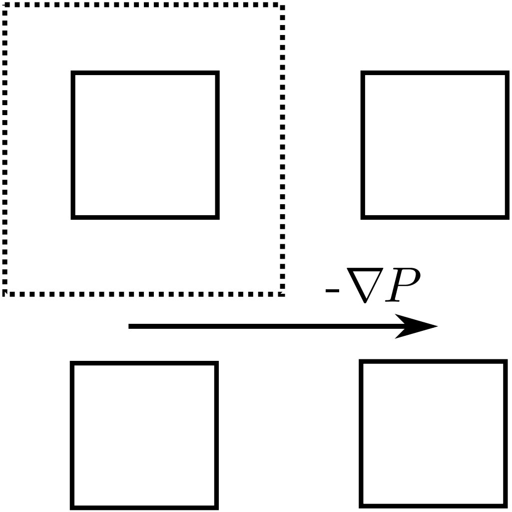
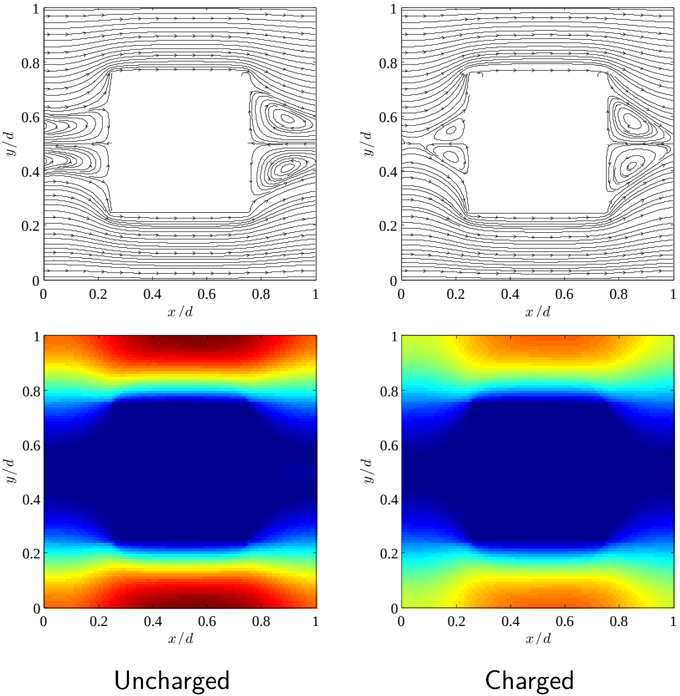


Figure: Comparison between velocity profiles computed using a mean current (dotted) and by using the actual local current (dashed) for the streaming potential. The solution in the channel is a KCl solution defined by parameters in table **??**. In this simulation, $\sigma_0 = 0.89\mu$C/m^2, $\partial_x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

Flow through square array





1
0.8
0.6
0.4
0.2
0
0
0.2
0.4
0.6
0.8
1
y/d
x/d
Uncharged
Charged

Flow through square array

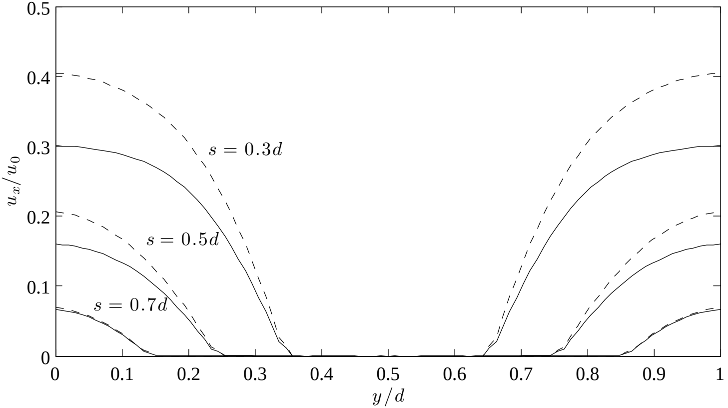
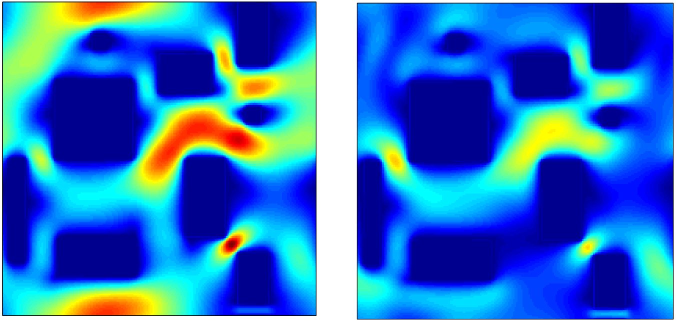


Figure: Velocity profiles across the square array at $x = d/2$ in the cell. The sides of the squares are varied between $0.3d$, $0.5d$ and $0.7d$ where $d = 10\mu$m is the length of the cell. The flow is driven by a pressure gradient and the uncharged (dashed) and charged (solid) squares are compared.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

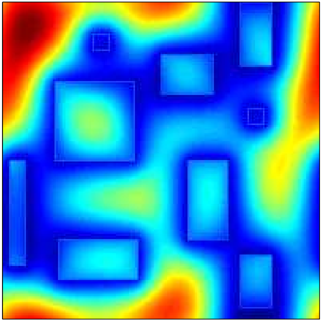
A more complicated geometry



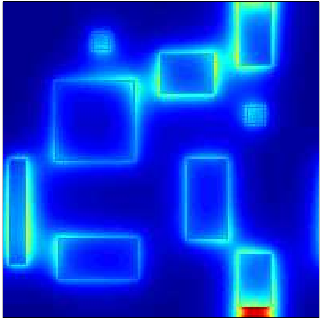
(a) $|\mathbf{u}|$ Uncharged

(b) $|\mathbf{u}|$ Charged

A more complicated geometry



(c) c_-



(d) c_+

Thanks for listening!

Questions?