Monolithic FEM multigrid techniques for the simulation of viscoelastic flow

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- **Generalized Navier-Stokes equations**

$$\rho \frac{\partial u}{\partial t} + \rho\, u \cdot \nabla u - \nabla \cdot \sigma + \nabla p = \rho f(x, y, \Theta),\; \nabla \cdot u = 0,$$

$$\frac{\partial \Theta}{\partial t} + u \cdot \nabla \Theta - \nabla \cdot (k \nabla \Theta) - D(u) : \sigma = 0,$$

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

- **Viscous stress**

$$\sigma^s = 2\eta_s(D_{\mathrm{II}}, p, \Theta) D\,,\; D_{\mathrm{II}} = tr(D(u)^2)$$

- **Elastic stress**

$$\sigma^p + \mathrm{We}\frac{\delta_a \sigma^p}{\delta t} = 2\eta_p D(u)$$

Viscoelastic flow models

Quasi-Newtonian models

- **Viscous stress**

$$\sigma^s = 2\eta_s(D_{\mathrm{II}}, p, \Theta)D\,,\; D_{\mathrm{II}} = tr(D(u)^2)$$

➢ **Power law model**

$$\eta_s(z, p, \Theta) = \eta_0 z^{\frac{r}{2}-1} \quad (\eta_0 > 0,\; r > 1)$$

➢ **Carreau model**

$$\eta_s(z, p, \Theta) = \eta_{\infty+(}\eta_0 - \eta_\infty)(1 - z)^{\frac{r}{2}-1}$$

$$(\eta_0 > \eta_\infty \geq 0,\; r > 1)$$

➢ **Schaeffer model (granular flow)**

$$\eta_s(z, p, \Theta) = \sqrt{2}\sin\phi\, p z^{-\frac{1}{2}}$$

➢ **Non-isothermal model**

$$\eta_s(z, p, \Theta) = \eta_0 e^{\left(a_1 + \frac{a_2}{a_3 + \Theta}\right)}(b_1 + b_2 z)^{\frac{r}{2}-1}$$

$$(a_i,\; b_j \text{ material parameters}, r > 1)$$

Constitutive models

- **Elastic stress (Oldroyd/Maxwell/Jeffreys)**

$$\sigma^p + \mathrm{We}\,\frac{\delta_a \sigma^p}{\delta t} = 2\eta_p D(u)$$

  - **Upper/Lower convective derivative**

$$\frac{\delta_a \sigma}{\delta t} = \left(\frac{\partial}{\partial t} + u \cdot \triangledown\right)\sigma + g_a(\sigma, u)$$

  - **Johnson Segelman terms**

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

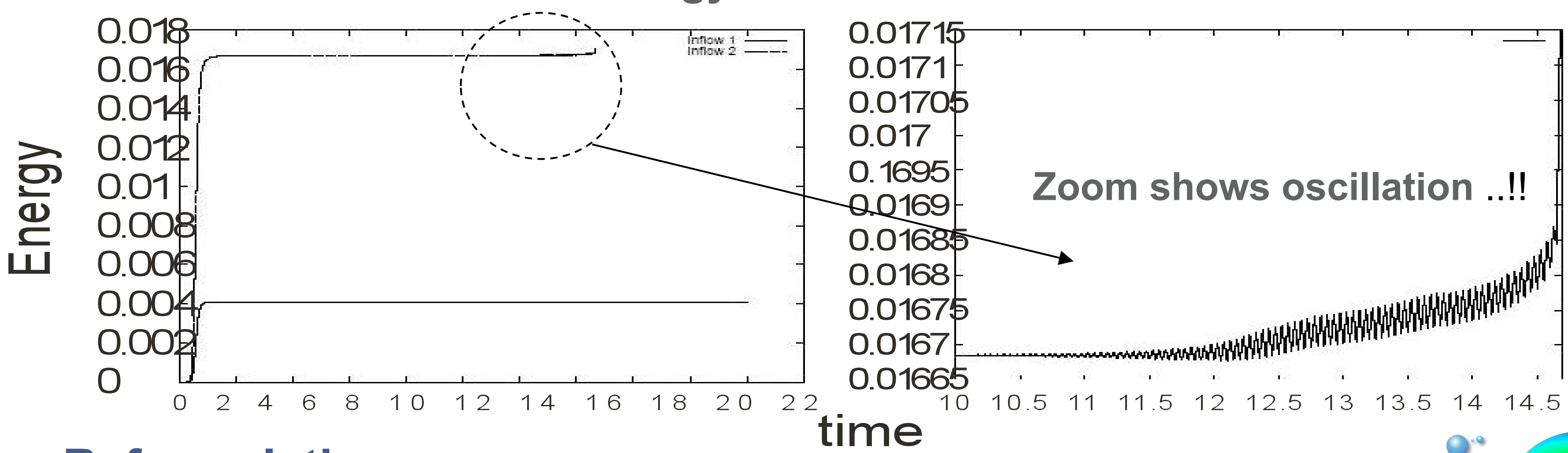
- **Problems**
  - **Blow up phenomena for time dependent problem**
  - **High Weissenberg Number Problem (HWNP !)**

- **Different highly developed models**
  - **Oldroyd A/B, Maxwell A/B, Jeffreys**
  - **Phan-Thien Tanner, Phan-Thien, Giesekus**

- **Different numerical methods**
  - **FEM, FVM, FDM, DEVSS,DG, SUPG**

- **HWNP remains**

Kinetic energy for two different We numbers



- **Reformulation**

Problem reformulation

Conformation tensor reformulation

- **Conformation Tensor (Oldroyd-B) (Lee & Xu)**

  - **Using the identity** $$\frac{\delta_1 \mathrm{I}}{\delta t} = -2D(u)$$

  - **Change of variable** $$\sigma^c = \sigma^p + \frac{\eta_p}{\mathrm{W}e}\mathrm{I}$$

  - **Conformation tensor reformulation**

    - **Rate type expression** $$\sigma^c + \mathrm{W}e\frac{\delta_1 \sigma^c}{\delta t} = \frac{\eta_p}{\mathrm{W}e}\mathrm{I}$$

    - **Integral expression**

$$\sigma^c(t) = \int_{\infty}^{t} \frac{\eta_p}{\mathrm{W}e^2} exp\left(-\frac{t-s}{\mathrm{W}e}\right) F(s,t)F(s,t)^{\mathrm{T}} ds$$

✓ **positive definite**

✓ **of exponential type**

Positivity preserving discretizations

- **Conformation reformulation (Fattal & Kupferman)**
  - **The diagonalizing transformation**

$$\sigma^c = R \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} R^{\mathrm{T}}$$

  - **Transformation and decomposition of velocity gradient**

$$R^{\mathrm{T}} \nabla u R =: \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \quad \nabla u = \tilde{G} + \tilde{W} + N\sigma^{-1}$$

    - **The symmetric part**

$$\tilde{G} = R \begin{pmatrix} m_{11} & 0 \\ 0 & m_{22} \end{pmatrix} R^{\mathrm{T}}$$

    - **The anti-symmetric part**

$$\tilde{W} := R \begin{pmatrix} 0 & s \\ -s & 0 \end{pmatrix} R^{\mathrm{T}}$$

$$s := \frac{\lambda_2 m_{12} + \lambda_1 m_{21}}{\lambda_2 - \lambda_1}$$

$$n := \frac{m_{12} + m_{21}}{\lambda_2^{-1} - \lambda_1^{-1}}$$

$$N := R \begin{pmatrix} 0 & n \\ -n & 0 \end{pmatrix} R^{\mathrm{T}}$$

- **Conformation reformulation (Fattal & Kupferman)**

  - **New conformation tensor reformulation**

$$\left(\frac{\partial}{\partial t} + u \cdot \nabla\right) \sigma^c - \left(\tilde{W}\,\sigma^c - \sigma^c \tilde{W}\right) - 2\tilde{G}\,\sigma^c = \frac{1}{\mathrm{We}}\left(\frac{\eta_p}{\mathrm{We}}\mathrm{I} - \sigma^c\right)$$

- **Log Conformation Reformulation (LCR)**

  - **Change of variable** $\sigma^{lc} = \log(\sigma^c)$

$$\left(\frac{\partial}{\partial t} + u \cdot \nabla\right) \sigma^{lc} - \left(\tilde{W}\,\sigma^{lc} - \sigma^{lc} \tilde{W}\right) - 2\tilde{G} = \frac{1}{\mathrm{We}}\left(-\frac{\eta_p}{\mathrm{We}}\mathrm{I} + e^{-\sigma^{lc}}\right)$$

Positivity preserving via LCR

LCR equations

$$
\begin{aligned}
\rho \frac{\partial u}{\partial t} + \rho\, u \cdot \nabla u - \nabla \cdot (2\eta_s(D_{\mathrm{II}}, p, \Theta) D(u)) + \nabla p& \\
- \nabla \cdot \exp(\sigma^{lc}) = \rho f(x, y, \Theta)&, \\
\nabla \cdot u = 0&, \\
\frac{\partial \Theta}{\partial t} + u \cdot \nabla \Theta - \nabla \cdot (k \nabla \Theta) - 2\eta_s D(u) : D(u)& \\
- D(u) : \exp(\sigma^{lc}) = 0&, \\
\left(\frac{\partial}{\partial t} + u \cdot \nabla \right) \sigma^{lc} - \left(\tilde{W} \sigma^{lc} - \sigma^{lc} \tilde{W} \right)& \\
-2\tilde{G} - \frac{1}{\mathrm{We}} \exp(-\sigma^{lc}) = - \frac{\eta_p}{\mathrm{We}^2} \mathrm{I}&.
\end{aligned}
$$

- **Standard Navier-Stokes**

$$a(u,v) = \int_\Omega \alpha\, u\, v d\Omega + \int_\Omega 2\eta_s D(u) : D(v)\, d\Omega$$

$$+ \int_\Omega \rho(u\cdot\nabla)u\, v\, d\Omega$$

$$b(p,v) = -\int_\Omega p\nabla\cdot v\, d\Omega$$

- **New non-symmetric bilinear forms due to LCR**

$$c(\sigma^{lc}, v) = \int_\Omega \exp\left(\sigma^{lc}\right) : D(v)\, d\Omega$$

$$\tilde{c}(\tau, u) = 2\int_\Omega \tilde{G}(\nabla u, \sigma^c) : \tau\, d\Omega$$

- **New nonlinear tensor variational form due to LCR**

$$d(\sigma^{lc},\tau) = \int_\Omega \left(\alpha\,\sigma^{lc} + \frac{-1}{\mathrm{We}}\exp(-\sigma^{lc}) + (u\cdot\nabla)\sigma^{lc}\right) : \tau\, d\Omega$$
$$- \int_\Omega \left(\tilde{W}\,\sigma^{lc} - \sigma^{lc}\tilde{W}\right) : \tau\, d\Omega$$

- **Energy equation with friction**

$$e(\Theta,\Phi) = \int_\Omega \alpha\,\Theta\,\Phi d\Omega + \int_\Omega k\,\nabla\Theta\nabla\Phi d\Omega + \int_\Omega (u\cdot\nabla)\Theta\,\Phi d\Omega$$
$$- \int_\Omega 2\eta_s[D(u):D(u)]\Phi d\Omega - \int_\Omega D(u) : \exp(\sigma^{lc})\Phi d\Omega$$

- **Source terms**

$$L(u,\sigma^{lc},\Theta,p) = \quad \int_\Omega f\,v\,d\Omega - \frac{\eta_p}{\mathrm{We}^2}\int_\Omega \mathbf{I} : \tau\, d\Omega$$

- **Set** $X := H_0^1(\Omega)]^2 \times [L^2(\Omega)]^4 \times H^1(\Omega)$

$$Q := L_0^2(\Omega) \qquad \tilde{A} := \begin{bmatrix} A & C & 0 \\ \tilde{C}^{\mathrm{T}} & D & 0 \\ E_{f_D} & E_{f_{\sigma^{lc}}} & E \end{bmatrix}$$

$$\tilde{u} := (u, \sigma^{lc}, \Theta)$$

- **Find** $(\tilde{u}, p) \in X \times Q$ **such that**

$$\langle K(\tilde{u}, p), (\tilde{v}, q)\rangle = \langle L(\tilde{u}, p), (\tilde{v}, q)\rangle \quad \forall (\tilde{v}, q) \in X \times Q$$

$$K := \begin{bmatrix} \tilde{A} & B \\ B^{\mathrm{T}} & 0 \end{bmatrix}$$

Typical saddle point problem !

- **Compatibility condition for existance and uniqueness**

$$\sup_{u\in[H_0^1(\Omega)]^2} \frac{\int_\Omega \nabla\cdot u\, q\, dx}{\|u\|_{1,\Omega}} \geq \beta_1 \|q\|_{0,\Omega} \quad \forall q\in L_0^2(\Omega)$$

$$\sup_{\sigma\in[L^2(\Omega)]^4} \frac{\int_\Omega \sigma : \nabla u\, dx}{\|\sigma\|_{0,\Omega}} \geq \beta_2 \|u\|_{1,\Omega} \quad \forall u\in [H_0^1(\Omega)]^2$$

What about LCR !

- **The `NEW´ non-symmetric bilinear forms due to LCR**

$$\mathrm{T}_{\mathrm{PD}} := \{\tau \in [L^2(\Omega)]^4; \tau \text{ is positive definite}\}$$

$$\begin{aligned} c(\tau, v) =& \int_\Omega \exp(\tau) : D(v)\, d\Omega \\ \geq& \beta_2 \|\exp(\tau)\|_{0,\Omega} \|v\|_{1,\Omega} \\ \geq& \beta_2 \|\tau\|_{0,\Omega} \|v\|_{1,\Omega} \qquad \forall \tau \in \mathrm{T}_{\mathrm{PD}}, \forall v \in [H_0^1(\Omega)]^2 \end{aligned}$$

$$\begin{aligned} \tilde{c}(\tau, v) =& 2 \int_\Omega \tau : \nabla_{\sigma^c} v \, d\Omega \qquad \sigma^c \in \mathrm{T}_{\mathrm{PD}} \\ \geq& \beta_2 \|\tau\|_{0,\Omega} \|v\|_{1,\Omega} \qquad \forall \tau \in [L^2(\Omega)]^4, \forall v \in [H_0^1(\Omega)]^2 \end{aligned}$$

- **FEM discretization**
  - $Q_2/Q_2/Q_2/P_1^{\text{disc}}$ approximations for velocity-stress-temperature-pressure
- **Edge-oriented stabilization for (in preparation)**
  - Same finite element interpolation velocity and stress

$$J_u = \sum_{\text{edge E}} \gamma_u h_E \int_E [\nabla u][\nabla v] ds$$

  - convective dominated problem

$$J_u = \sum_{\text{edge E}} \gamma_u^* h_E^2 \int_E [\nabla u][\nabla v] ds$$

$$J_\Theta = \sum_{\text{edge E}} \gamma_\Theta h_E^2 \int_E [\nabla \Theta][\nabla \Phi] ds$$

$$J_\sigma = \sum_{\text{edge E}} \gamma_\sigma h_E^2 \int_E [\nabla \sigma][\nabla \tau] ds$$

Practically the convective terms are the main source of the instability !

- **Newton with damping results in the solution of the form**

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

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

- **Inexact Newton**
  - **The Jacobian matrix is approximated using finite differences**

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

$$\left[\frac{\partial R(\mathbf{x}^n)}{\partial \mathbf{x}} \right] = K + K^* =: \tilde{K}$$

$$= \begin{bmatrix} \tilde{A} + \tilde{A}^* & B + B^* \\ B^{\mathrm{T}} & 0 \end{bmatrix}$$

Typical saddle point problem !

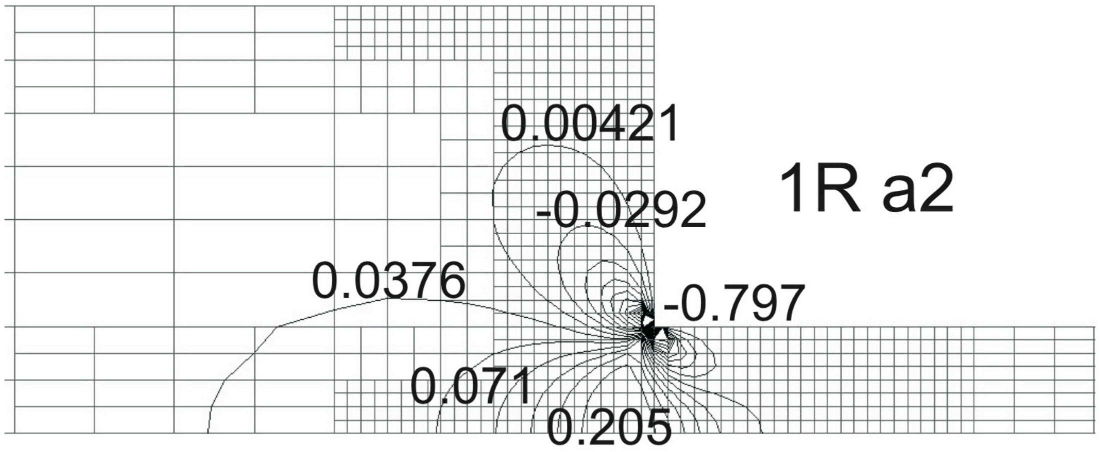
- **Monolithic multgrid solver**
  - **Standard geometric multigrid aproach**
  - **Full Q_2, P_1^{disc} restrictions and prolongations**
  - **Local MPSC via Vanka-like smoother**

$$\begin{bmatrix} u^{l+1} \\ \sigma^{l+1} \\ \Theta^{l+1} \\ p^{l+1} \end{bmatrix} = \begin{bmatrix} u^{l} \\ \sigma^{l} \\ \Theta^{l} \\ p^{l} \end{bmatrix} + \omega^l \sum_{T \in_h} \left[(\tilde{K} + J)_{|T} \right]^{-1} \begin{bmatrix} Res_u \\ Res_\sigma \\ Res_\Theta \\ Res_p \end{bmatrix}_{|T}$$

Coupled Monolithic Multigrid Solver !

- **M-FEM Multgrid solver for 4:1 contraction**

Level / ϵ	1e-2	1e-3
We=0.1	NL/AVMG	
L1	9/3	6/4
L2	8/5	6/7
L2a1	8/11	6/15
L2a2	9/20	8/24
We=0.7	NL/AVMG	
L1	8/3	7/5
L2	8/5	7/7
L2a1	9/10	7/15
L2a2	9/12	8/25



Stable nonlinear solver w.r.t. adaptivity

Stable multigrid solver w.r.t. adaptivity

More investigation w.r.t discrete jacobian evaluation and stabilization

Q: Optimal way to apply Newton !

- **Driven cavity (Oldroyd-B)**

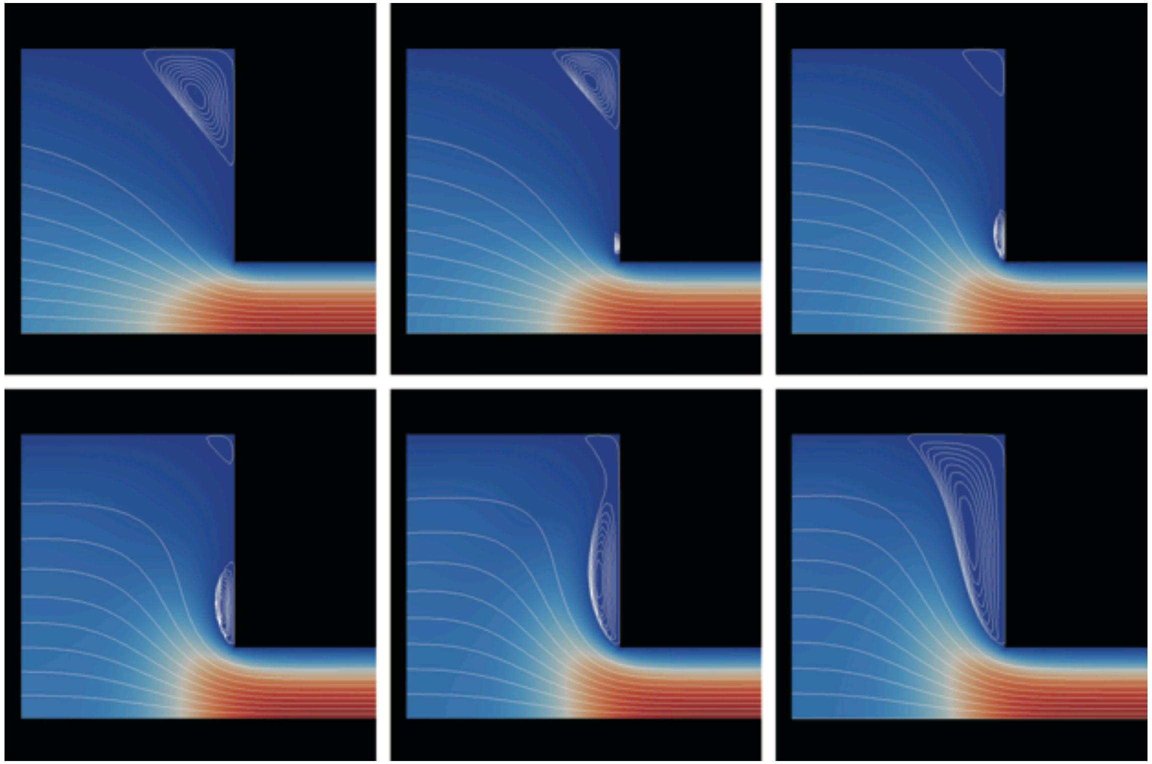
Streameline for $\mathrm{We} = 0.5$, $\mathrm{We} = 3$ **and** $We = 4.0$

With increasing of We

- **Shift of streameline to the right**
- **Increases of bottom right vortex**
- **Decreases of bottom left vortex**

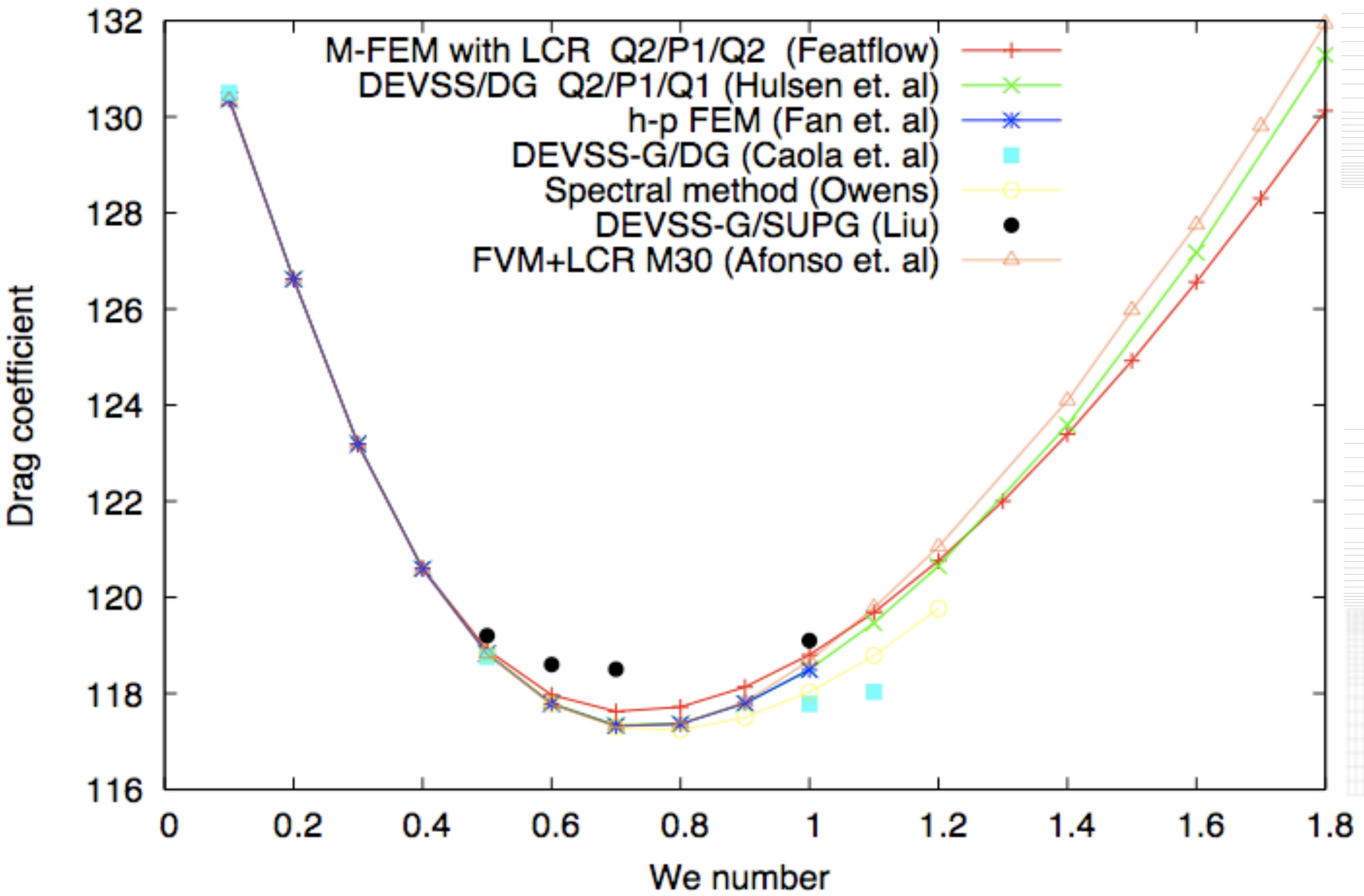
Direct steady simulation for non-steady derived formulation !

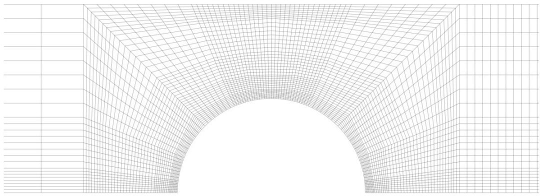
- **4:1 contraction (Oldroyd-B)**



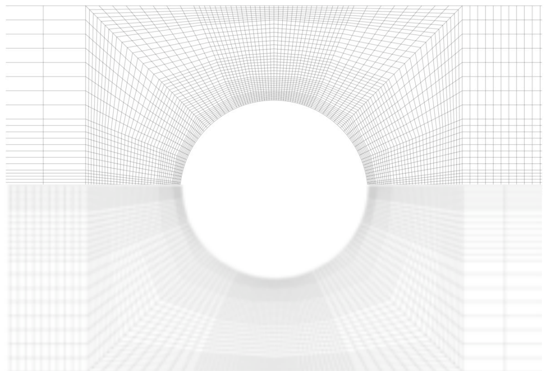
Lip vortex growth

- **Planar flow around cylinder (Oldroyd-B)**



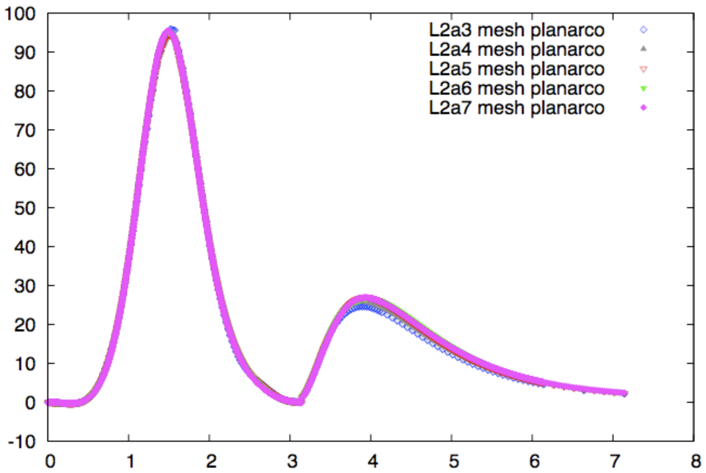


Half Domain
Vs.
Full Domain

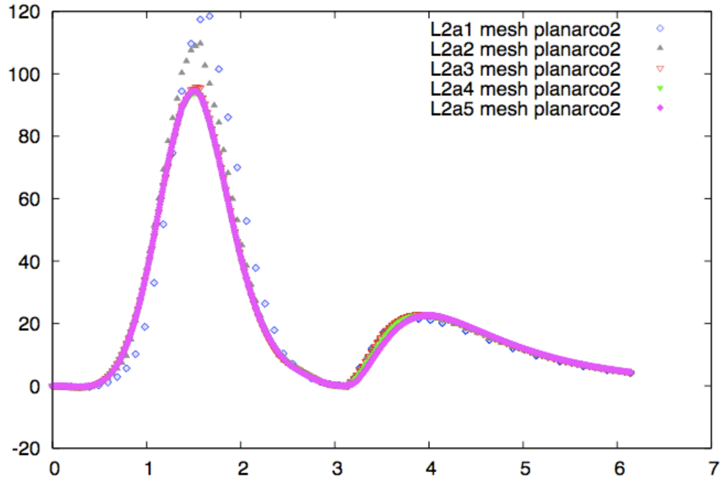


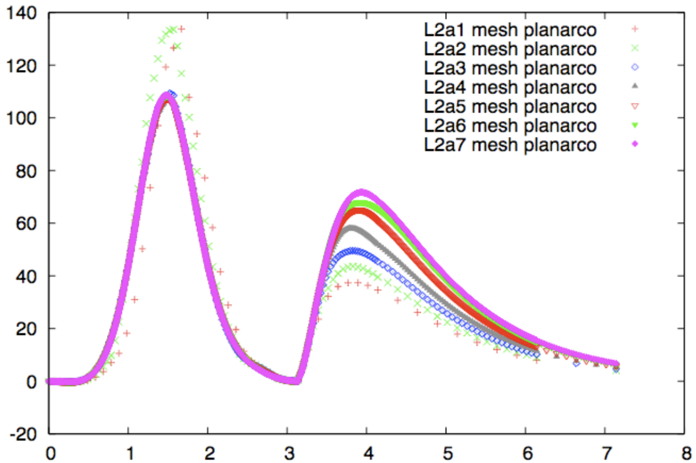
Only with LCR & next EO-FEM we hope that HWNP will be history !

- **Axial stress w.r.t. X-curved for half domain vs. full Domain (HD/FD) (Oldroyd-B)**

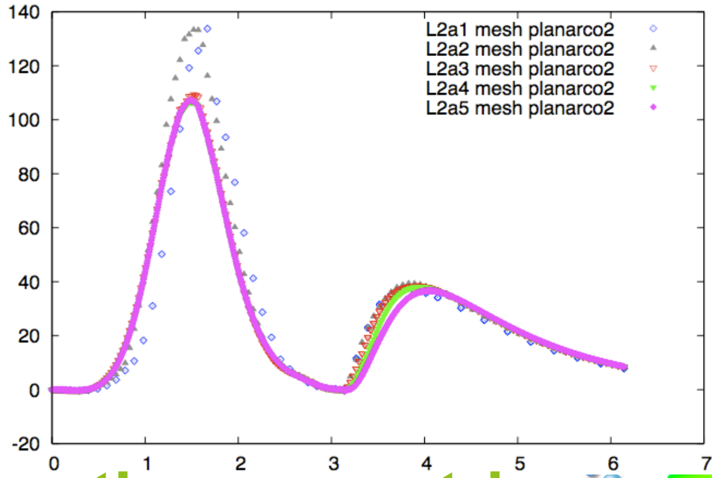


H.D.
vs.
F.D.
$We = 0.6$





H.D.
vs.
F.D.
$We = 0.7$



Q: is it appropriate to impose the symmetric condition for higher We number !

Summary

New numerical and algorithmic tools are available using

- ✓ Monolithic Finite Element Method (M-FEM)
- ✓ Log Conformation Reformulation (LCR)
- ✓ Edge Oriented stabilization (EO-FEM)
- ✓ Fast Multigrid Solver with local MPSC smoother

for the simulation of viscoelastic flow

Advantages

- ✓ No CFL-condition restriction due to the fully coupling
- ✓ Positivity preserving
- ✓ Large order and local adaptivity