Monolithic Newton multigrid FEM techniques for LCR reformulation of viscoelastic flow

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Non-Newtonian phenomena

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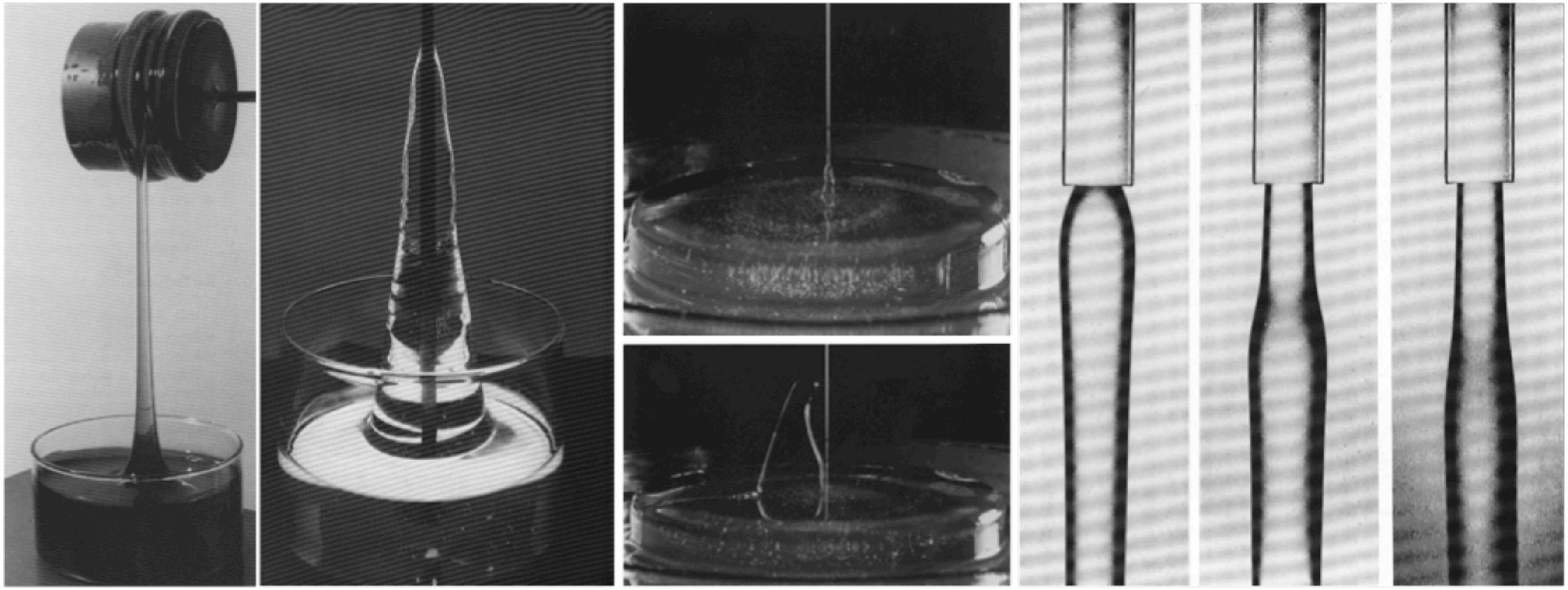
- **Effects due to normal stresses**
- **Effects due to elongational viscosity**
- **The drag reduction phenomenon**



Differential models

Governing equations

- **Generalized Navier-Stokes equations**

$$\rho\left(\frac{\partial}{\partial t}+u\cdot\nabla\right)u=-\nabla p+\nabla\cdot\sigma,\ \nabla\cdot u=0,$$

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

- **Viscous stress**

$$\sigma^{s}=2\eta_{s}(D_{\mathrm{II}},p)D\,,\ D_{\mathrm{II}}=tr(D(u)^{2}).$$

- **Elastic stress**

$$\sigma^{p}+\mathrm{We}\frac{\delta_{a}\sigma^{p}}{\delta t}=2\eta_{p}D(u).$$

Viscoelastic flow models

- **Viscous stress**

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

- **Power law model**

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

- **Carreau model**

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

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

- **Powder flow in the quasi-static and intermediate regimes**

$$\eta_s(z,p) = \sqrt{2}\left[\sin\phi z^{-\frac{1}{2}} + b\cos\phi z^{\frac{r-1}{2}}\right]$$

$$(\phi\,\text{is angle of internal friction}, r > 1)$$

- **Elastic stress**

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

- **Upper/Lower convective derivative**

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

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

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- **Generalized differential constitutive model**

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

- **Oldroyd**

$$\mathbf{G} = 0, \quad \mathbf{H} = 0$$

- **Giesekus**

$$\mathbf{G} = 0, \quad \mathbf{H} = \alpha\,\sigma^2$$

- **Phan-Thien and Tanner**

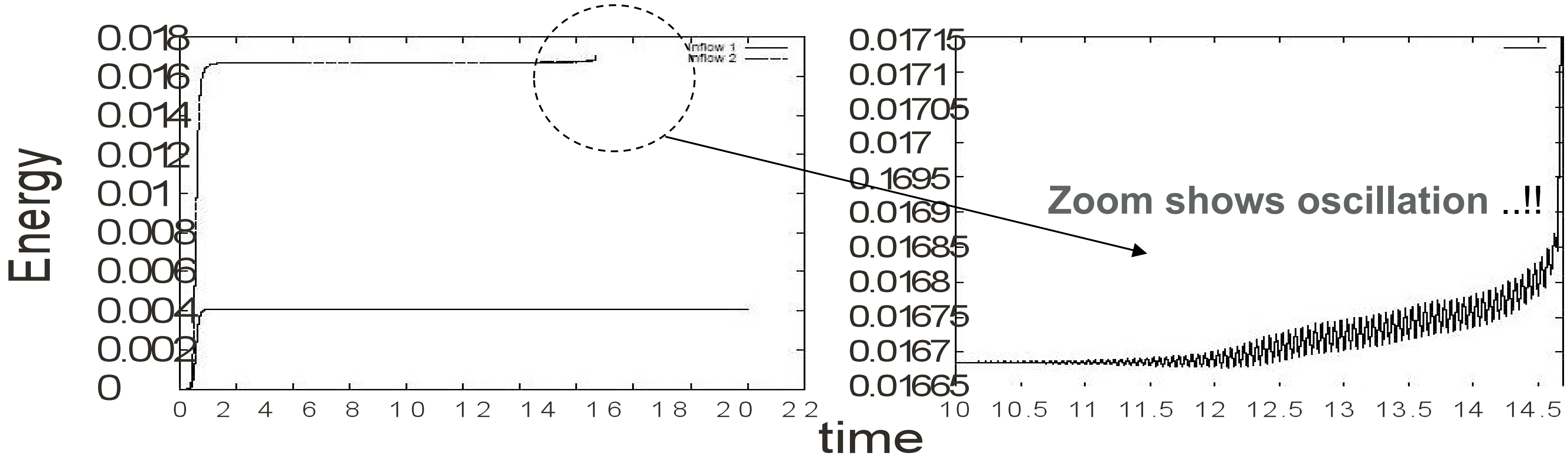
$$\mathbf{G} = 0, \quad \mathbf{H} = \left[\exp\left(\alpha\,\mathrm{tr}(\sigma)\right) - 1\right]\sigma$$

- **White and Metzner**

$$\mathbf{G} = \alpha\,(2\,D : D)^{1/2}, \quad \mathbf{H} = 0$$

- Blow up phenomena for time dependent problems
- High Weissenberg Number Problem (HWNP !)

Kinetic energy for two different We numbers



Problem 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**

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

    - ✓ **The symmetric part**

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

    - ✓ **The anti-symmetric part**

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

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

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

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

LCR formulation

- **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

- **LCR equations**

$$\rho\left(\frac{\partial}{\partial t} + u\cdot\nabla\right)u = -\nabla p + \nabla\cdot\left(2\eta_s(D_{\mathrm{II}},p)D(u)\right) + \nabla\cdot e^{\sigma^{lc}},$$

$$\nabla\cdot u = 0,$$

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

- **Oldroyd-B model**

$$f(\sigma^{lc}) = \left(e^{-\sigma^{lc}} - \frac{\eta_p}{\mathrm{We}}\mathrm{I}\right).$$

- **Giesekus model**

$$f(\sigma^{lc}) = \left(e^{-\sigma^{lc}} - \frac{\eta_p}{\mathrm{We}}\mathrm{I}\right) - \alpha\,e^{\sigma^{lc}}\left(e^{-\sigma^{lc}} - \frac{\eta_p}{\mathrm{We}}\mathrm{I}\right)^2.$$

- **Standard Navier-Stokes equations**

$$a(u,v) = \int_\Omega \frac{1}{\triangle t}\, u\, v \, d\Omega + \int_\Omega 2\eta_s D(u) : D(v)\, d\Omega + \int_\Omega \rho(u \cdot \nabla) u\, v\, d\Omega$$

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

- **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**

$$d(\sigma^{lc},\tau) = \int_\Omega \left(\frac{1}{\triangle t}\,\sigma^{lc} + u\cdot\nabla\sigma^{lc} \right) : \tau\, d\Omega$$

$$- \int_\Omega \frac{1}{\mathrm{We}} \left((1-\alpha)e^{-\sigma^{lc}} + \alpha\frac{\eta_p}{\mathrm{We}} e^{\sigma^{lc}} \right) : \tau\, d\Omega$$

$$- \int_\Omega \left(\tilde{W}\,\sigma^{lc} - \sigma^{lc}\tilde{W} \right) : \tau\, d\Omega$$

- **Source terms**

$$L(u,\sigma^{lc},p) = -\,(1-2\,\alpha)\,\frac{\eta_p}{\mathrm{We}^2} \int_\Omega \mathbf{I} : \tau\, d\Omega$$

Problem formulation

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

  $Q := L_0^2(\Omega)$

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

  $$\tilde{A} := \begin{bmatrix} A & C \\ \tilde{C}^{\mathrm{T}} & D \end{bmatrix}$$

- **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 !

- **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

- **High order $Q_2/Q_2/P_1^{\text{disc}}$ approximations for velocity-stress-pressure**

  - **Advantages:**
    - **Inf-sup stable for velocity and pressure**

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

    - **High order: good for accuracy**
    - **Discontinuous pressure: good for solver**

  - **Disadvantage**
    - **Stabilization for same approximation spaces for stress-velocity**
    - **a single d.o.f. belongs to four elements**

Compatibility condition between the stress and velocity spaces via EO-FEM !

- **Edge-oriented stabilization for**

  - **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**

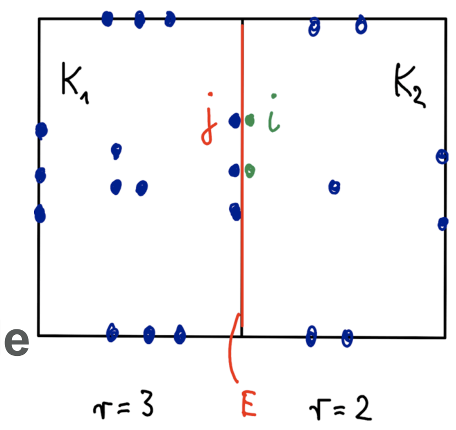
$$J_u = \sum_{\text{edge E}} \gamma_u^* h_E^2 \int_E [\nabla u] : [\nabla v] ds$$

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

Efficient Newton-type and multigrid solvers can be easily applied!

- **Larger FE space which allows the approximation of singular solution**

- **d.o.f.s belong to at most two elements which is good for parallelism**



- **Coupling of different polynomial order**

  - **Mortar condition: test space ≈ order at slave side**

$$|E|^{-1}\int_E v_h|_{K_2} L_{E,k}\,ds = |E|^{-1}\int_E v_h|_{K_1} L_{E,k}\,ds, \qquad 0 \le k < 2$$

  - **No hanging nodes**

Research in progress!

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

$$R(\mathbf{x}) = 0, \qquad \mathbf{x} = (u, \sigma, p)$$
$$\mathbf{x}^{n+1} = \mathbf{x}^n + \omega^n \left[\frac{\partial R(\mathbf{x}^n)}{\partial \mathbf{x}}\right]^{-1} R(\mathbf{x}^n)$$

- **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 !

Linear solver

- **Monolithic multgrid solver**

  - **Standard geometric multigrid approach**

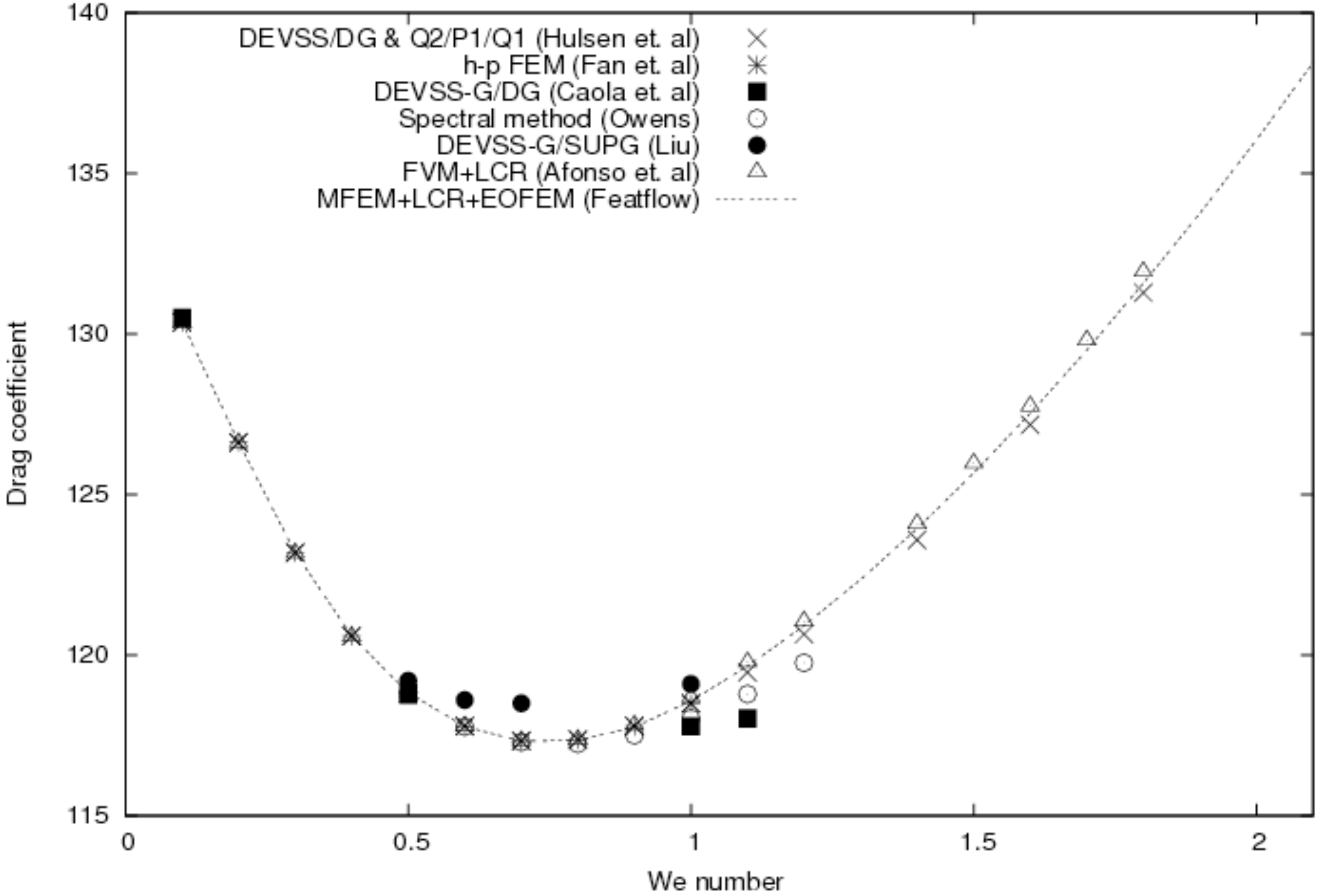
  - **Full** Q_2, P_1^{disc} **restrictions and prolongations**

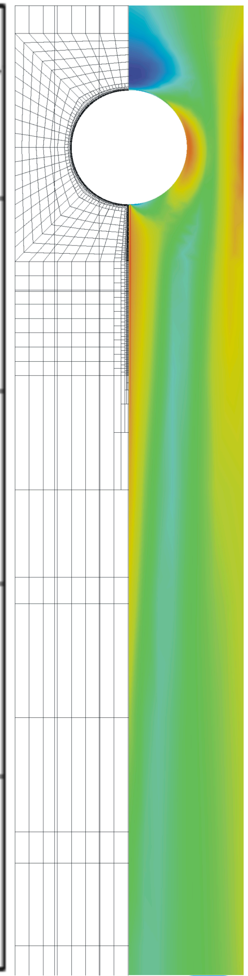
  - **Local MPSC via Vanka-like smoother**

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

Coupled Monolithic Multigrid Solver !

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

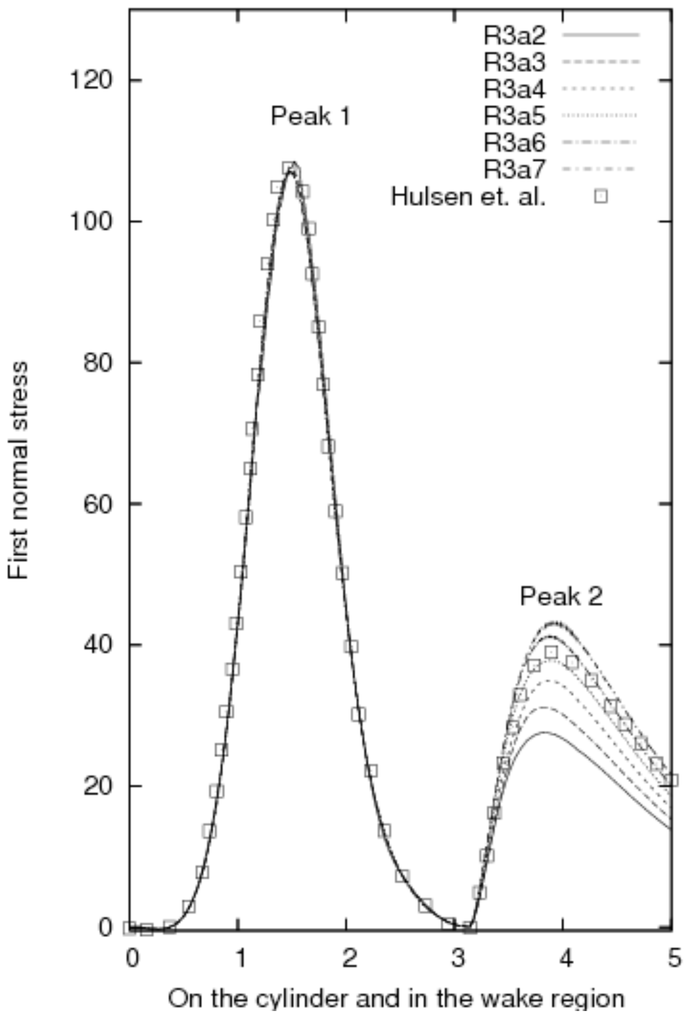




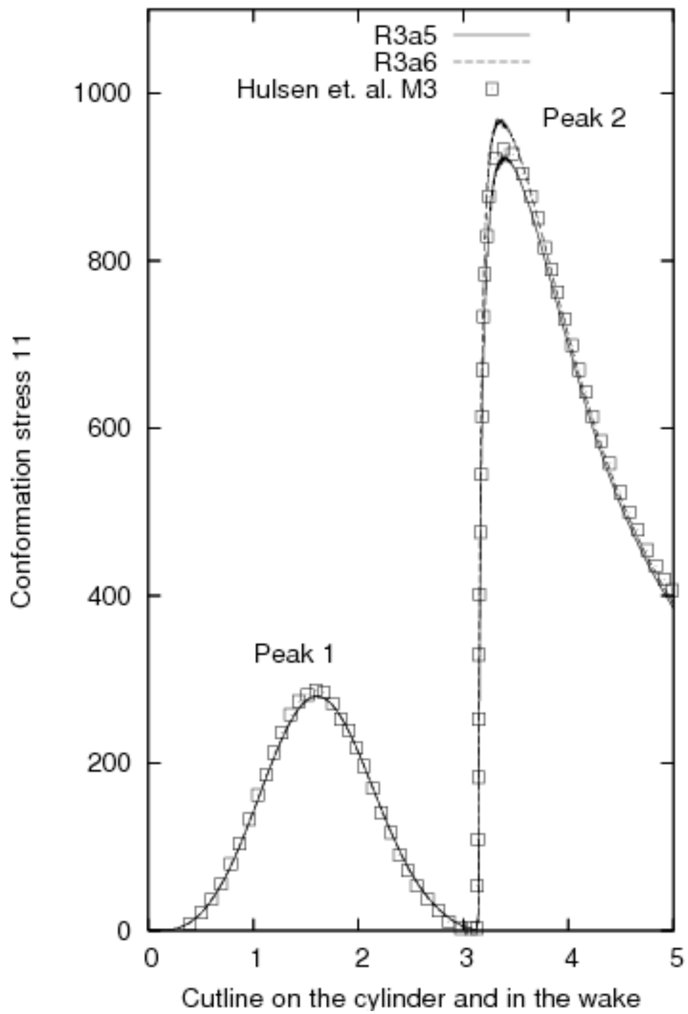
The numerical method is quantitatively validated

- **Axial stress w.r.t. X-curved: Oldroyd-B vs. Giesekus**

$We = 0.7$



$We = 5.0$



The lack of pointwise mesh convergence !

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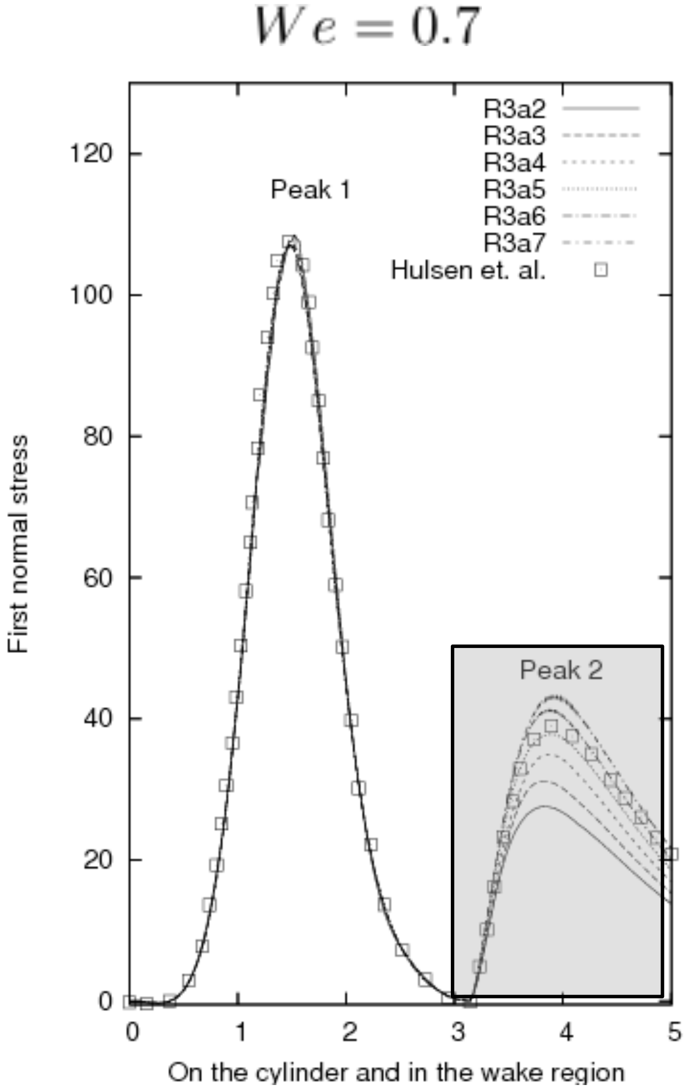

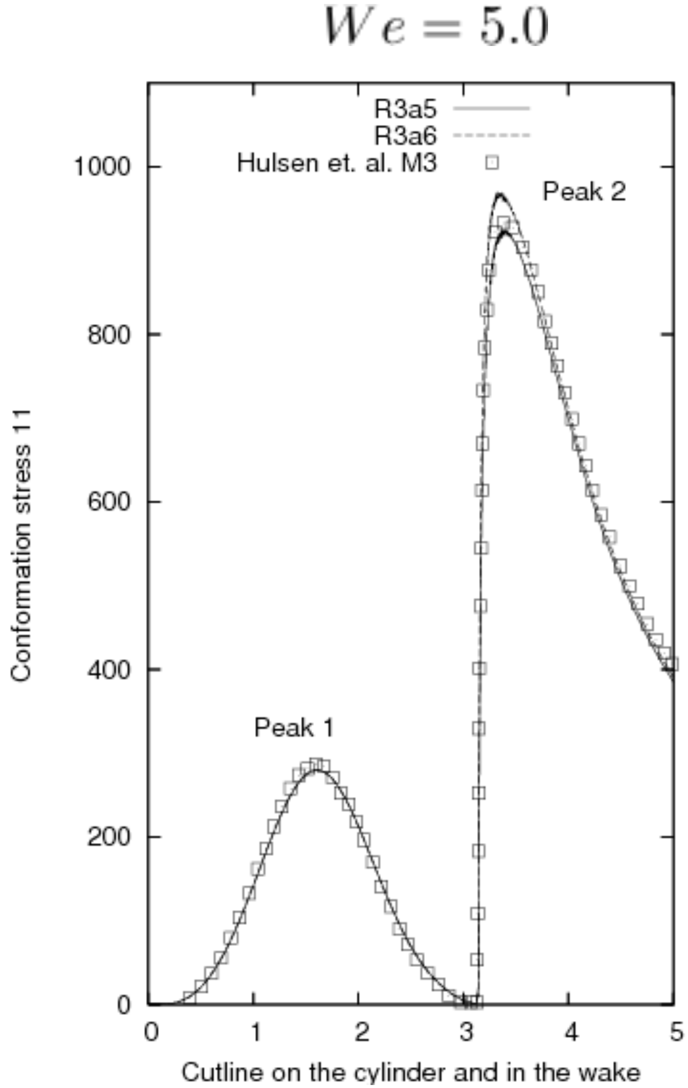

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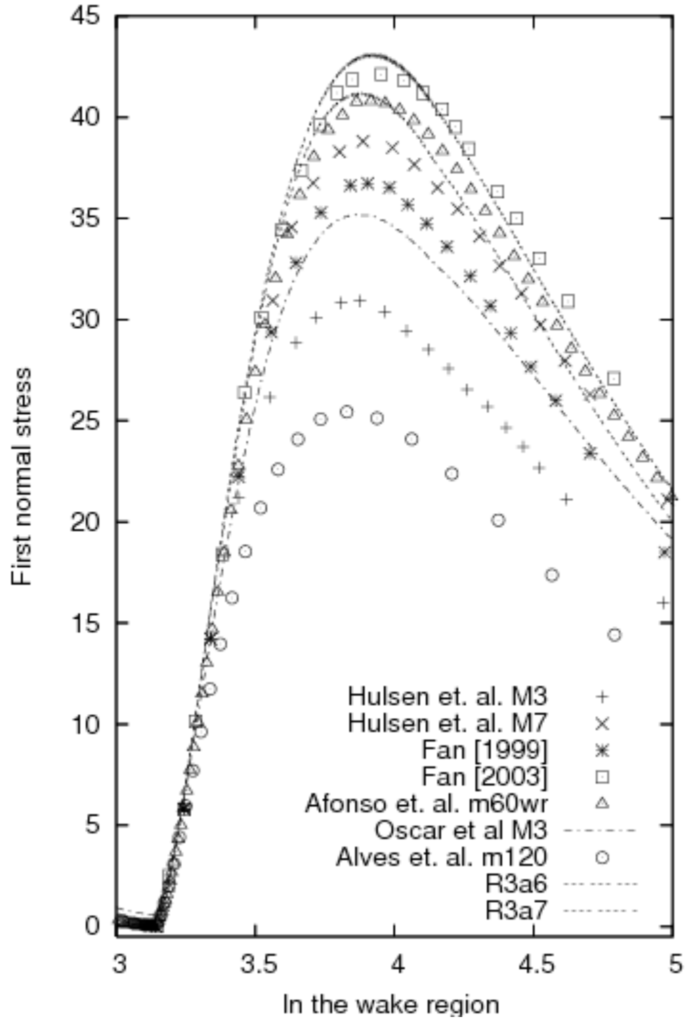

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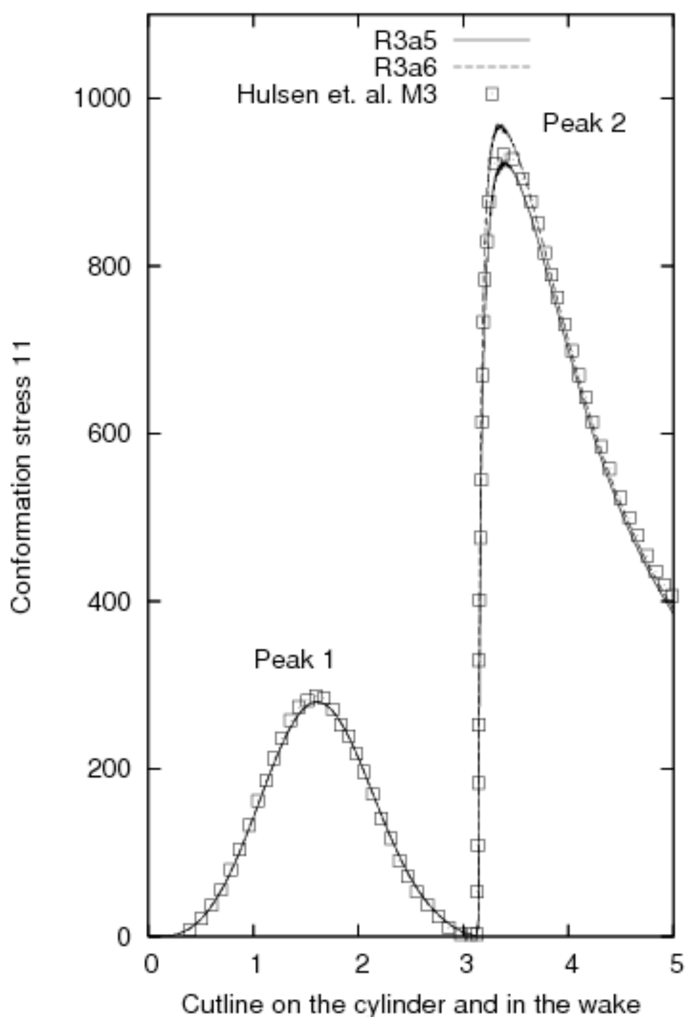


The lack of pointwise mesh convergence !

Solvers

- **M-FEM Newton solution Oldroyd-B vs. Giesekus**

Oldroyd-B

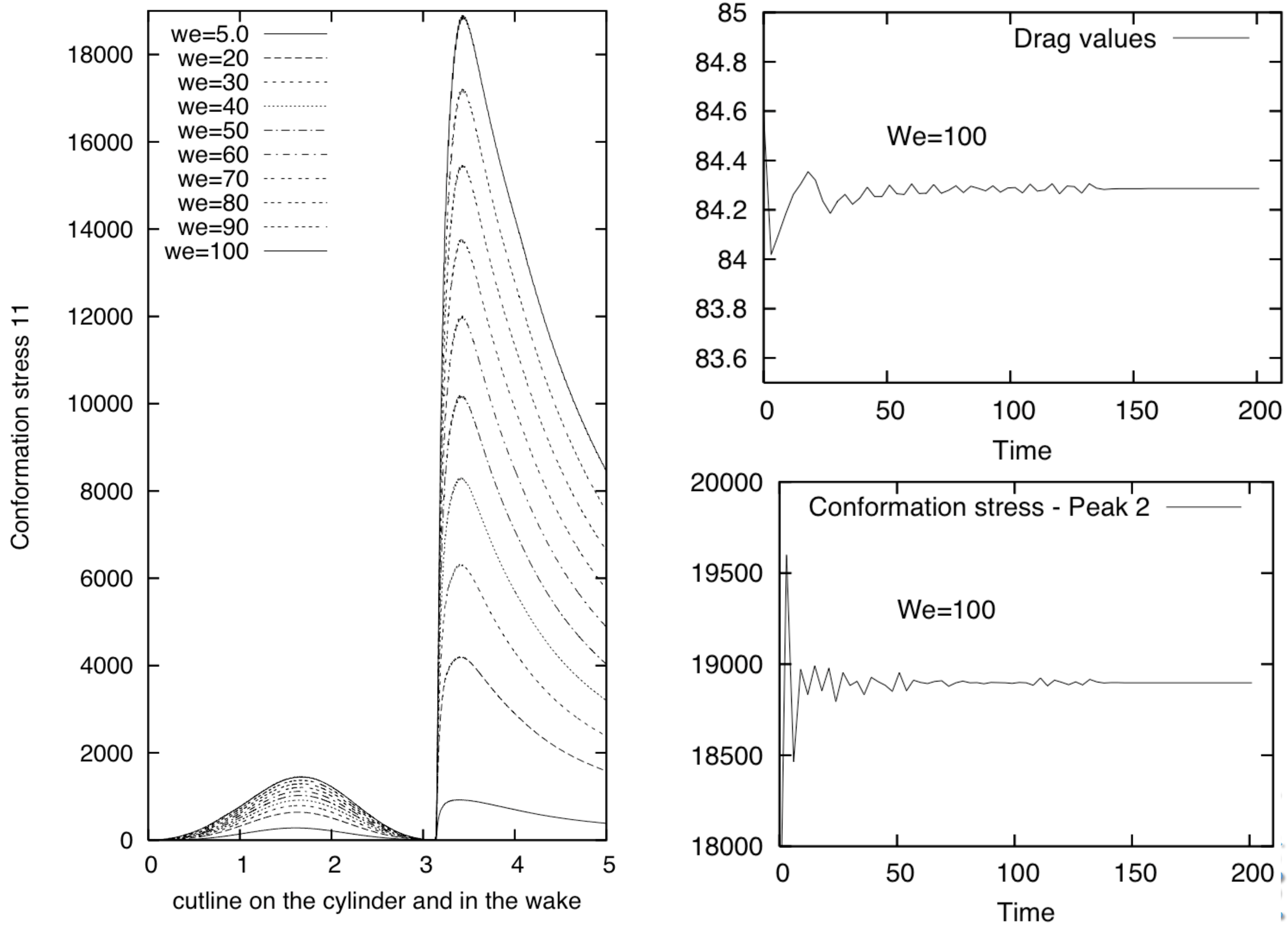
We	Drag	NL	We	Drag	NL	We	Drag	NL
0.1	130.366	8	0.8	117.347	4	1.5	125.665	4
0.2	126.628	5	0.9	117.762	4	1.6	127.523	4
0.3	123.194	4	1.0	118.574	6	1.7	129.494	4
0.4	120.593	4	1.1	119.657	6	1.8	131.578	4
0.5	118.828	4	1.2	120.919	5	1.9	133.754	4
0.6	117.779	4	1.3	122.350	4	2.0	136.039	5
0.7	117.321	4	1.4	123.936	4	2.1	138.438	5

Giesekus

We	Drag	Peak 2	NL	We	Drag	Peak 2	NL
5.0	96.943	924.45	14	60	85.859	12010.57	4
20	89.905	4204.51	12	70	85.356	13773.61	4
30	88.304	6318.79	5	80	84.937	15502.45	4
40	87.256	8311.32	5	90	84.585	17207.87	4
50	86.476	10199.10	4	100	84.287	18897.95	4

Stable Newton solver !

- **Direct steady vs. non-steady approach for Giesekus**



Summary

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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 full coupling**
- ✓ **Positivity preserving**
- ✓ **Higher order and local adaptivity**