Efficient numerics of non-isothermal highly viscous multiphase flows for the simulation of the production process of graded micro foams

FEM Multigrid Techniques for Viscoelastic Flow

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Nonlinear Flow Models

Generalized Navier-Stokes equations

$$\rho \frac{\partial u}{\partial t} + u \cdot \nabla u - \nabla \cdot \sigma + \nabla p = \rho f \quad , \quad \nabla \cdot u = 0,$$

$$\frac{\partial \Theta}{\partial t} + u \cdot \nabla \Theta - \nabla \cdot (k \nabla \Theta) - D : \sigma,$$

$$\sigma = \sigma^s + \sigma^p \quad , \quad D = \frac{1}{2} \left(\nabla u + (\nabla u)^{\mathrm{T}} \right).$$

Quasi-Newtonian part $\sigma^s = 2\eta_s(D_{\mathrm{II}}, \Theta) D \quad , \quad D_{\mathrm{II}} = tr(D^2).$

Viscoleastic part

$$\sigma^p + \Lambda \frac{\delta_a \sigma^p}{\delta t} = 2\eta_p D,$$

$$\frac{\delta_a \sigma^p}{\delta t} = \left(\frac{\partial}{\partial t} + u \cdot \nabla \right) \sigma + \frac{1-a}{2} \left(\sigma \nabla u + (\nabla u)^{\mathrm{T}} \sigma \right)$$

$$- \frac{1+a}{2} \left(\nabla u \sigma + \sigma (\nabla u)^{\mathrm{T}} \right).$$

Required: 1. Special Models

$$T + \Lambda \frac{\delta_a T}{\delta t} = 2\,\eta_0 \left(D + \Lambda_r \frac{\delta_a D}{\delta t} \right)$$

Oldroyd A

Oldroyd B

Maxwell A

Maxwell B

Jeffreys

$$T + \Lambda \frac{\delta_a T}{\delta t} + B(T) = 2\eta D$$

Phan-Thien Tanner

Phan-Thien

Giesekus

Required: 2. Special Numerics

Special FEM Techniques

Multigrid Solvers

Stabilization for high Re and Wi Numbers

Implicit Approaches

Space-Time Adaptivity

Grid Deformation Methods

Newton Methods

Our Numerical Approach

Fully implicit monolithic multigrid FEM solver

Numerical Techniques:

FEM discretization

- Stable FE spaces — $Q_2/P_1/(?)$
  - velocity / pressure — $\tilde{Q}_1/P_0/(?)$
  - velocity / extra-stress — $\tilde{Q}_2/P_1/(?)$

- Special treatment of the convective terms

$$u \cdot \nabla u\,,\; u \cdot \nabla \Theta\,,\; u \cdot \nabla \sigma$$

edge-oriented/interior penalty FEM, TVD/FCT

Numerical Techniques:

Solvers

- The nonlinear solver has to deal with different source of nonlinearity
  - Nonlinear viscosities: Newton method via divided differences
  - Strong coupling of equations: Monolitic multigrid approach

Numerical Techniques:

Problem formulation

- The reactive term

$$\frac{1-a}{2}\left(\sigma\nabla u+(\nabla u)^{\mathrm{T}}\sigma\right)-\frac{1+a}{2}\left(\nabla u\,\sigma+\sigma(\nabla u)^{\mathrm{T}}\right.$$

is responsible for

- High weissenberg number problem (HWNP)
- Blow up phenomena for time dependent solution

Newton Solver

Solve for the residual of the nonlinear system algebraic equations

$$R(\mathbf{x}) = 0 \quad , \quad \mathbf{x} = (u, \Theta, \sigma, p)$$

Newton method with damping results in iterations of the form

$$\mathbf{x}^{n+1} = \mathbf{x}^n + \omega^n \left[\frac{\partial R(\mathbf{x}^n)}{\partial \mathbf{x}} \right]^{-1} R(\mathbf{x}^n)$$

- Continuous Newton: on variational level (before discretization)

→ The continuous Frechet operator can be calculated

- Inexact Newton: on matrix level (after discretization)

→ The Jacobian matrix is **approximated** using finite differences as

$$\left[\frac{\partial R(\mathbf{x}^n)}{\partial \mathbf{x}} \right]_{ij} \approx \frac{R_j(\mathbf{x}^n + \epsilon e_j) - R_i(\mathbf{x}^n - \epsilon e_i)}{2\epsilon}$$

Multigrid Solver

- Standard geometric multigrid approach
- Full $Q_2, \tilde{Q}_1, P_1^{\text{disc}}$ and P_0 grid transfer
- Smoother: Local/Global MPSC

Coupled multigrid solver: Local MPSC via Vanka-like smoother

$$\begin{bmatrix} u^{l+1} \\ \sigma^{l+1} \\ \Theta^{l+1} \\ p^{l+1} \end{bmatrix} = \begin{bmatrix} u^{l} \\ \sigma^{l} \\ \Theta^{l} \\ p^{l} \end{bmatrix} + \omega^l \, [K+S]_T^{-1} \begin{bmatrix} Res_u \\ Res_\sigma \\ Res_\Theta \\ Res_p \end{bmatrix}_T$$

Decoupled multigrid solver: Global MPSC

- solve for an intermediat $\tilde{\mathbf{u}}$ (generalized momentum equation)
- Solve for $\mathbf{p}$

  pressure Poisson equation
- Update of $\mathbf{u}$ and $\mathbf{p}$ incompressibility condition
- Solve for $\boldsymbol{\Theta}$ energy equation
- Solve for σ constitutive equation

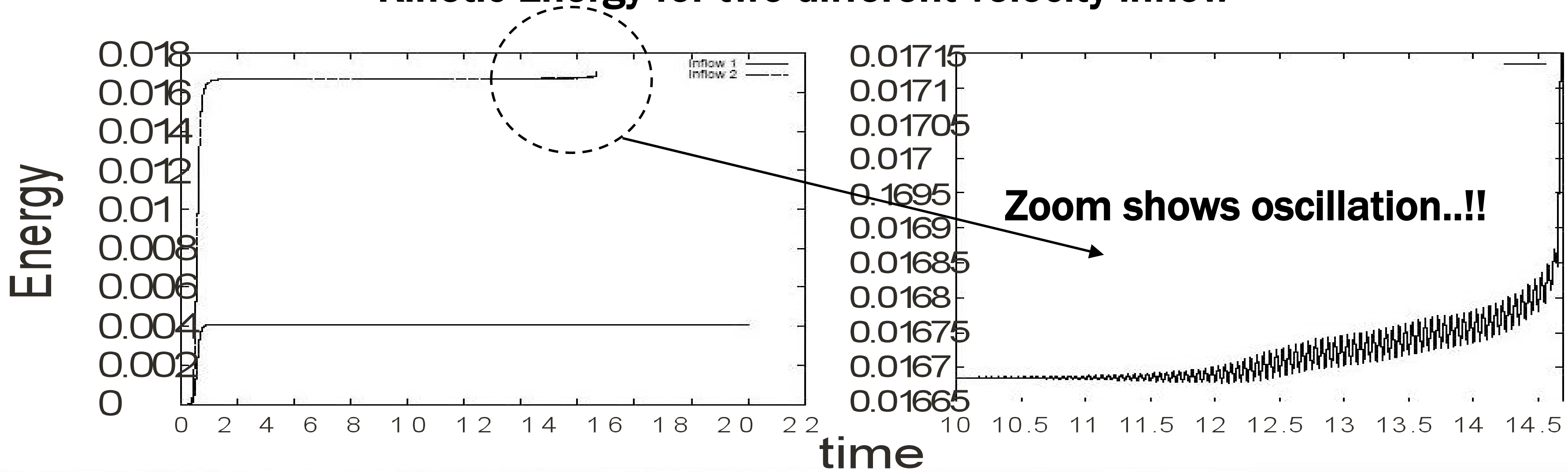
Viscoelastic Models

Different highly developed models

Oldroyd A/B, Maxwell A/B, Jeffreys, PTT, Giesekus

…nevertheless, despite „good“ models and „good“ Numerics, the HWNP („High Weissenberg Number problem“) stills exists for critical Wi, resp., De numbers…

Kinetic Energy for two different velocity inflow



Problem Reformulation

Standard rate-type non-Newtonian formulation → (u, p, σ^p)

$$\left.\begin{aligned} \rho\left(\frac{\partial u}{\partial t} + u\cdot\nabla u\right) = \nabla p - 2\eta_s \nabla\cdot D - \frac{\eta_p}{\Lambda}\nabla\cdot\sigma^p, \\ \nabla\cdot u = 0, \\ \frac{\delta_a \sigma^p}{\delta t} + \Lambda(\sigma^p - \mathbf{I}) = 0. \end{aligned}\right\} \quad (1)$$

Conformation tensor: **Using the identity** $\frac{\delta_a \mathbf{I}}{\delta t} = -2aD$

Change of variable $\sigma^p = \frac{\eta_p}{\Lambda a}(\tau - \mathbf{I})$

$$\left.\begin{aligned} \rho\left(\frac{\partial u}{\partial t} + u\cdot\nabla u\right) = \nabla p - 2\eta_s \nabla\cdot D - \frac{\eta_p}{\Lambda}\nabla\cdot\tau, \\ \nabla\cdot u = 0, \\ \frac{\delta_a \tau}{\delta t} + \Lambda(\tau - \mathbf{I}) = 0. \end{aligned}\right\} \quad (2)$$

This tensor is symmetric and positive definite

For large class of constitutive equations !!

Properties of Conformation Tensor

$$\tau(X,t) = \int_{\infty}^{t} \frac{\eta_p}{\Lambda} \exp\left(\frac{-(t-s)}{\sqrt{\Lambda}}\right) F(s,t)F(s,t)^{\mathrm{T}}\, ds$$

Positive by design,
so we can take its logarithm

Observations:

- positive definite → positive preserving discretizations : FCT/TVD
- exponential behaviour → approximation by polynomials???

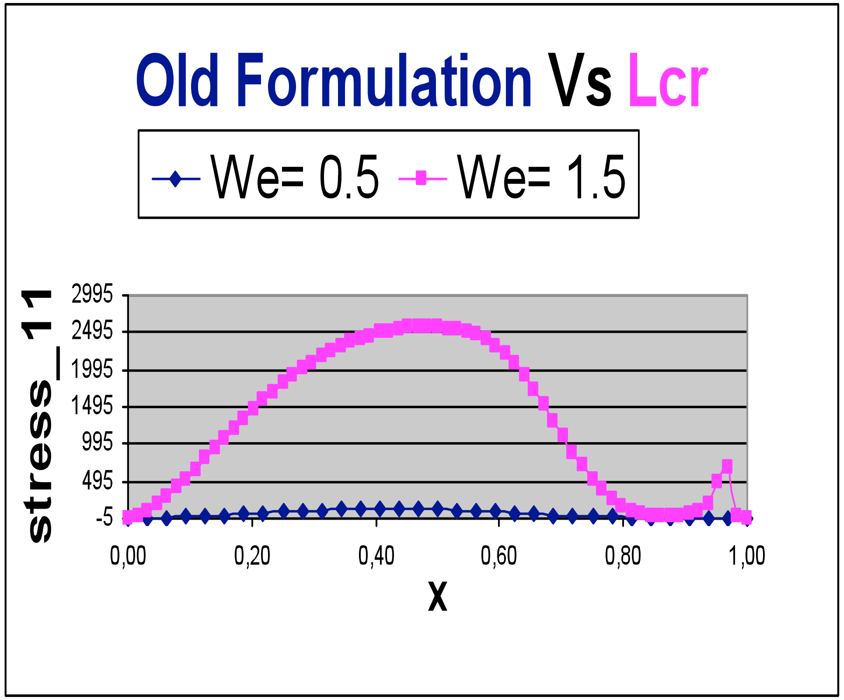
Numerical experiences:

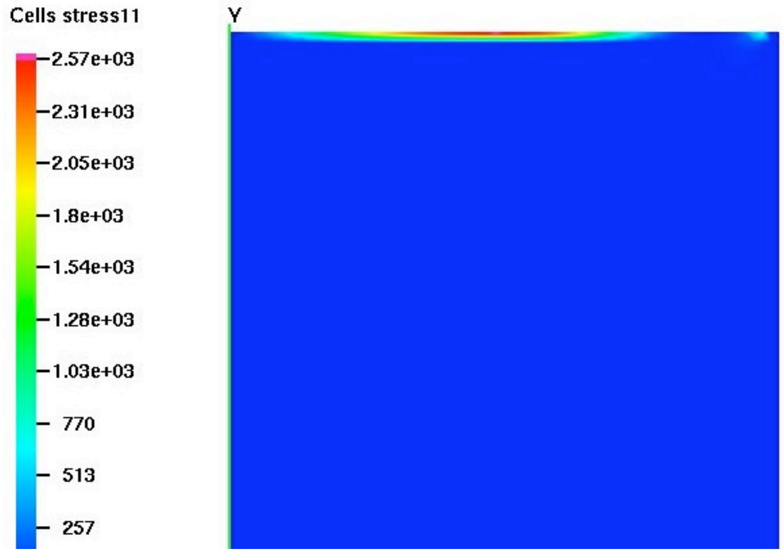
- Stresses grow exponentially
- Stretching part creates numerical problem

$$\frac{1-a}{2}\left(\sigma\nabla u + (\nabla u)^{\mathrm{T}}\sigma\right) - \frac{1+a}{2}\left(\nabla u\,\sigma + \sigma(\nabla u)^{\mathrm{T}}\right.$$

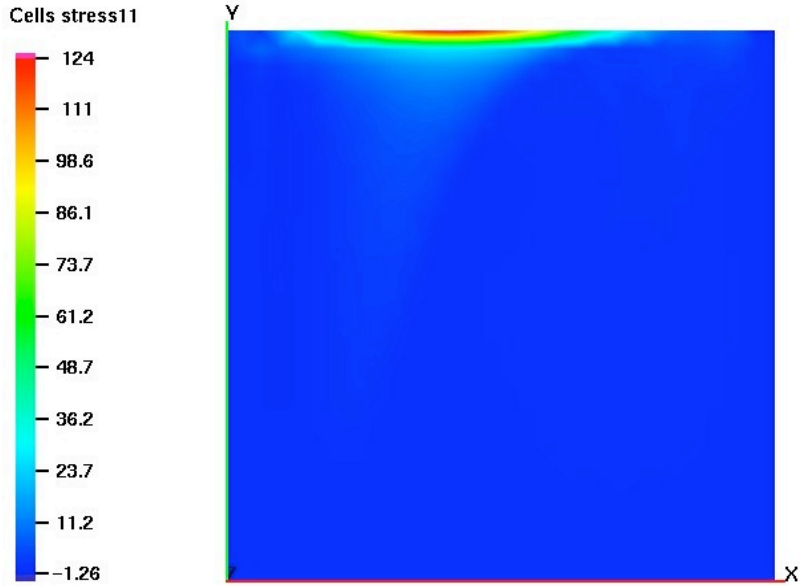
Driven Cavity

Cutline of Stress_11 component at y = 1.0





(LCR)



(Old)

LCR Formulation (I)

Direct change of variable $\tau = \exp\psi$ in the conformation tensor constitutive equation (the idea is due to M. Behr)

$$\left.\begin{aligned} \rho\left(\frac{\partial u}{\partial t} u \cdot \nabla u\right) = \nabla p - 2\eta_s \nabla \cdot D - \frac{\eta_p}{\Lambda}\nabla \cdot \exp\psi, \\ \nabla \cdot u = 0, \\ \frac{\delta_a \exp\psi}{\delta t} + \frac{1}{\Lambda}(\exp\psi - \mathbf{I}) = 0. \end{aligned}\right\} \quad (3)$$

Gradient of exponential of ψ $\Diamond$ $???$

Solvers → ???

LCR Formulation (II)

The change of variable $\tau = \exp \psi$ as an evolution equation for the purely extension part of ∇u (the idea is due to Kupferman)

- Decompose the velocity gradient into a purely extension and commutable part B and to a purely rotation part Ω

$$\nabla u = \Omega + B + N\tau^{-1}$$

using the eigenvalue problem

$$\psi = R \log(\lambda_r) R^{\mathrm{T}}$$

- The conformation tensor equation can be rewriten as

$$\left(\frac{\partial}{\partial t} + u \cdot \nabla\right)\tau - (\Omega\tau - \tau\Omega) + 2\,B\tau = \frac{1}{\Lambda}(1-\tau)$$

LCR Formulation (II)

$$\frac{\partial \tau}{\partial t} = 2B\tau \Longrightarrow \frac{\partial \psi}{\partial t} = 2B$$

$$\left.\begin{aligned}(\Omega\tau + \tau\Omega)^{\mathrm{T}} &= (\Omega\tau + \tau\Omega)\\ \tfrac{\partial \tau}{\partial t} &= (\Omega\tau + \tau\Omega)\end{aligned}\right\} \Longrightarrow \frac{\partial \psi}{\partial t} = (\Omega\psi + \psi\Omega)$$

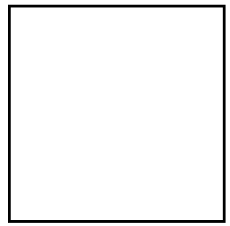
$$\left.\begin{aligned}\rho\left(\frac{\partial u}{\partial t} + u\cdot\nabla u\right) &= \nabla p - 2\eta_s \nabla\cdot D - \frac{\eta_p}{\Lambda}\nabla\cdot\tau,\\ \nabla\cdot u &= 0,\\ \left(\frac{\partial}{\partial t} + u\cdot\nabla\right)\psi - (\Omega\psi - \psi\Omega) + 2B &= \frac{1}{\Lambda}(\exp(-\psi) - \mathbf{I}).\end{aligned}\right\} \quad (4)$$

→ **Increases the critical Wi number dramatically !!**

Numerical Results:

steady problem tests

1. **Driven cavity**



Velocity profile at the upper wall: $v_{in} \; x^2(1-x)^2$

Dirichtlet Bc's everywhere $v_{in} = 16$

Stress field: Neuman Bc's

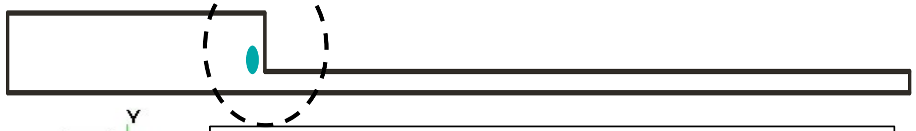
2. **4 to 1 contraction**

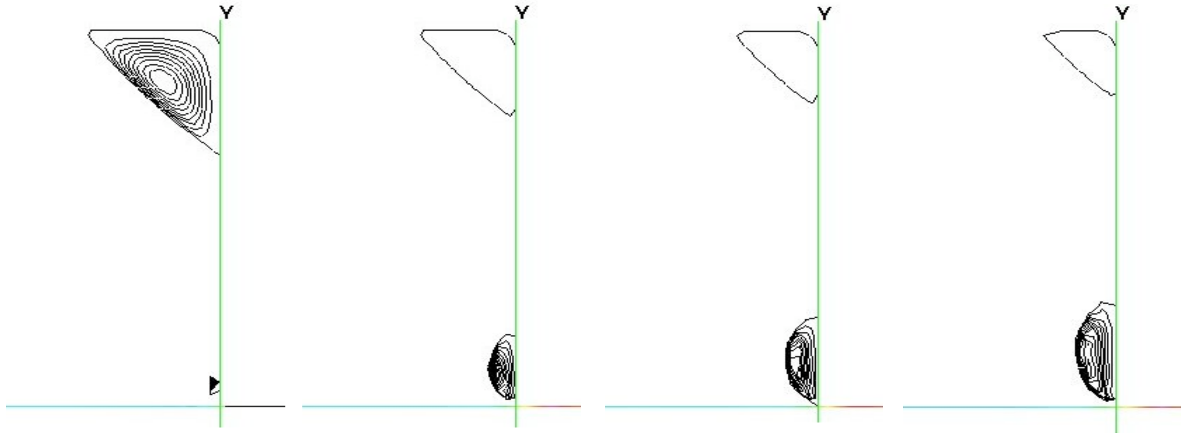
Velocity profile at the inlet: $\frac{3}{128} v_{in} \left(16 - y^2\right)$

Out flow: Neuman Bc's

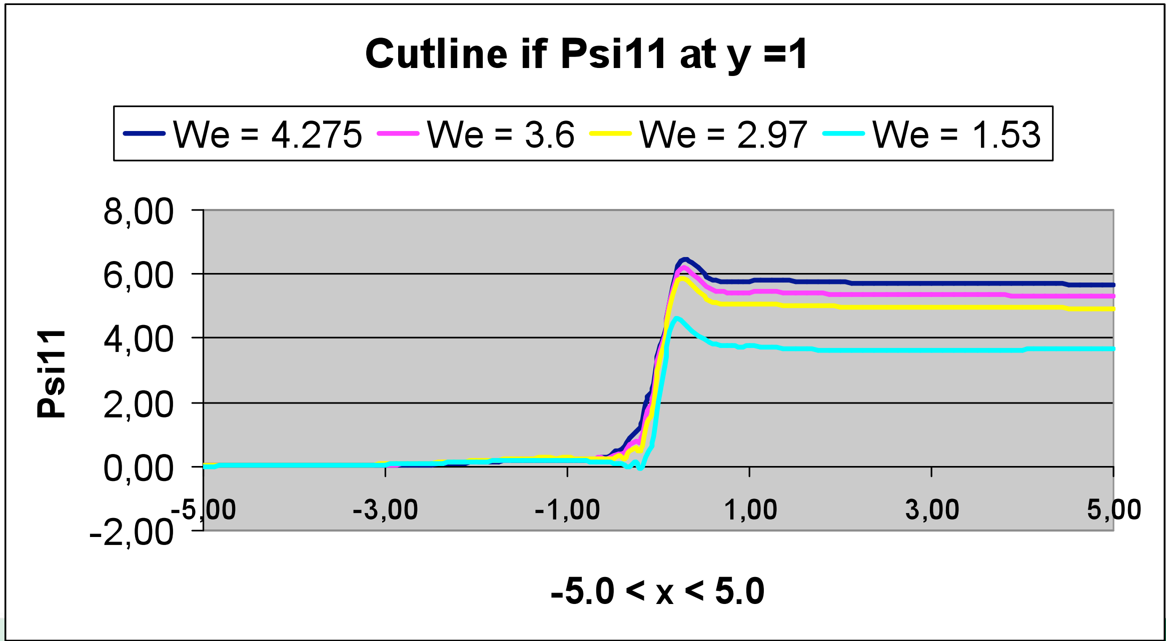
Stress field: Neuman Bc's $v_{in} = 1.0$

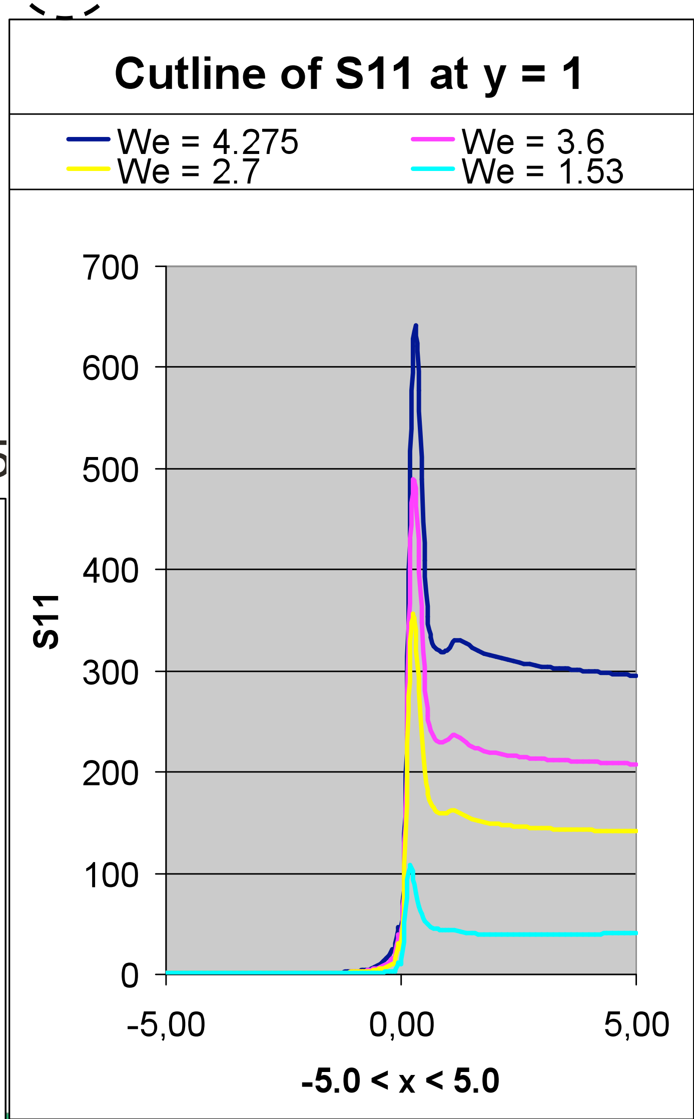
Lip-Vortex Growth





We=1.53 We=2.97 We=3.6 We=4.275





Numerical Results:
unsteady problem tests

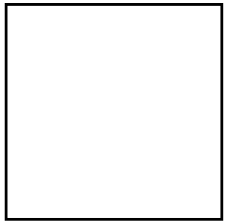
Driven cavity

Velocity profile at the upper wall:

$$v_{in}\, x^2 (1-x)^2$$

$$v_{in} = 8\left(1 + \tanh\left(8(t-0.5)\right)\right)$$

For t > 1, v_{in} = 16

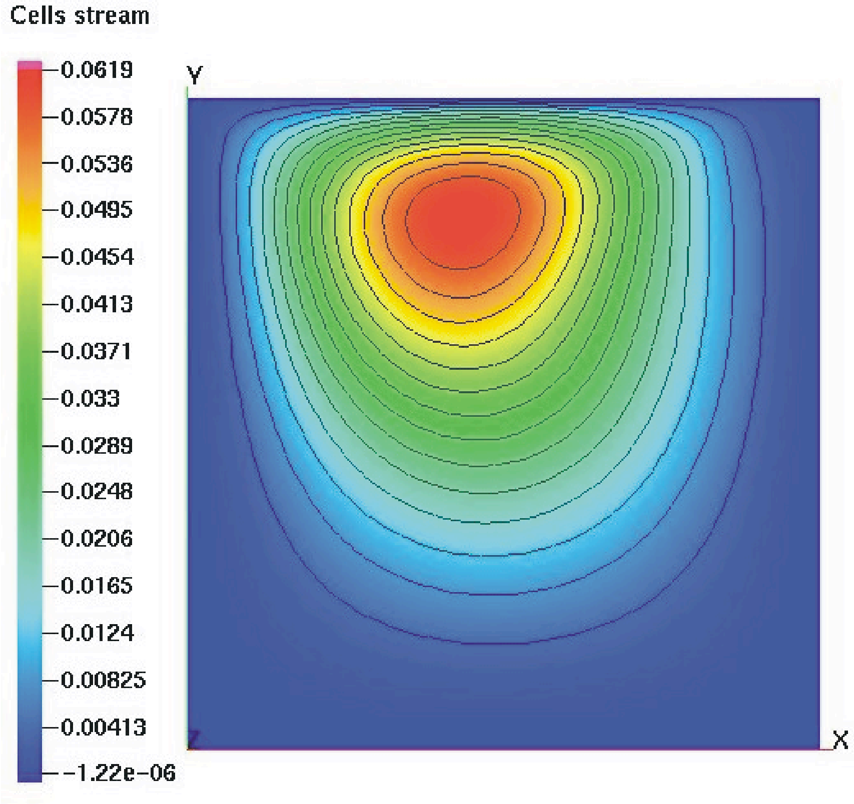


Dirichtlet Bc's everywhere
Stress field: Neuman Bc's

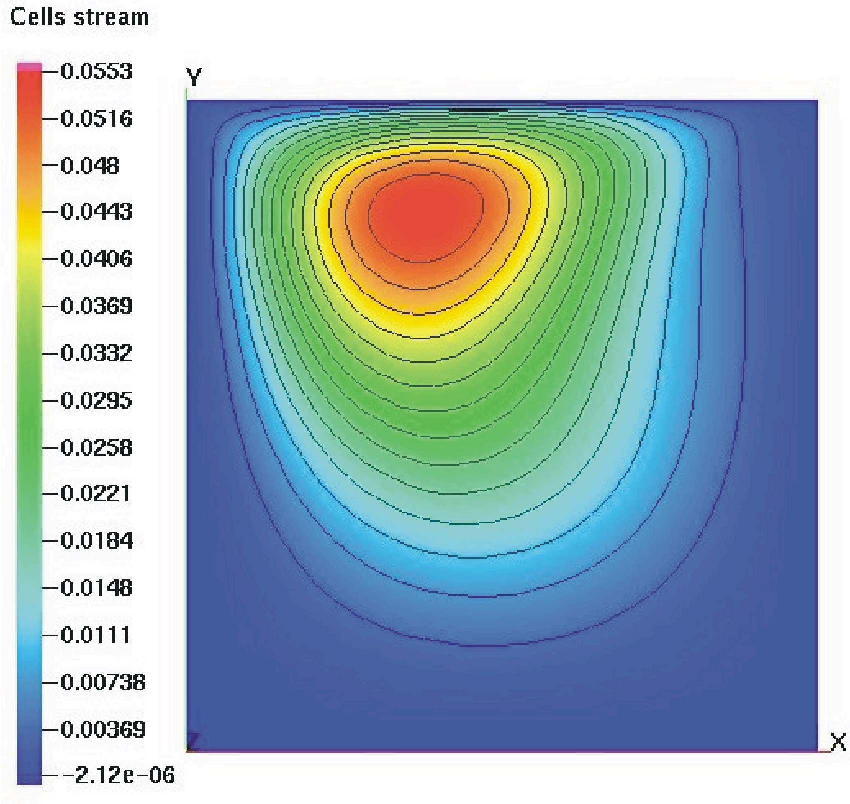
Stream function

t = 8

We = 1



We = 3

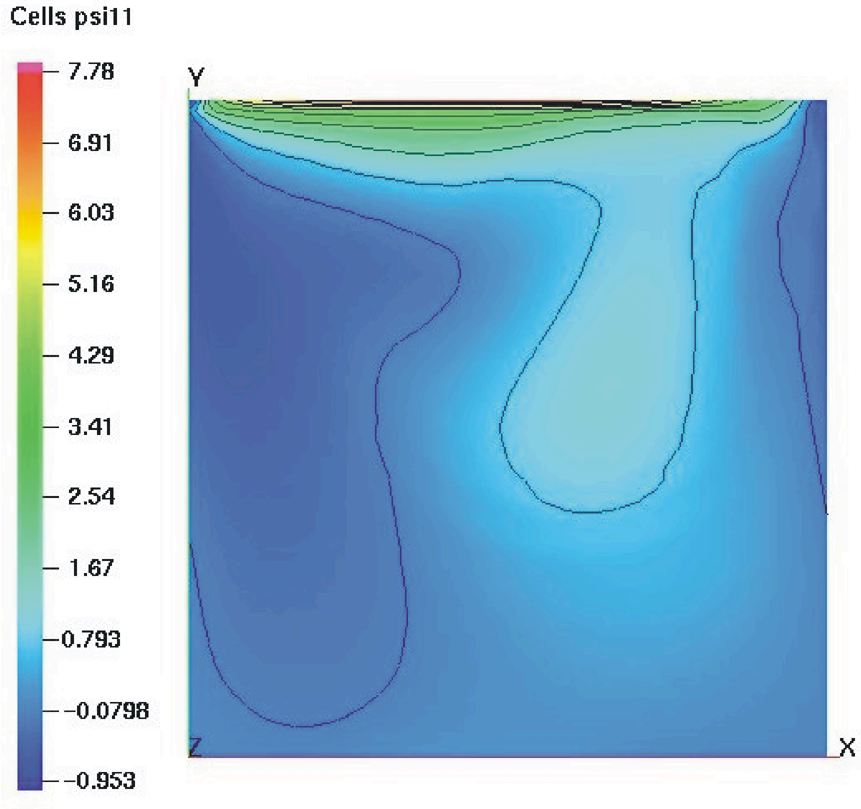


Increasing Wi number shifts the stream to the left

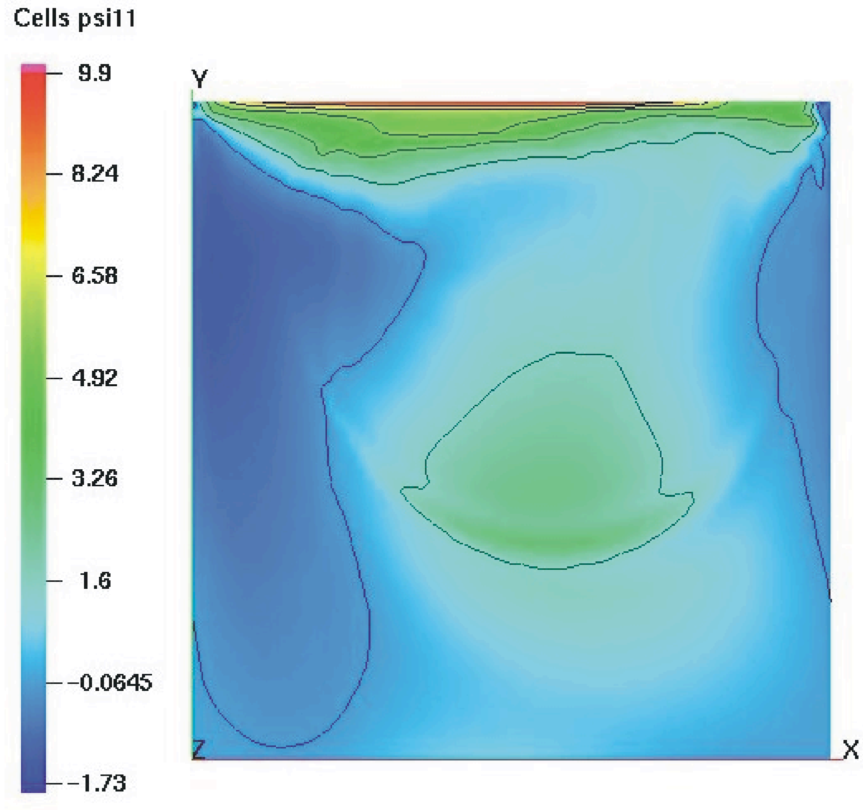
ψ_{11}

t = 8

We = 1



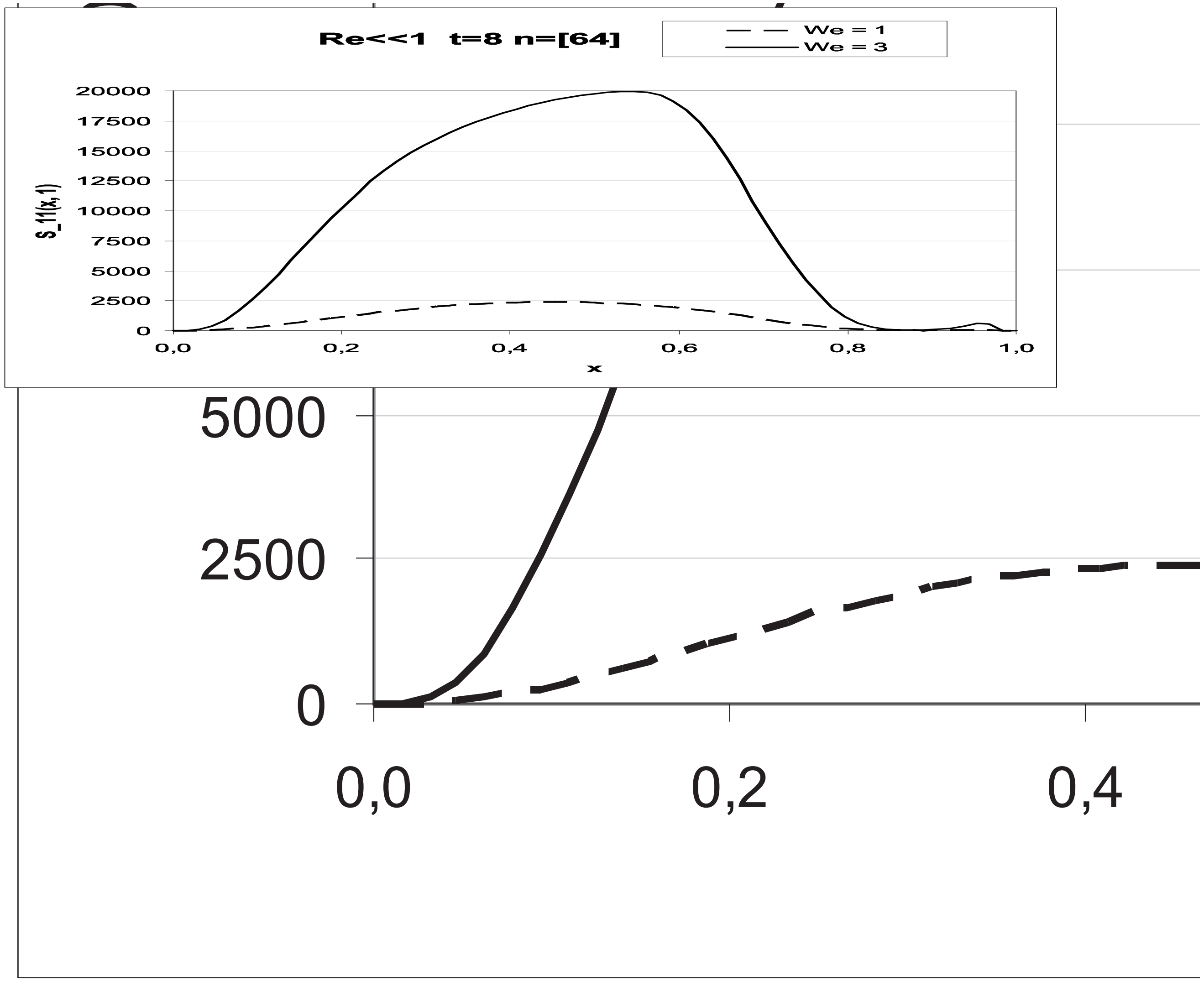
We = 3



Increasing Wi number increases psi by a factor of 1

σ_{11}

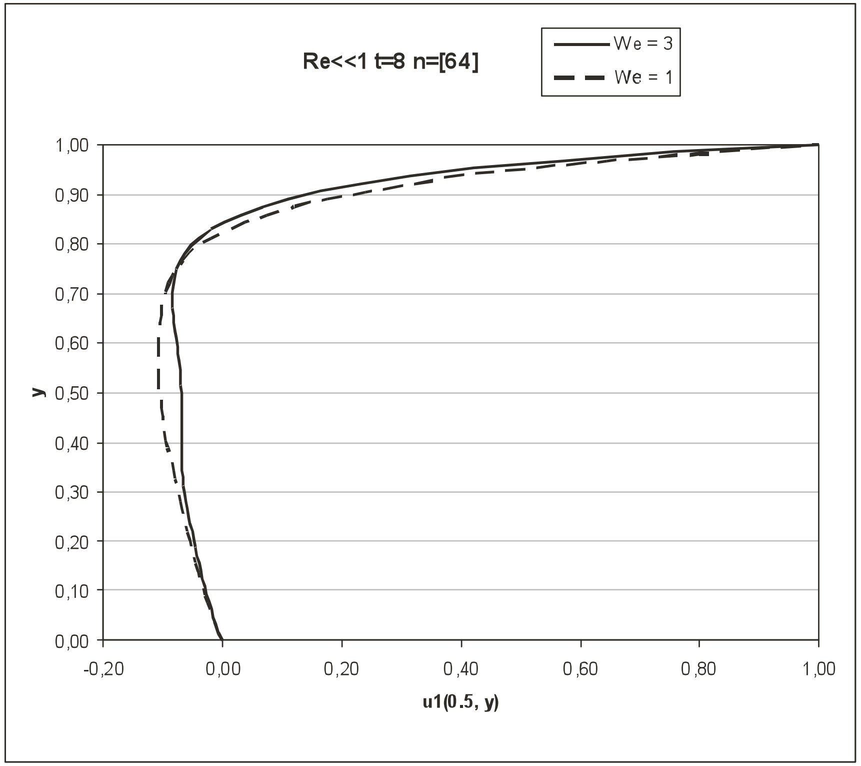
t = 8


Re<<1 t=8 n=[64]
We = 1
We = 3
20000
17500
15000
12500
10000
7500
5000
2500
0
$_11(x,1)
0,0
0,2
0,4
0,6
0,8
1,0
x
5000
2500
0
0,0
0,2
0,4

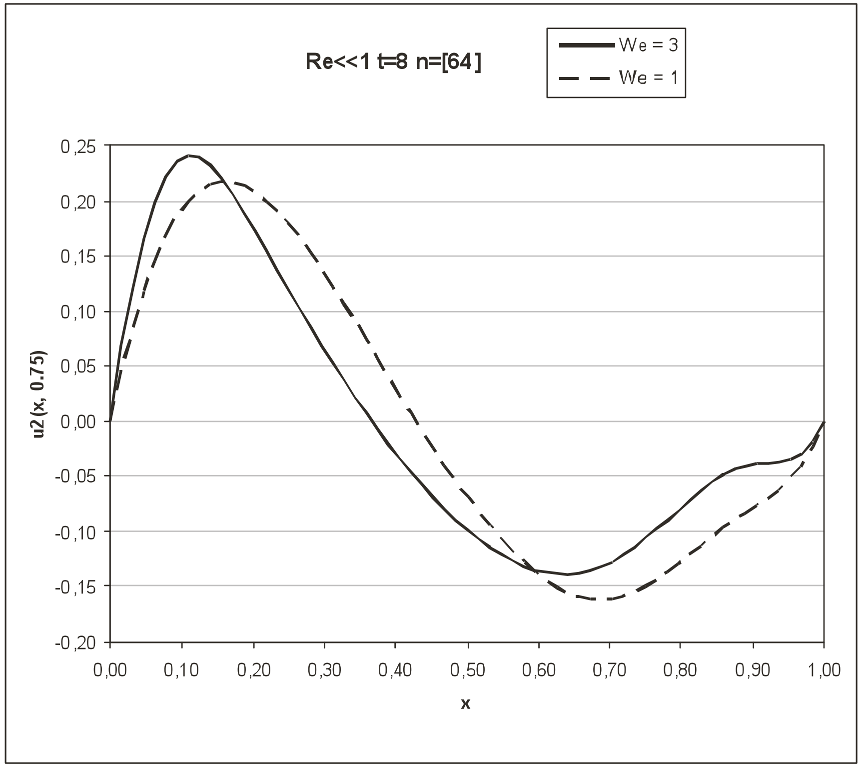
Velocities

t = 8

$V_{x = 0.5}$



$V_{y = 0.75}$



Increasing Wi number does not give much impact to the velocity field

Summary

With LCR, we are now able to simulate much higher Wi numbers

→ **Wi ~ 1.0 for 4 to 1 configuration**

→ **Wi ~ 0.5 for square**

NEW:

→ **Wi >> 4.5 for 4 to 1 contraction (steady state)**

→ **Wi >> 1.5 for square (steady state)**

Additional stabilization will help for high Re + Wi numbers

→ **LCR + Edge Oriented/TVD stabillization**

Application to other viscoelastic flow models