Numerical Studies of Electro-Osmotic flows of Viscoelastic fluids

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

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[2] Departamento de Engenharia Mecânica e Gestão Industrial, CEFT, Faculdade de Engenharia da Universidade do Porto, Portugal, fpinho@fe.up.pt

Outline

1. Introduction
   - Electro-Osmotic Flow (EOF): Theory
2. Governing Equations
   - EOF of Viscoelastic Fluid
   - Electrokinetics
3. Numerical Solutions
   - Channel flows
   - Complex geometries
4. Conclusions

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Electro-Osmotic Flow (EOF)

Surface charge

Surface charge:

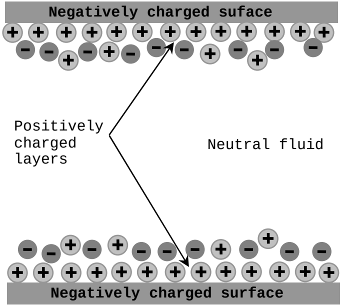
- Solution of ions
- Overall charge neutrality

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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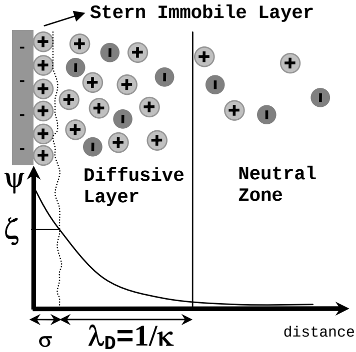

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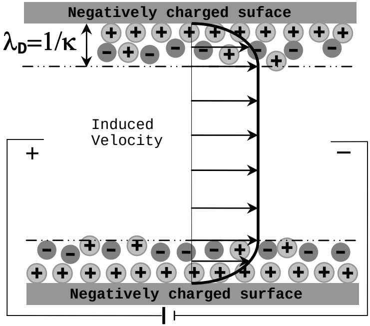

Aplications:

- micro flow injection analysis, microfluidic chromatography, microreactors, microenergy, microelectronic cooling systems and micro-mixing.

Interesting Flow Instabilities:

- Newtonian fluids[1].
- Viscoelastic fluids[2].

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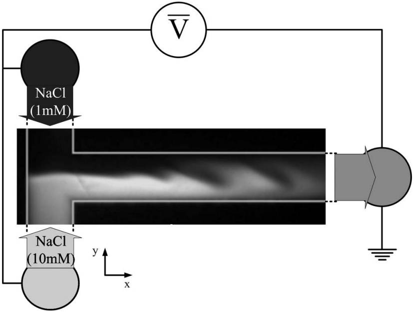

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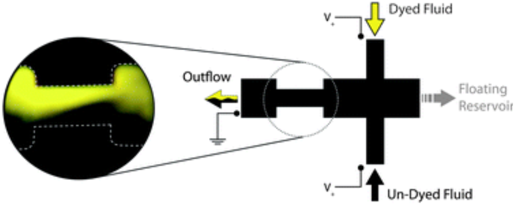

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Mass Conservation:

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

Momentum Conservation:

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} - \rho_e \nabla (\phi + \psi)$$

Constitutive Equation:

$$f(\tau_{kk})\boldsymbol{\tau} + \lambda \overset{\nabla}{\boldsymbol{\tau}} = 2\eta \mathbf{D} \qquad \overset{\nabla}{\boldsymbol{\tau}} = \frac{D\boldsymbol{\tau}}{Dt} - \boldsymbol{\tau}.\nabla\mathbf{u} - \nabla\mathbf{u}^T.\boldsymbol{\tau}$$

Phan-Thien & Tanner (PTT)

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

Upper Convected Maxwell (UCM)

$$\varepsilon = 0 \Rightarrow f(\tau_{kk}) = 1$$

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Nernts-Plankt Equations

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

$$\nabla^2 \psi = -\frac{ez}{\epsilon} (n^+ - n^-)$$

$$\rho_e = ez (n^+ - n^-)$$

$$\frac{\partial n^\pm}{\partial t} + \mathbf{u} \cdot \nabla n^\pm = \nabla \cdot (D^\pm \nabla n^\pm) \pm \nabla \cdot \left[D^\pm n^\pm \frac{ez}{k_B T} \nabla \Phi \right]$$

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Poisson-Boltzmann Equations (PB)

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

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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]: $\mathtt{sinh(X)}=\mathtt{sinh(X)}^{n}+(\mathtt{X}^{n-1}-\mathtt{X}^{n})\mathtt{cosh(X)}^{n}$

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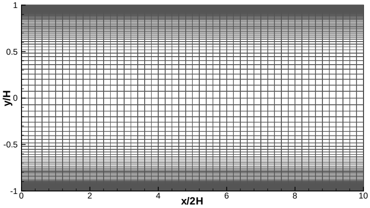

Computational meshes

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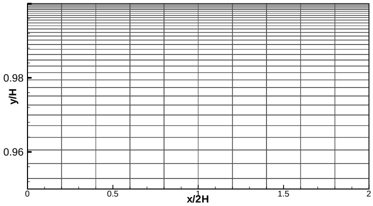

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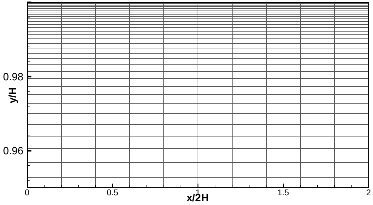

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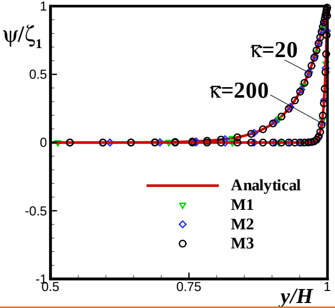

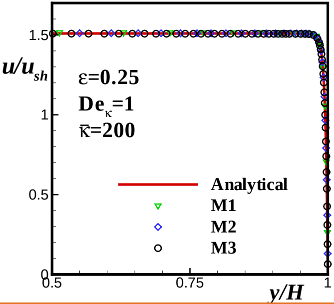

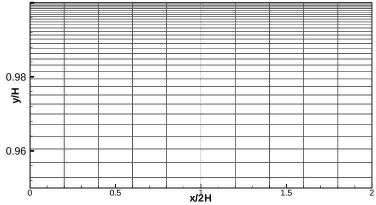

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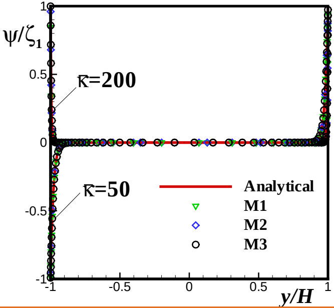
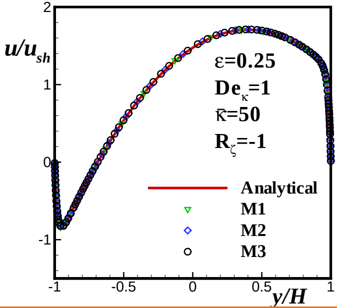
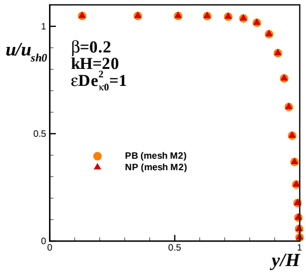
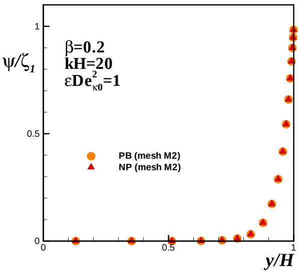




Numerical Solutions

Channel Flow - NP/PB equations





Analytical Solution

$$\frac{u(y)}{u_{sh_0}} = \frac{1}{\beta}\left(1 - \frac{\sinh(\bar{\kappa}y)}{\cosh(\bar{\kappa})} - (1-\beta)\left[\Omega(1) - \frac{\sinh(\bar{\kappa}y)}{\cosh(\bar{\kappa})}\Omega(y)\right]\right)$$

$$\Omega(y) = \sum_{n=0}^{\infty}\left[\frac{\left(\frac{1}{3}\right)_n\left(\frac{1}{2}\right)_n\left(\frac{2}{3}\right)_n}{\left(\frac{3}{2}\right)_n\left(\frac{3}{2}\right)_n}\frac{\left(-\frac{27}{2}\beta\varepsilon De_{\kappa_0}^2\left(\frac{\sinh(\bar{\kappa}y)}{\cosh(\bar{\kappa})}\right)^2\right)^n}{n!}\right]$$

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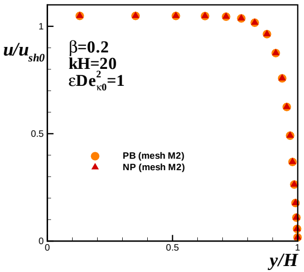

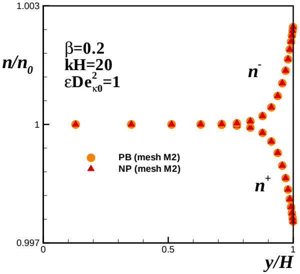

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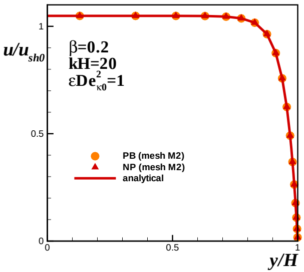

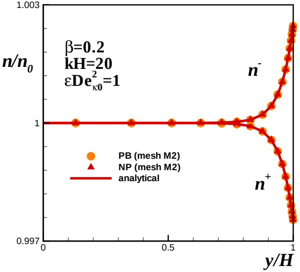

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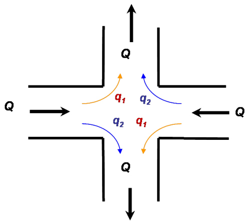

Computational mesh (same refinement of M1)

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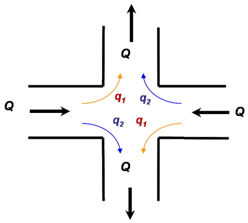
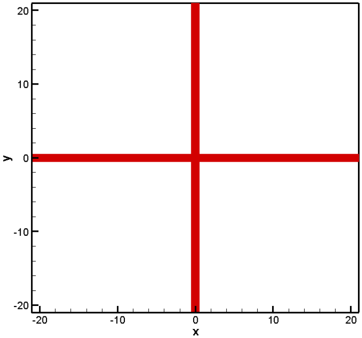
Numerical Solutions

Cross Slot: meshes





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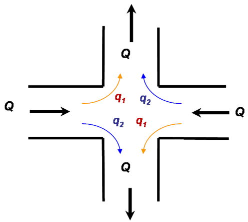

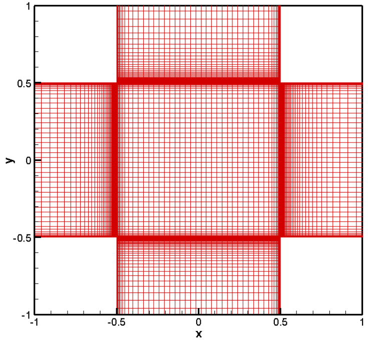

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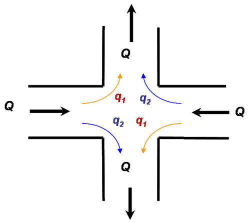
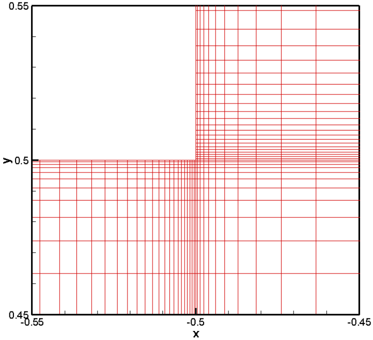


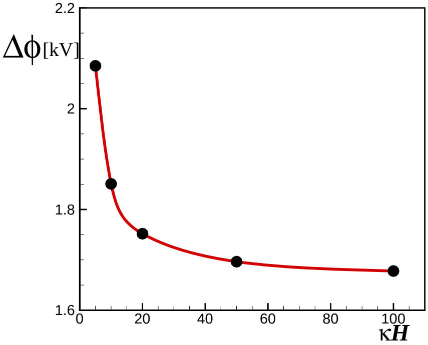


Computational mesh (same refinement of M1)

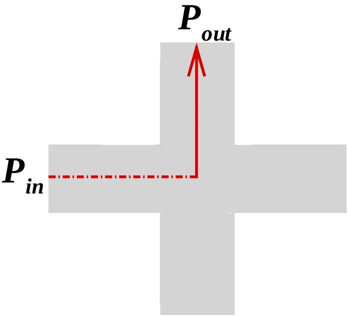
	nº cells	$\triangle x_{min}$x10^{-4}	$\triangle y_{min}$x10^{-4}
MCS	12801	4	4

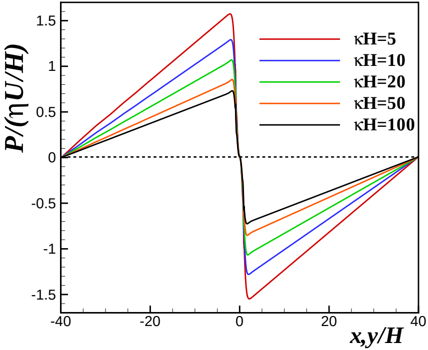
Numerical Solutions

Pure newtonian EOF: external potential

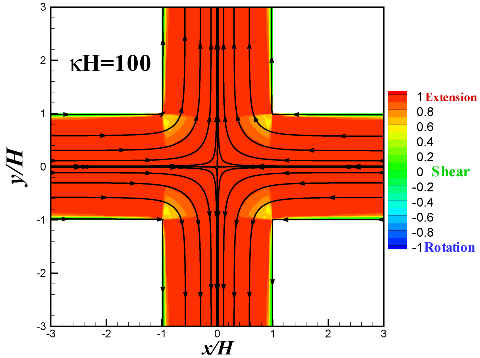


Numerical Solutions
Pressure profiles in the Cross-slot



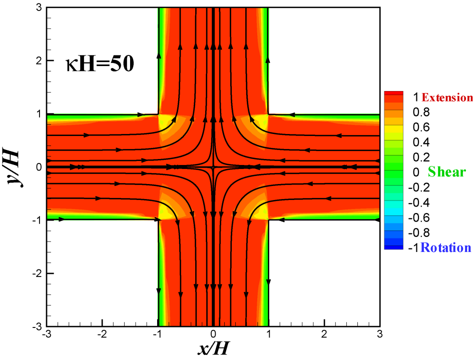


Effect of Debye Layer size ($\kappa H = 100$)

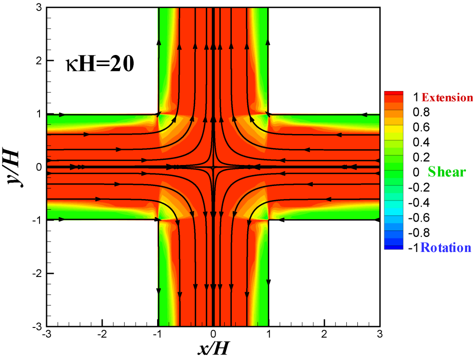


Numerical Solutions

Effect of Debye Layer size ($\kappa H = 50$)

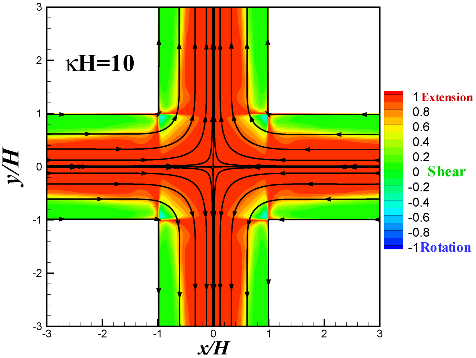


Effect of Debye Layer size ($\kappa H = 20$)

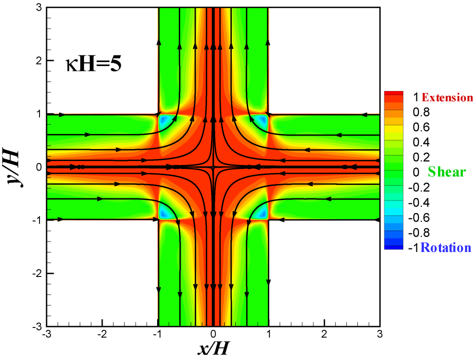


Numerical Solutions

Effect of Debye Layer size ($\kappa H = 10$)



Effect of Debye Layer size ($\kappa H = 5$)

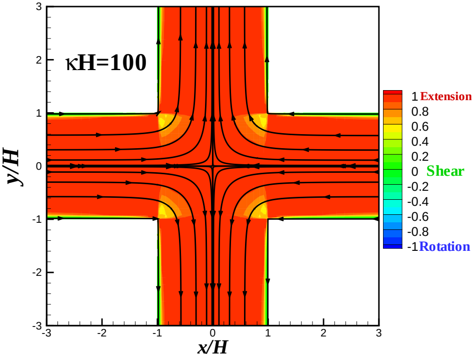


Numerical Solutions

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

Results κH=100

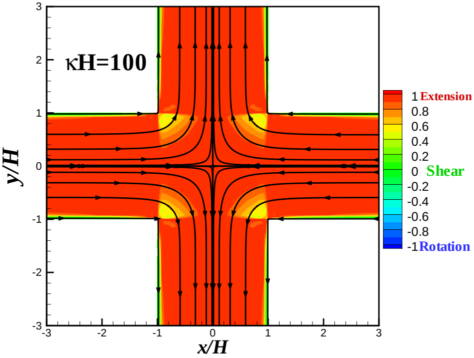
$De_\kappa = \lambda U \kappa$	$De_H = \frac{\lambda U}{H}$
0	0
1	0.01
2	0.02
3	0.03
4	0.04
4.88	0.0488
4.9	0.049
5	0.05
10	0.1



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

Results κH=100

$De_\kappa = \lambda U \kappa$	$De_H = \frac{\lambda U}{H}$
0	0
1	0.01
2	0.02
3	0.03
4	0.04
4.88	0.0488
4.9	0.049
5	0.05
10	0.1



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0	0
1	0.01
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4.9	0.049
5	0.05
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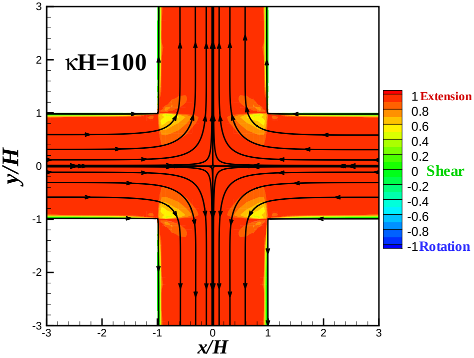

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$De_\kappa = \lambda U \kappa$	$De_H = \frac{\lambda U}{H}$
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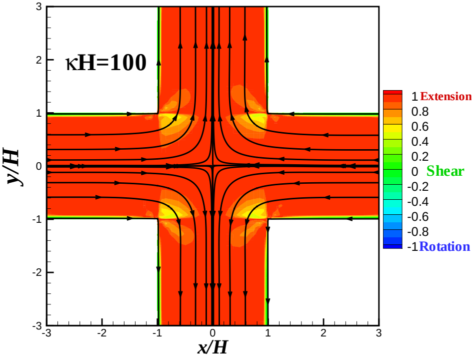
1	0.01
2	0.02
3	0.03
4	0.04
4.88	0.0488
4.9	0.049
5	0.05
10	0.1



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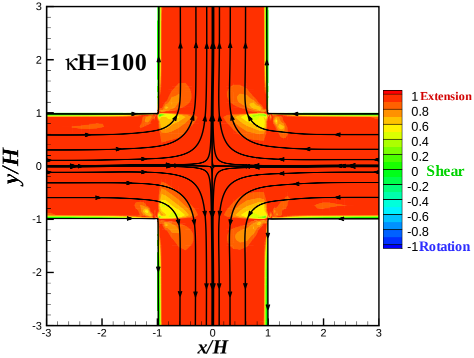
10	0.1



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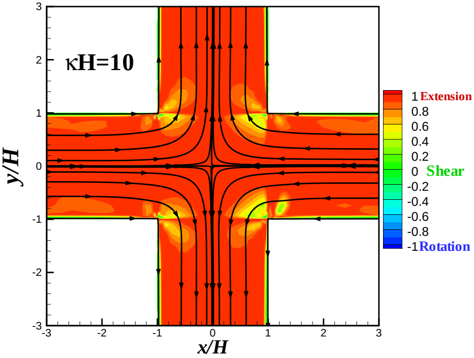

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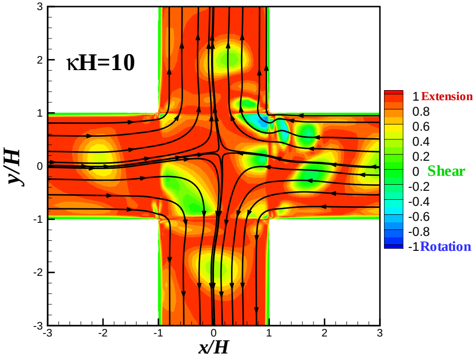

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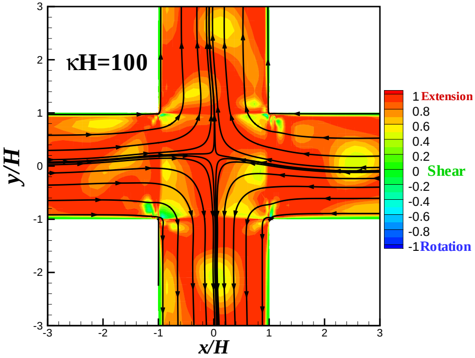

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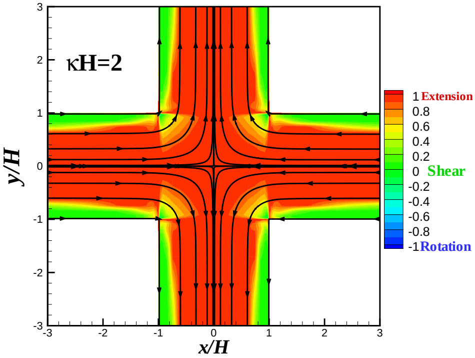
5	0.05
10	0.1

Results κH=20

$De_\kappa = \lambda U \kappa$	$De_H = \frac{\lambda U}{H}$
0	0
0.8	0.04
2.	0.1
4	0.2
4.6	0.23
4.7	0.235
4.8	0.24



Numerical Solutions

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

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0.8	0.04
2.	0.1
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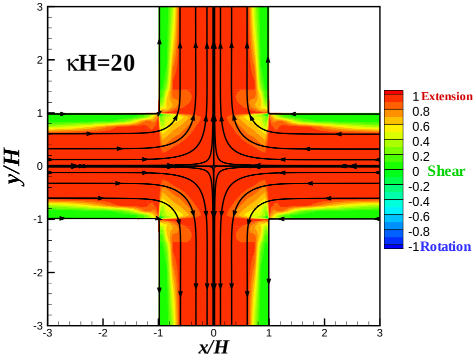

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0	0
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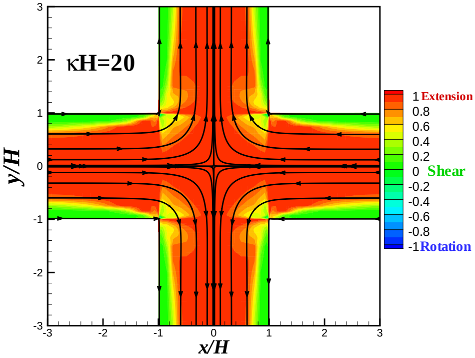

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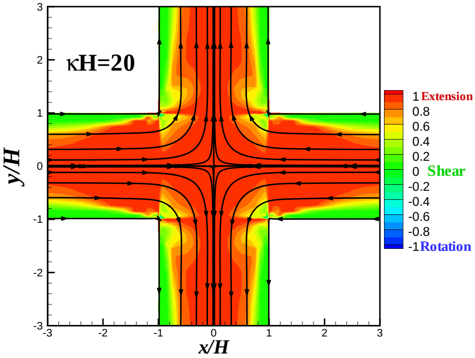

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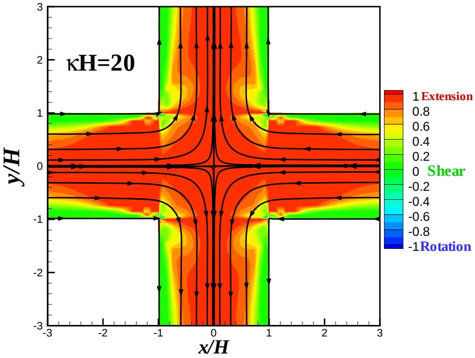

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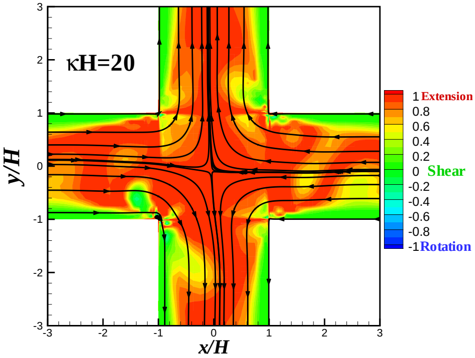

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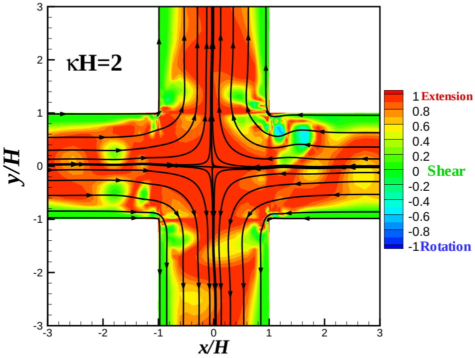
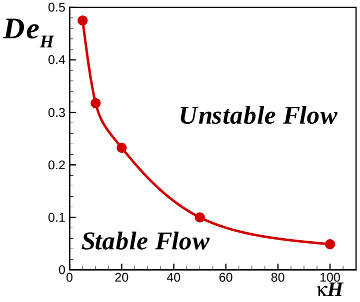
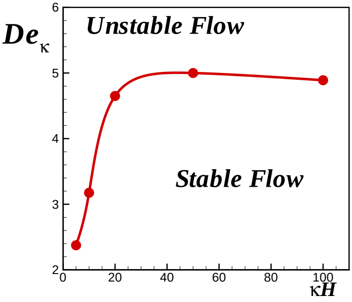


Numerical Solutions

Stability Maps: De.vs.κH





Conclusions

Numerical solutions

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

Elastic instabilities

- Elastic instabilities present in the viscoelastic EOF flow in Cross-Slot geometry;
- The critical Deborah number increased with Debye layer relative size (κH);
- No steady assymetric flow [2] were obtained, rounded corners are needed;

[1] Park and Lee, JCIS (2009) [2] Poole, Alves and Oliveira, PRL (2007)

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- Fundação para a Ciência e a Tecnologia (FCT), Portugal:
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  - Scholarship SFRH/BD/28828/2006 (A.M. Afonso).

Thanks!

Questions?