Numerical and Analytical Studies of Two-Dimensional Electro-Osmotic flows of Viscoelastic fluids

A.M. Afonso[1], F.T. Pinho[2] and M.A. Alves[1]

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Outline

1 Introduction
- Electro-Osmotic Flow (EOF): Theory

2 Governing Equations
- EOF of Viscoelastic Fluid

3 Analytical Solutions for Channel flows
- Newtonian fluids
- Viscoelastic fluids

4 Numerical Solutions
- Channel flows
- Complex geometries

5 Conclusions

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Electro-Osmotic Flow (EOF)

a classical electrokinetic phenomena

Electro-Osmotic Flow (EOF)[1]

is the motion of the liquid adjacent to a charged surface due to an externally imposed electric field.

[1] A.V. Delgado, *Interfacial Electrokinetics and Electrophoresis*, (New York: Marcel Dekker, 2002), pp 8.

Surface charge:

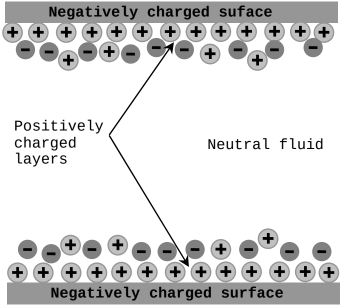
- Solution of ions
- Overall charge neutrality

Electric Double Layer (EDL):

- Mobile diffusive layer
- Immobile layer (Stern Model)
- Debye layer: $\lambda_D = \frac{1}{\kappa} = \sqrt{\frac{\epsilon k_B T}{2 n_o e^2 z^2}}$

Electro-Osmotic Velocity:

- Apply an external potential
  Electric force $\mathbf{F} = \rho_e \mathbf{E}$
- Viscous forces drag the solution.



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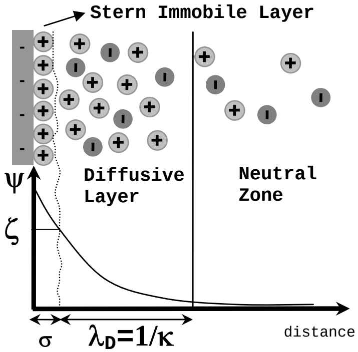

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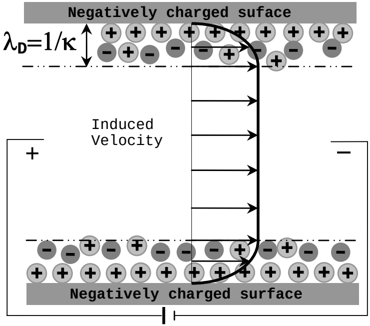

Mass Conservation:

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

Momentum Conservation:

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} - \rho_e \nabla \Phi$$

Constitutive Equation:

$$f(\tau_{kk})\boldsymbol{\tau} + \lambda \overset{\nabla}{\boldsymbol{\tau}} = 2\eta \mathbf{D}$$

Electrokinetics:

$$\nabla^2 \Phi = -\frac{\rho_e}{\epsilon}$$

Phan-Thien & Tanner Model (PTT)

$$\overset{\nabla}{\boldsymbol{\tau}} = \frac{D\boldsymbol{\tau}}{Dt} - \boldsymbol{\tau} . \nabla \mathbf{u} - \nabla \mathbf{u}^T . \boldsymbol{\tau}$$

$$f(\tau_{kk}) = 1 + \frac{\varepsilon \lambda}{\eta} \tau_{kk}$$

Electric Body Force:

$$\mathbf{\Phi} = \phi + \psi$$

$$\rho_e = -2 n_o e z \sinh\left(\frac{ez}{k_B T}\psi\right)$$

Poisson-Boltzmann Equations:

$$\nabla^2 \phi = 0$$

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Debye-Hückel approximation:

$$\nabla^2 \psi = 2\frac{n_o e z}{\epsilon} \underbrace{\sinh\left(\frac{ez}{k_B T}\psi\right)}_{\sinh x \approx x} \approx \kappa^2 \psi$$

Symmetric case:

B.C. $\psi_{|y=H} = \zeta_1$ *and* $\frac{d\psi}{dy}_{|y=0} = 0$:

$$\psi(y) = \zeta_1 \left(\frac{e^{\kappa y} + e^{-\kappa y}}{e^{\kappa H} + e^{-\kappa H}}\right)$$

κ is the screening length

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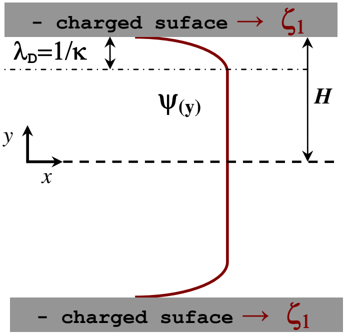

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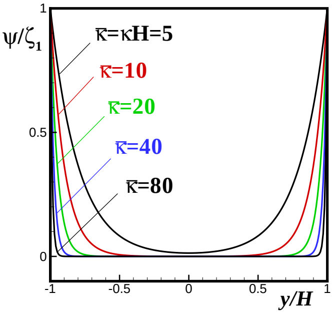

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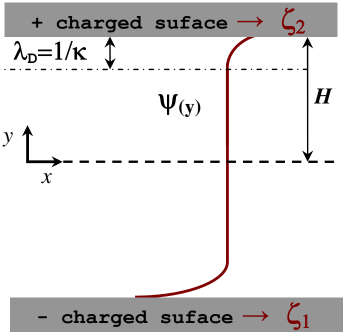
Asymmetric Case (e.g. PDMS/Glass)

B.C. $\psi_{|y=H} = \zeta_2$ and $\psi_{|y=-H} = \zeta_1$:

$$\psi(y) = \zeta_1\left(\frac{\left(R_\zeta e^{\kappa H} - e^{-\kappa H}\right)}{2\sinh(2\kappa H)}e^{\kappa y} - \frac{\left(R_\zeta e^{-\kappa H} - e^{\kappa H}\right)}{2\sinh(2\kappa H)}e^{-\kappa y}\right)$$

Ratio of zeta potentials: $R_\zeta = \frac{\zeta_2}{\zeta_1}$



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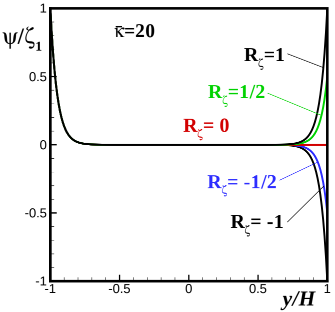

Momentum Conservation:

$\frac{du}{dy} = \epsilon\kappa^2 E_x \psi(y)$

Symmetric case:

B.C. $u_{|y=H} = 0$, $\frac{du}{dy}_{|y=0} = 0$:

$$u(y) = \frac{\epsilon E_x \zeta_1}{\eta}\left(\frac{\psi(y)}{\zeta_1} - \zeta_1\right)$$

Helmholtz-Smoluchowski Velocity:

When $\lambda_D \to 0$ $(\kappa \to \infty)$*:*

$$u_{sh} = -\frac{\epsilon E_x \zeta_1}{\eta}$$

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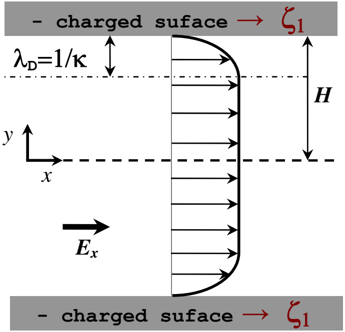

Analytical Solutions - Channel Flow

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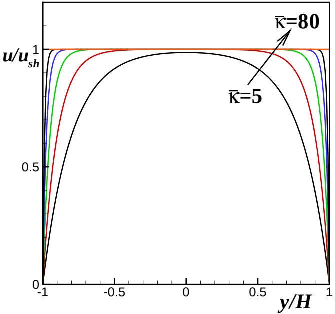

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$$\frac{u(\overline{y})}{u_{sh}} = \frac{1}{2}\left(R_\zeta - 1\right)\left(\overline{y} + 1\right) + 1 - \frac{\psi(\overline{y})}{\zeta_1}$$

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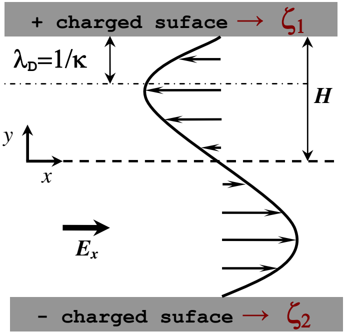

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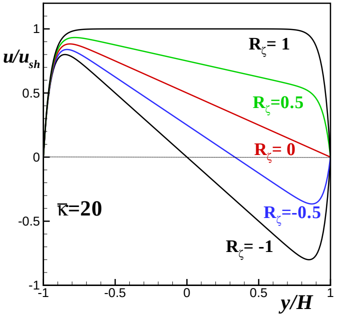

Superposition principle:

$$u = u^E + u^P$$

$$\frac{u(y)}{u_{sh}} = 1 - \overline{\psi}(y) + \frac{1}{2}\Gamma\left(\overline{y}^2 - 1\right)$$

Ratio of Pressure to EO gradient forces:

$$\Gamma = -\frac{H^2}{\epsilon\zeta_1}\frac{p_{,x}}{E_x}$$

- Favourable Pressure gradient $\Gamma < 0$;
- Adverse Pressure gradient $\Gamma > 0$.

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Analytical Solutions - Channel Flow

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Analytical Solutions - Channel Flow

Velocity profiles for mixed driving forces

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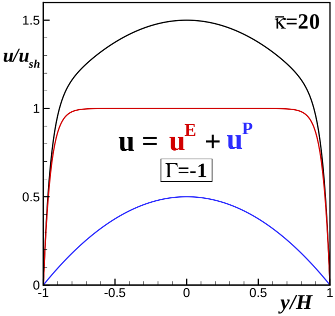

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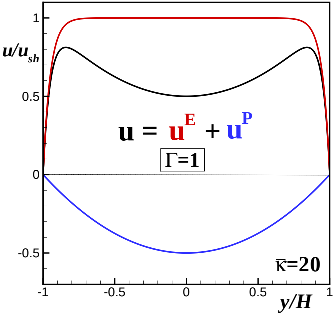

Analytical Solutions - Channel Flow

Viscoelastic fluid (PTT model):

Superposition principle is not valid[1]!

$$u = u^P + u^E + u^{EP}$$

$$u^P = \frac{1}{2}\left[\frac{p_{,x}}{\eta}\right]\left(y^2 - H^2\right)\left[1 + \varepsilon\lambda^2\left[\frac{p_{,x}}{\eta}\right]^2\left(y^2 + H^2\right)\right]$$

$$u^E = \frac{\epsilon\zeta_1 E_x}{\eta}\left[(1 - 2\overline{C}\varepsilon\lambda^2\kappa^2\left[\frac{\epsilon\zeta_1 E_x}{\eta}\right]^2)(\overline{A} - 1) + \frac{2}{3}\varepsilon\lambda^2\kappa^2\left[\frac{\epsilon\zeta_1 E_x}{\eta}\right]^2\left(\overline{A}^3 - 1\right)\right]$$

$$u^{EP} = \frac{3}{2}\varepsilon\lambda^2\left[\frac{\epsilon\zeta_1 E_x}{\eta}\right]^2\left[\frac{p_{,x}}{\eta}\right]\left[1 - \overline{A}^2 + (\kappa^2 H^2 - \kappa^2 y^2)\overline{C} + 2\kappa\overline{D}\left(y\overline{A}\,\overline{B} - H\right)\right]$$
$$+12\frac{\varepsilon\lambda^2}{\kappa^2}\left[\frac{\epsilon\zeta_1 E_x}{\eta}\right]\left[\frac{p_{,x}}{\eta}\right]^2\left[\kappa\overline{D}\left(H - y\overline{B}\right) + (1 + \tfrac{1}{2}\kappa^2 y^2)\overline{A} - (1 + \tfrac{1}{2}\kappa^2 H^2)\right]$$

$\overline{A} = \frac{\cosh(\kappa y)}{\cosh(\kappa H)}$, $\overline{B} = \frac{\sinh(\kappa y)}{\sinh(\kappa H)}$, $\overline{C} = \frac{1}{\cosh^2(\kappa H)}$ and $\overline{D} = \tanh(\kappa H)$.

Deborah number

$$De_\kappa = \frac{\lambda u_{sh}}{\lambda_D} = \lambda\kappa u_{sh}$$

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$$u^{EP} = \frac{3}{2}\varepsilon\lambda^2\left[\frac{\epsilon\zeta_1 E_x}{\eta}\right]^2\left[\frac{p_{,x}}{\eta}\right]\left[1 - \overline{A}^2 + (\kappa^2 H^2 - \kappa^2 y^2)\overline{C} + 2\kappa\overline{D}\left(y\overline{A}\,\overline{B} - H\right)\right]$$

$$+12\frac{\varepsilon\lambda^2}{\kappa^2}\left[\frac{\epsilon\zeta_1 E_x}{\eta}\right]\left[\frac{p_{,x}}{\eta}\right]^2\left[\kappa\overline{D}\left(H - y\overline{B}\right) + (1 + \frac{1}{2}\kappa^2 y^2)\overline{A} - (1 + \frac{1}{2}\kappa^2 H^2)\right]$$

$\overline{A} = \frac{\cosh(\kappa y)}{\cosh(\kappa H)}$, $\overline{B} = \frac{\sinh(\kappa y)}{\sinh(\kappa H)}$, $\overline{C} = \frac{1}{\cosh^2(\kappa H)}$ and $\overline{D} = \tanh(\kappa H)$.

Deborah number

$$De_\kappa = \frac{\lambda u_{sh}}{\lambda_D} = \lambda\kappa u_{sh}$$

[1] Afonso, Alves and Pinho, JNNFM (2009); Oliveira and Pinho, JFM (1999).

Analytical Solutions - Channel Flow

Viscoelastic fluid (PTT model):

Superposition principle is not valid[1]!

$$u = u^P + u^E + u^{EP}$$

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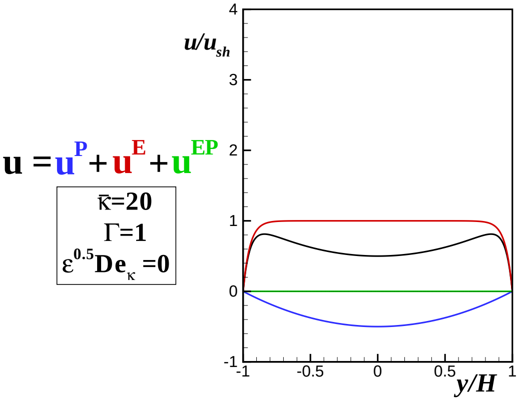

The non-linear term, u^{EP}, increases with $\sqrt{\varepsilon} De_{\kappa}$

Analytical Solutions - Channel Flow

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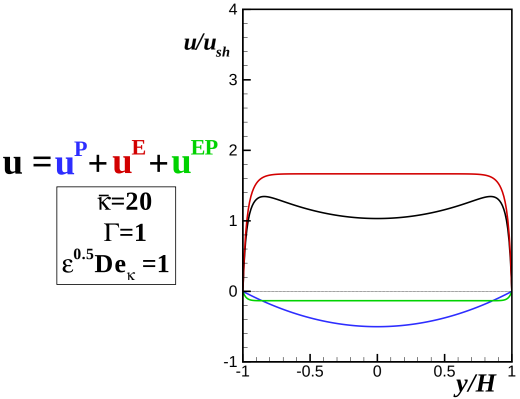

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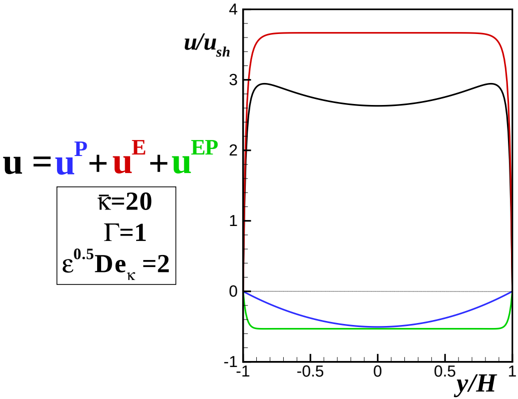

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Finite Volume Method[1]

- Structured, collocated and non-orthogonal meshes.
- Discretization (formally 2nd order)
  - Diffusive terms: central differences (CDS)
  - Advective terms, high resolution scheme: CUBISTA[2]
- Dependent variables evaluated at cell centers;
- Special formulations for cell-face velocities and stresses;
- Log-conformation for the extra-stress tensor[3].
- sinh linearization[4]: $\sinh(X) = \sinh(X)^n + (X^{n-1} - X^n)\cosh(X)^n$

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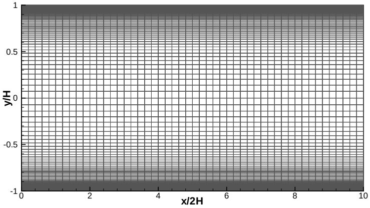
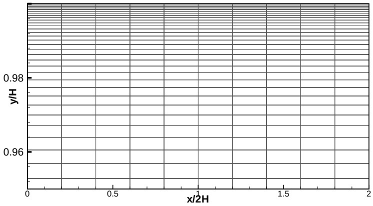


Computational meshes

	nº cells	$\triangle x_{min}$	$\triangle y_{min}$x10^{-4}
$M1$	1800	0.2	8
$M2$	3600	0.2	4
$M3$	7200	0.2	2



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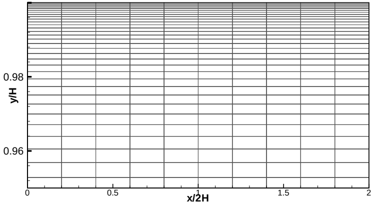

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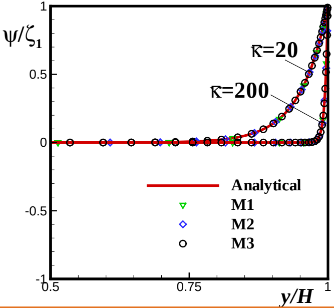
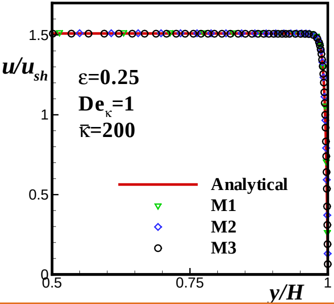
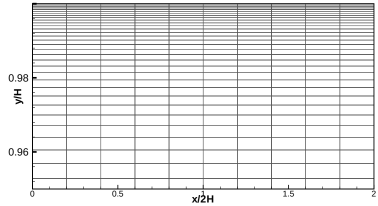




Numerical Solutions

Channel Flow - Mesh convergence



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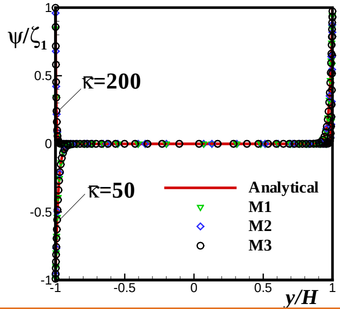
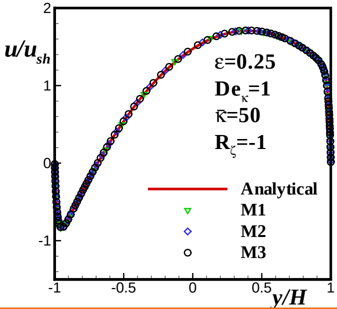
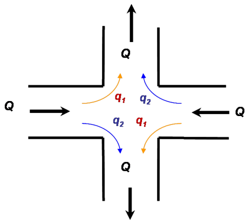




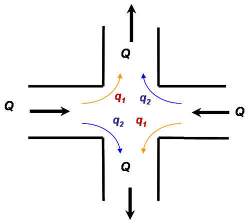


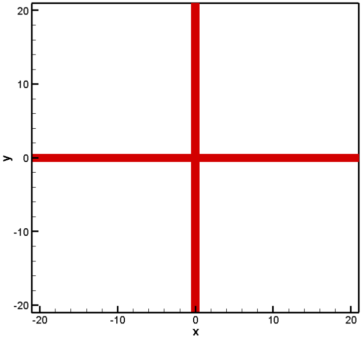
Computational mesh (same refinement of M1)

	nº cells	$\triangle x_{min}$x10^{-4}	$\triangle y_{min}$x10^{-4}
MCS	12801	4	4

Numerical Solutions

Cross Slot: meshes





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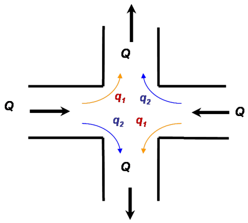

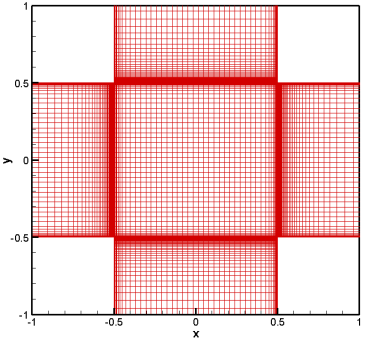

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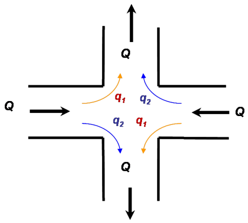

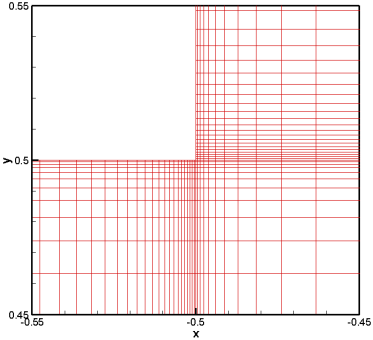

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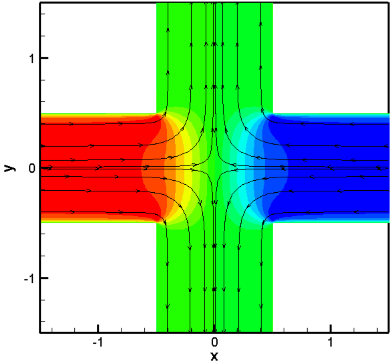
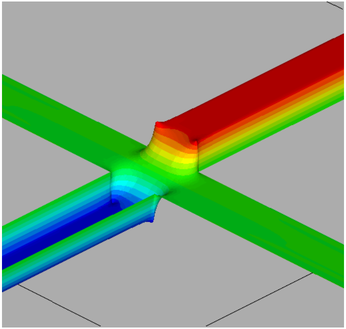
Numerical Solutions

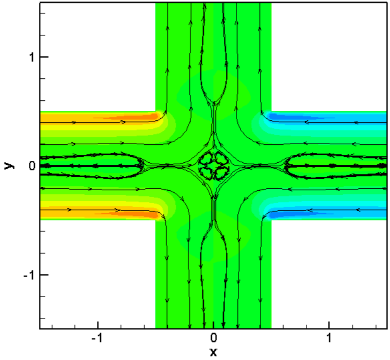
Pure newtonian EOF: $(\Gamma \simeq 0)$

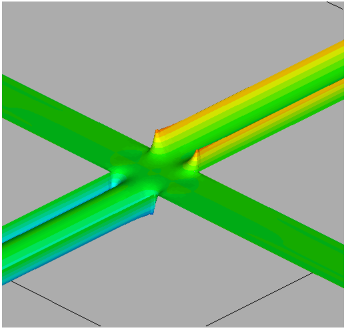




Numerical Solutions

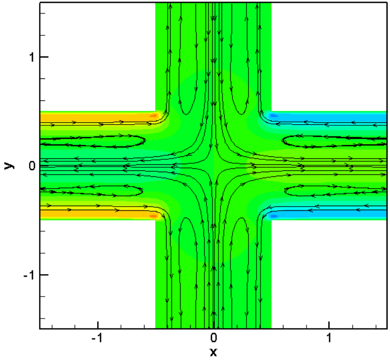
Adverse pressure gradient: $(\Gamma \simeq 2)$

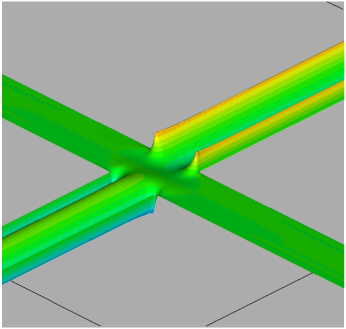




Numerical Solutions

Adverse pressure gradient: $(\Gamma \simeq 2.5)$



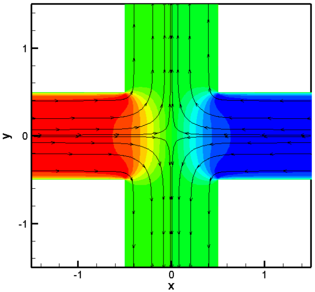


Numerical Solutions

Creeping flow of pure Viscoelastic EOF ($\Gamma \simeq 0$) using UCM ($\varepsilon = 0$)

Deborah numbers (κ=40 and h=H/2)

$De_\kappa = \lambda u_{sh} \kappa$	$De_\kappa = \frac{\lambda u_{sh}}{h}$
0	0
2	0.1
4	0.2
5	0.25
5.5	0.275
6	0.3



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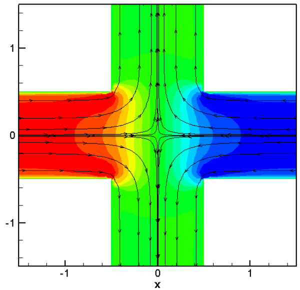

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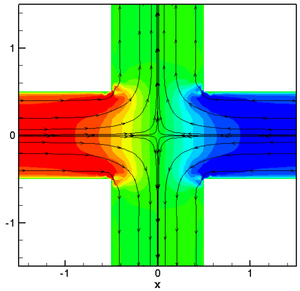

Numerical Solutions

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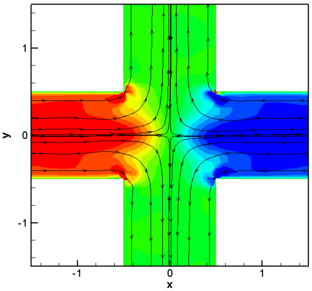

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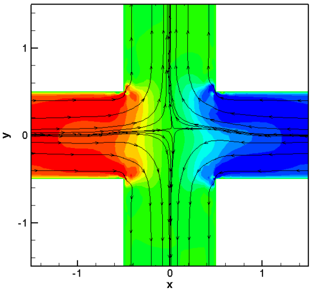

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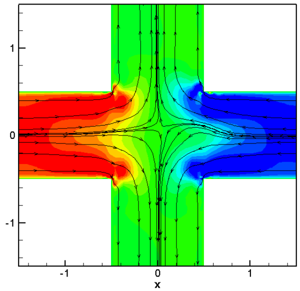
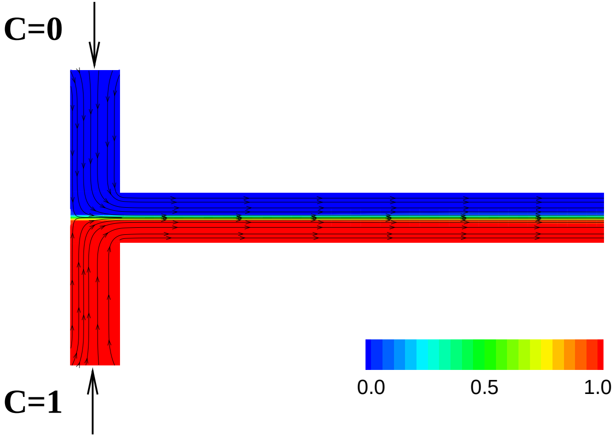


Numerical Solutions

Mixing in a T-channel



Creeping flow, $Re_\kappa = \frac{\rho u_{sh}}{\eta \kappa} \ll 1$, and low diffusivity $Pe_\kappa = \frac{u_{sh}}{D\kappa} = 10^4$,

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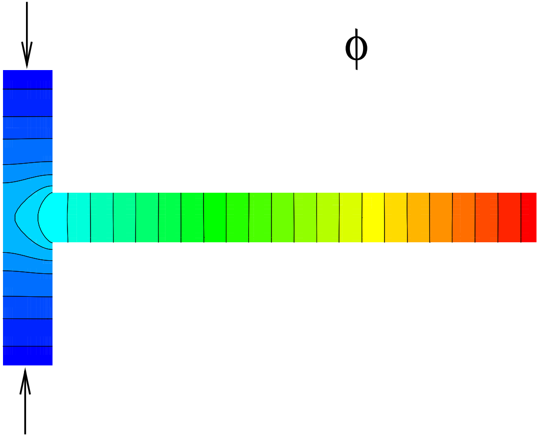
Numerical Solutions
The electric field



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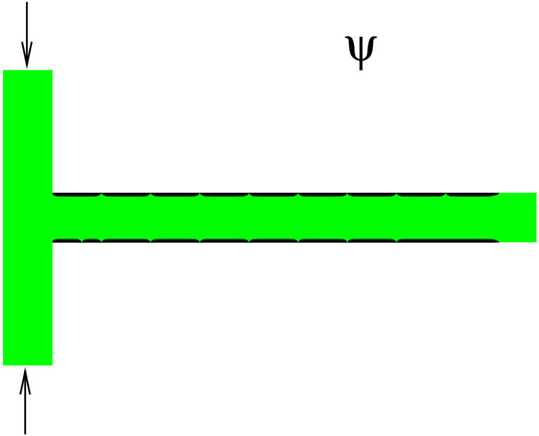
Numerical Solutions

ψ pattern in the walls



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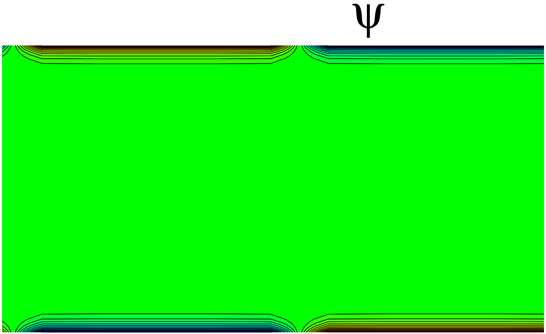
Numerical Solutions

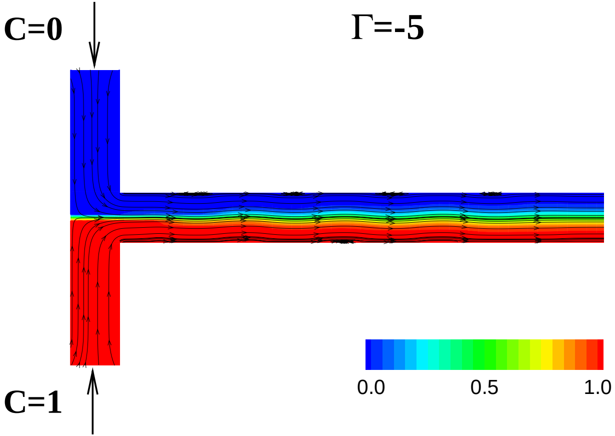
ψ pattern in the walls (detail view)



Creeping flow, $Re_\kappa = \frac{\rho u_{sh}}{\eta\kappa} \ll 1$, and low diffusivity $Pe_\kappa = \frac{u_{sh}}{D\kappa} = 10^4$, $\overline{\kappa} = 20$

Numerical Solutions

Increasing external electric potential (decreasing Γ)



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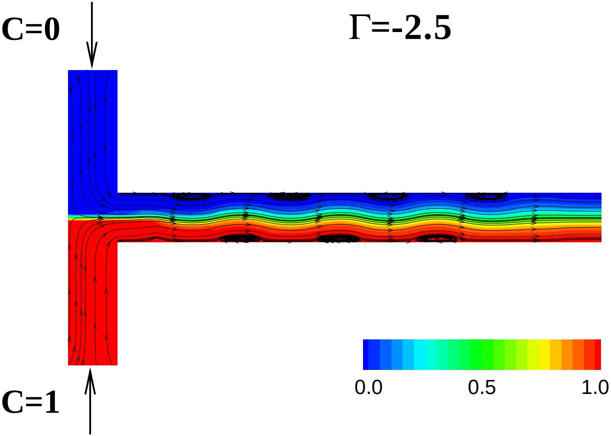

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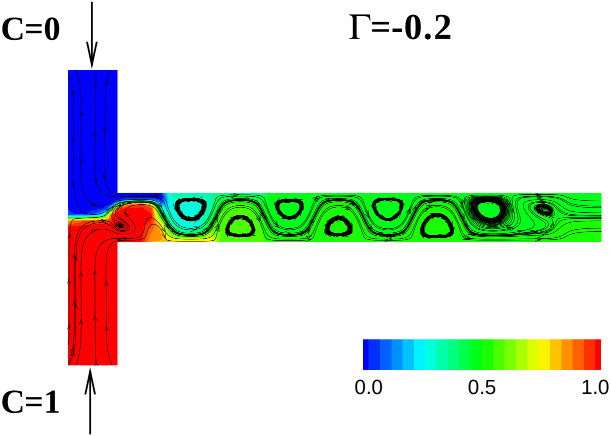

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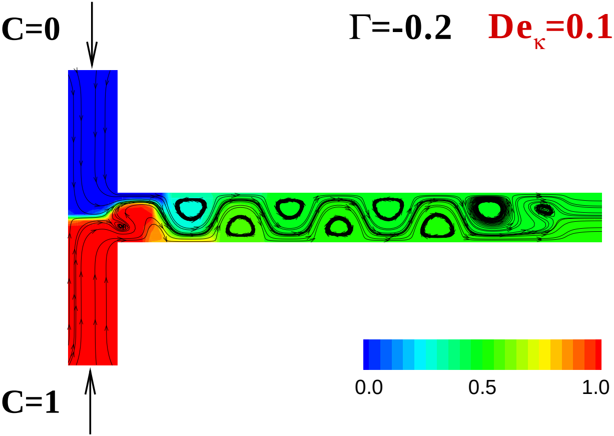

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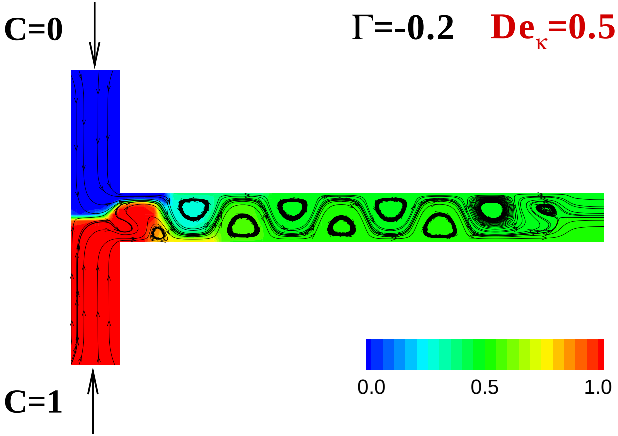

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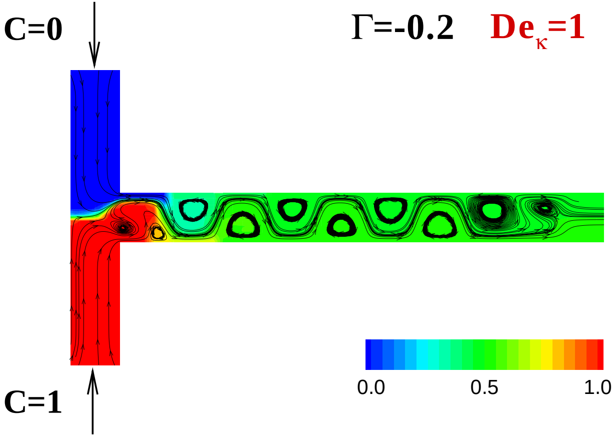

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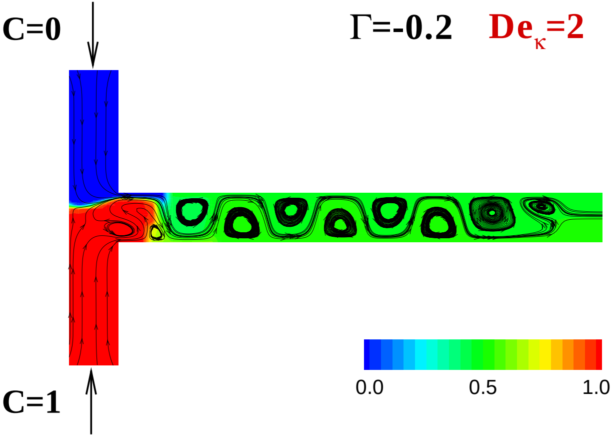

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Conclusions

Analytical solutions

- Superposition principle is not valid for viscoelastic fluids;
- Velocity increases with elasticity ($\sqrt{\varepsilon} De_\kappa$).

Numerical solutions

- Excellent agreement with analytical solutions;
- Sharp refinement near the EDL (Alternative: Viscoelastic Helmholtz-Smoluchowski Velocity at the wall (Slip velocity)[1]);

EOF of viscoelastic fluids

- is an open field to explore;
- Electrokinetic instabilities (EKI) even for Newtonian fluids[2]
  - EKI+ elastic instabilities!!

[1]Park and Lee, JCIS (2009)[1]Oddy, PhD Thesys (2005)

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Acknowledgements

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Thanks!

Questions?