Monolithic FEM Techniques for Viscoelastic Flow

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ECCOMAS CFD 2010, Lissabon

Governing Equations

- **Generalized Navier-Stokes equations**

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

$$D(u) = \frac{1}{2}(\nabla u + (\nabla u)^{\mathrm{T}})$$

$$\boxed{\sigma = \sigma^{s} + \sigma^{p}}$$

- **Viscous stress**

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

- **Elastic stress**

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

- **Viscous stress**

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

➢ **Power law model**

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

➢ **Carreau model**

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

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

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

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

(ϕ 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**

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

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

Constitutive Models (III)

- **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**

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

Problem Reformulation

Old → $(\mathrm{u}, \mathrm{p}, \boldsymbol{\sigma}^p)$

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

Conformation tensor →(u, p, τ) which is positive definite by design

Replace σ^p in (1) with $\sigma^p = \dfrac{\eta_p}{\Lambda}(\tau - \mathrm{I})$ → special discretization: TVD

$$
\left.
\begin{aligned}
&\rho\left(\frac{\partial \mathrm{u}}{\partial t} + \mathrm{u}\cdot\nabla\mathrm{u}\right) = -\nabla p + 2\eta_s \nabla\cdot D + \frac{\eta_p}{\Lambda}\nabla\cdot\tau,\\
&\nabla\cdot\mathrm{u} = 0,\\
&\frac{\delta_{\mathrm{a}}\tau}{\delta t} + \frac{1}{\Lambda}(\tau - \mathrm{I}) = 0
\end{aligned}
\right\} \quad (2)
$$

Conformation Tensor Properties

$$\tau(t) = \int_{\infty}^{t} \frac{1}{\mathrm{We}} \exp\left(\frac{-(t-s)}{\mathrm{We}} \right) F(s,t)\, F(s,t)^T\, ds$$

Positive by design,
so we can take its logarithm

2 Observations:

- positive definite → special discretizations like FCT/TVD
- exponential behaviour → approximation by polynomials???

Problem Reformulation

Replace τ in (2) with $\tau = \exp\psi$

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

Gradient of exponential of ψ → ???

Solvers → ???

Experiences:

- Stresses grow exponentially
- Conformation tensor is positive by design

Idea:

- Decompose the velocity gradient inside the stretching part

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

- Take the logarithm as a new variable $\psi = \log \tau$ using eigenvalue decomposition

$$\psi = R \log(\lambda_\tau)\, R^T$$

LCR for Oldroyd-B Model

$$\tau(t) = \int_{\infty}^{t} \frac{1}{\mathrm{We}} \exp\left(\frac{-(t-s)}{\mathrm{We}}\right) F(s,t)\, F(s,t)^{T}\, ds$$

Oldroyd-B

$$\mathrm{We}\frac{\delta_a \sigma^p}{\delta t} + \sigma^p - 2\eta_p D = 0,$$

$$\sigma^p = \frac{\eta_p}{\mathrm{We}}(\tau - I)$$

$$\frac{\delta_a \tau}{\delta t} + \frac{1}{\mathrm{We}}(\tau - I) = 0,$$

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

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

$$\tau = \exp\ \psi \qquad \psi = R \log(\lambda_\tau)\, R^T$$

LCR

$$\partial_t \psi + (\nabla u)\psi - (\Omega.\psi - \psi.\Omega) + 2B = \frac{1}{\mathrm{We}}(\exp(-\psi) - I)$$

- **LCR equations**

$$\rho(\frac{\partial}{\partial t}+u\cdot\nabla)u = -\nabla p+\nabla\cdot(2\eta_s(D_{\mathrm{II}},p)D(u))+\frac{\eta_p}{\mathrm{We}}\nabla\cdot e^{\psi},$$

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

$$(\frac{\partial}{\partial t}+u\cdot\nabla)\psi-(\Omega\psi-\psi\Omega)-2\mathrm{B}=\frac{1}{\mathrm{We}}f(\psi).$$

- **Oldroyd-B model**

$$f(\psi)=(e^{-\psi}-I).$$

- **Giesekus model**

$$f(\psi)=(e^{-\psi}-I)-\alpha e^{\psi}(e^{-\psi}-I)^2.$$

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- **FEM techniques have to handle the following challenging points**
  - Stable FE spaces for velocity/pressure and velocity/extra-stress fields
    → Q2/P1/Q2 or Q1(nc)/P0/Q1(nc) (new: Q2(nc)/P1/Q2(nc))
  - Special treatment of the convective terms $\mathrm{u} \cdot \nabla \mathrm{u}$, $\mathrm{u} \cdot \nabla \sigma$
    → Edge-Oriented/interior penalty EO-FEM, TVD/FCT
  - High Weissenberg number problem (HWNP) via LCR

- **Solvers have to deal with different sources of nonlinearity**
  - nonlinear viscosity → Newton method via divided differences
  - strong coupling of equations → monolithic multigrid approach
  - complex geometries and meshes

FEM Discretization

- **High order $Q_2/Q_2/P_1^{\mathrm{disc}}$ 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**

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

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

EO-FEM

- **Edge-Oriented FEM stabilization for**

  - **convection 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 !

Nonlinear Solver

- **Damped Newton 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:** Jacobian 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

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- **Monolithic multgrid solver**

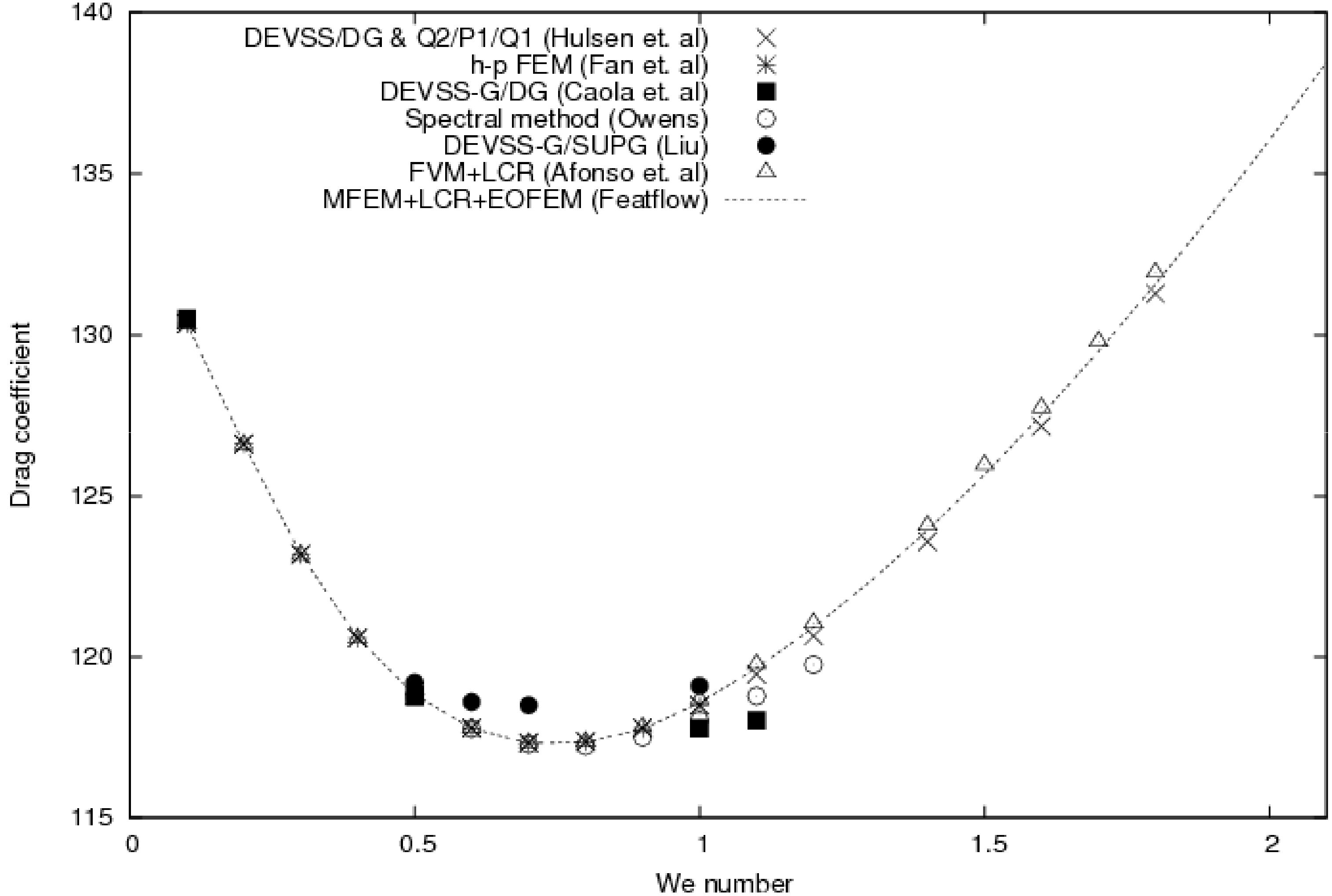
  - **Standard geometric multigrid approach**
  - **Full Q_2, P_1^{disc} restrictions and prolongations**
  - **Local MPSC via Vanka-like smoother**

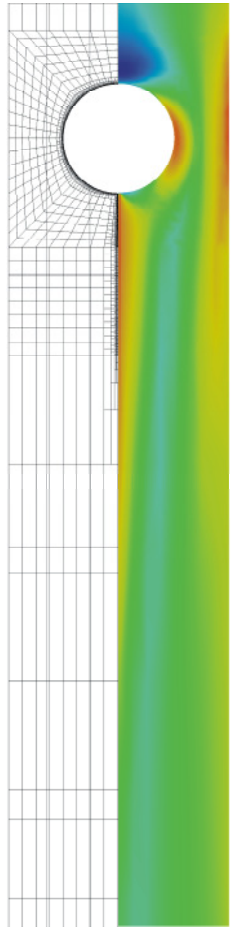
$$\begin{bmatrix} u^{l+1} \\ \sigma^{l+1} \\ p^{l+1} \end{bmatrix} = \begin{bmatrix} u^{l} \\ \sigma^{l} \\ p^{l} \end{bmatrix} + \omega^l \sum_{T \in \mathcal{T}_h} \left[(\tilde{K} + J)_{|T} \right]^{-1} \begin{bmatrix} Res_u \\ Res_\sigma \\ Res_p \end{bmatrix}_{|T}$$

Coupled Monolithic Multigrid Solver !

Viscoelastic Benchmark

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

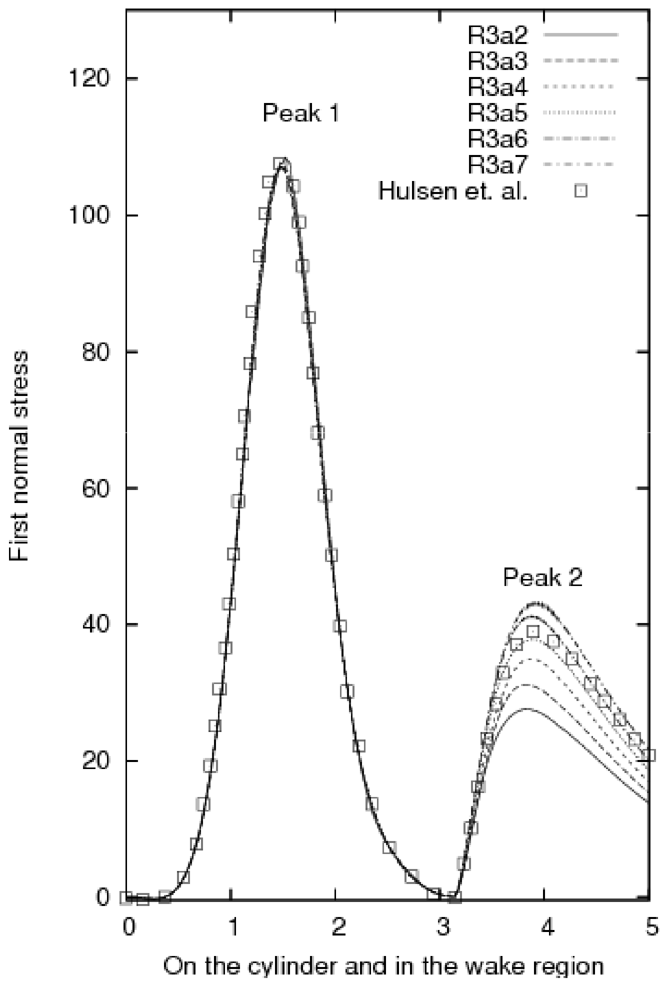




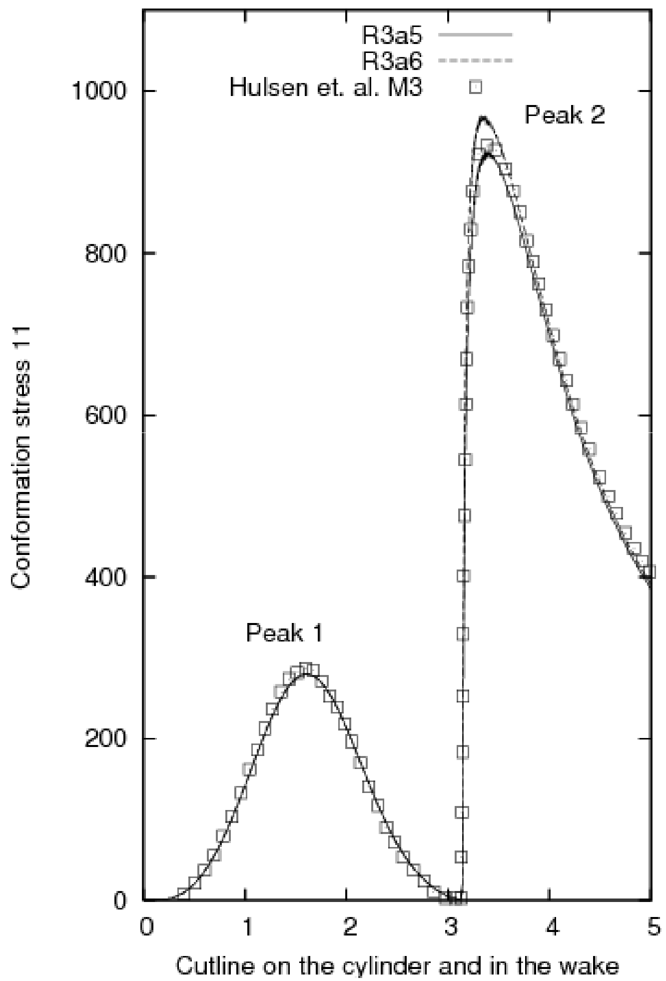
The numerical method is quantitatively validated

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

We 0.7



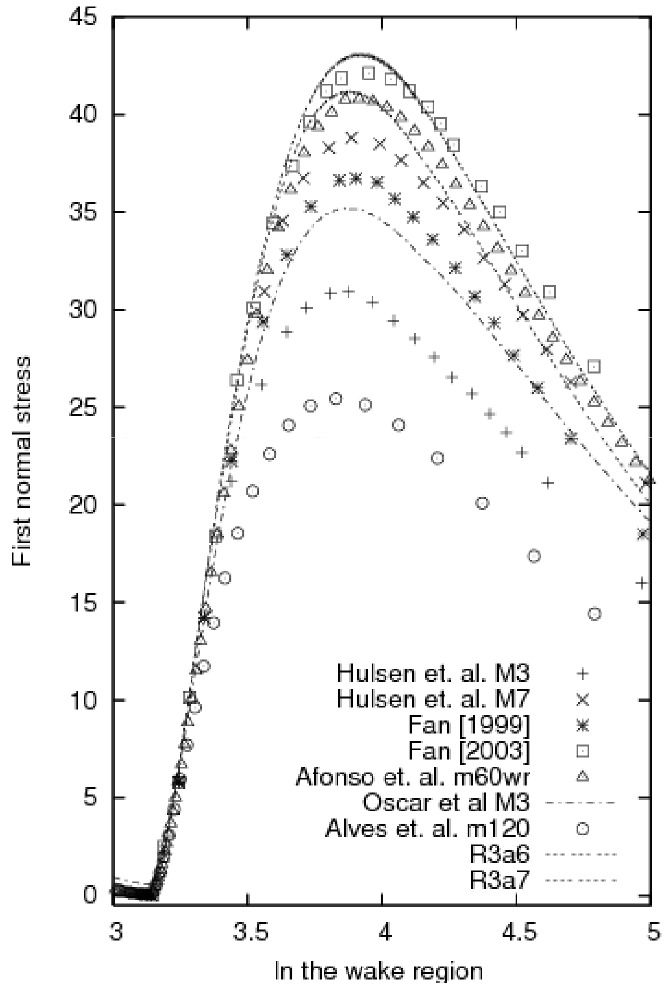
We 5.0



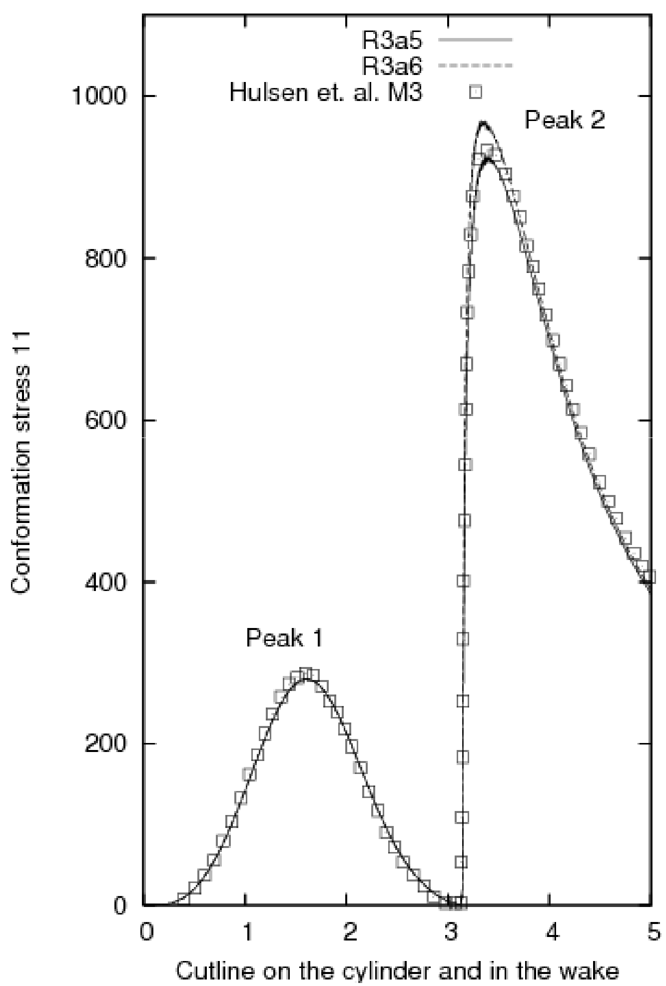
Lack of pointwise mesh convergence !

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

We 0.7



We 5.0



Lack of pointwise mesh convergence !

- **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	Peak2	NL	WE	Drag	Peak2	NL
5	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 !

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 Newton-Multigrid Solver with local MPSC smoother**

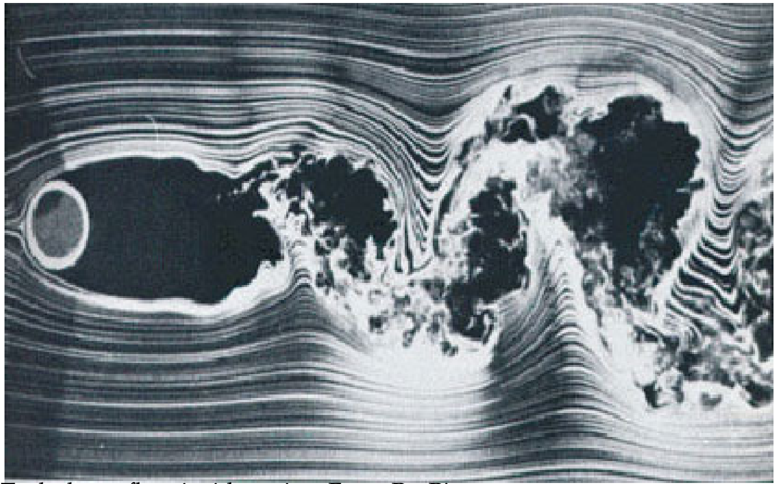
for the simulation of viscoelastic flow

Advantages

- ✓ **No CFL-condition restriction due to the full coupling**
- ✓ **Positivity preserving**
- ✓ **Higher order and local adaptivity**

Inertia turbulence

- Re>>1
- Numerical instabilities + problems



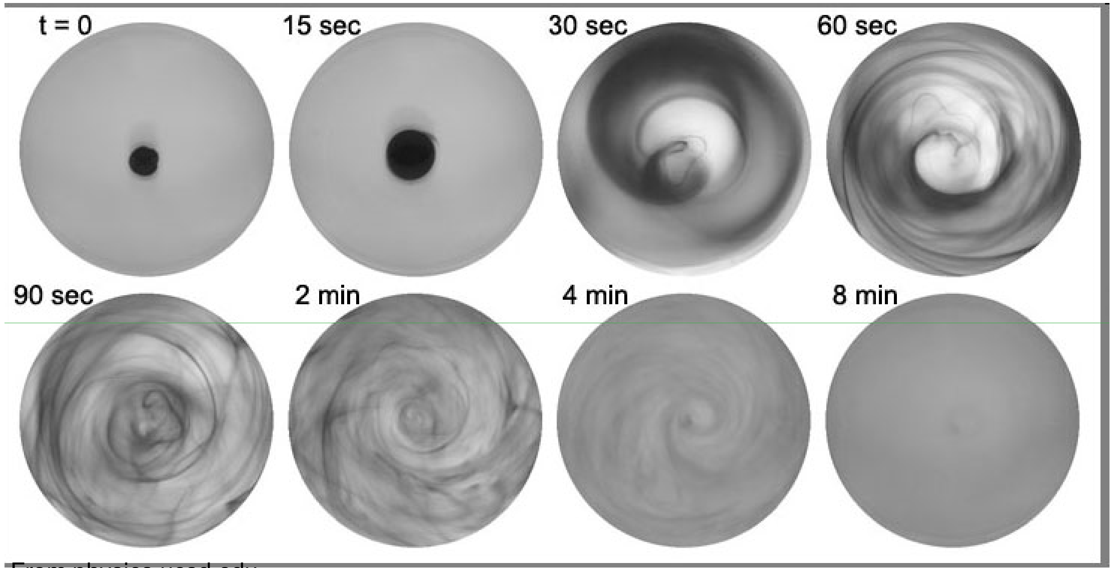
Turbulence flow inside a pipe. From ProPipe

→ Turbulence Models
→ Stabilization Techniques

Characteristics:
- Irregular temporal behaviour and spatially disordered
- Broad range of spatial/temporal scales

Elastic turbulence

- Re<<1, *We*>>1 (less inertia, more elasticity)
- Numerical instabilities + problems (HWNP)



From physics.ucsd.edu

→ Flow models: Oldroyd, Giesekus, Maxwell,…
→ Stabilization: EEME, EEVS, DEVSS/DG, SD, SUPG,…

Required: Special Numerics

Special FEM Techniques

Multigrid Solvers

Stabilization for high Re and We numbers

Implicit Approaches

Space-Time Adaptivity

Grid Deformation Methods

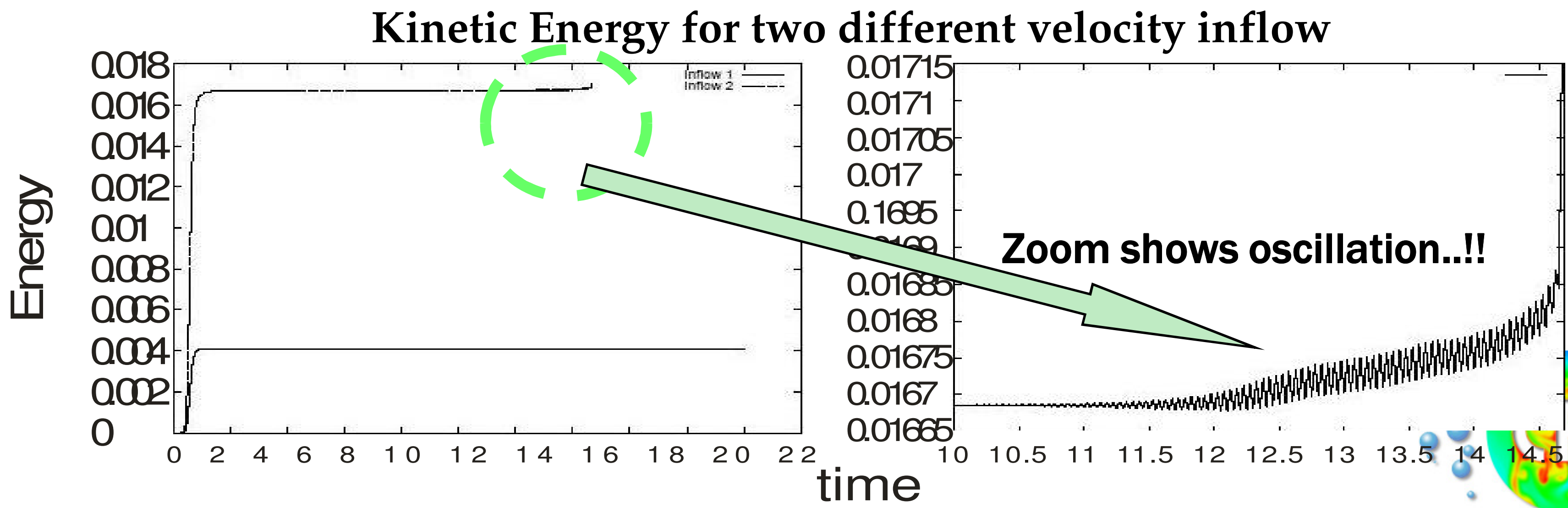
Newton Methods

Problems remain…

Different highly developed models

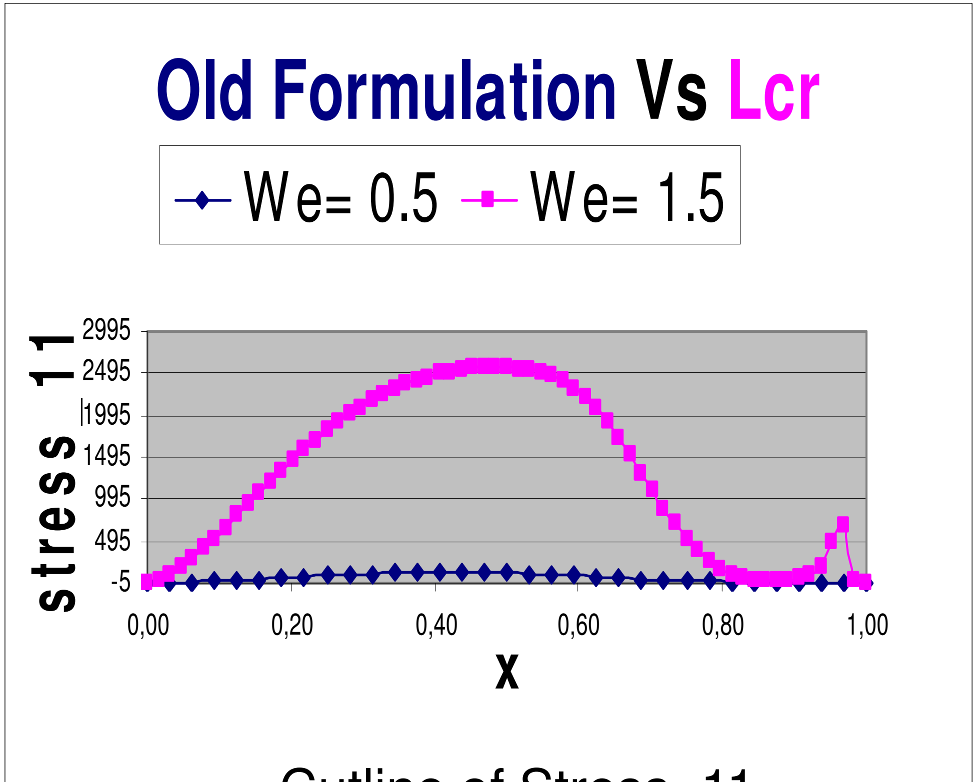
Oldroyd A/B, Maxwell A/B, Jeffreys, PTT, Giesekus

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

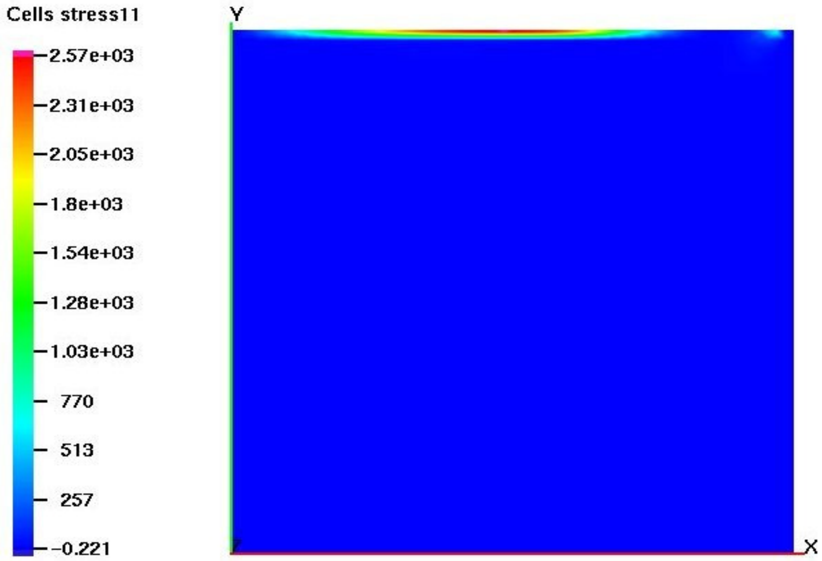


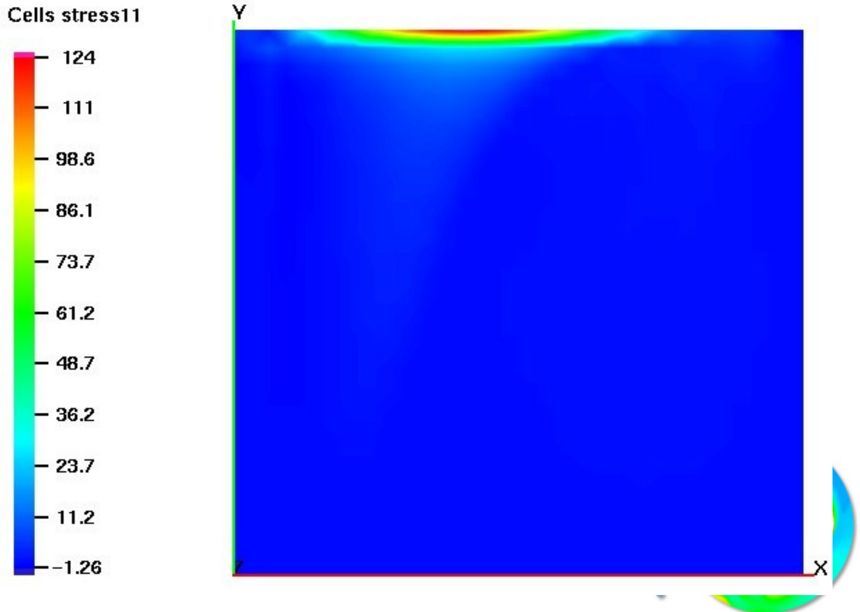
Fully implicit monolithic FEM Multigrid solver for LCR formulation!

Driven cavity example:
as We number changes from We=0.5 to We=1.5, the stress value jumps significantly



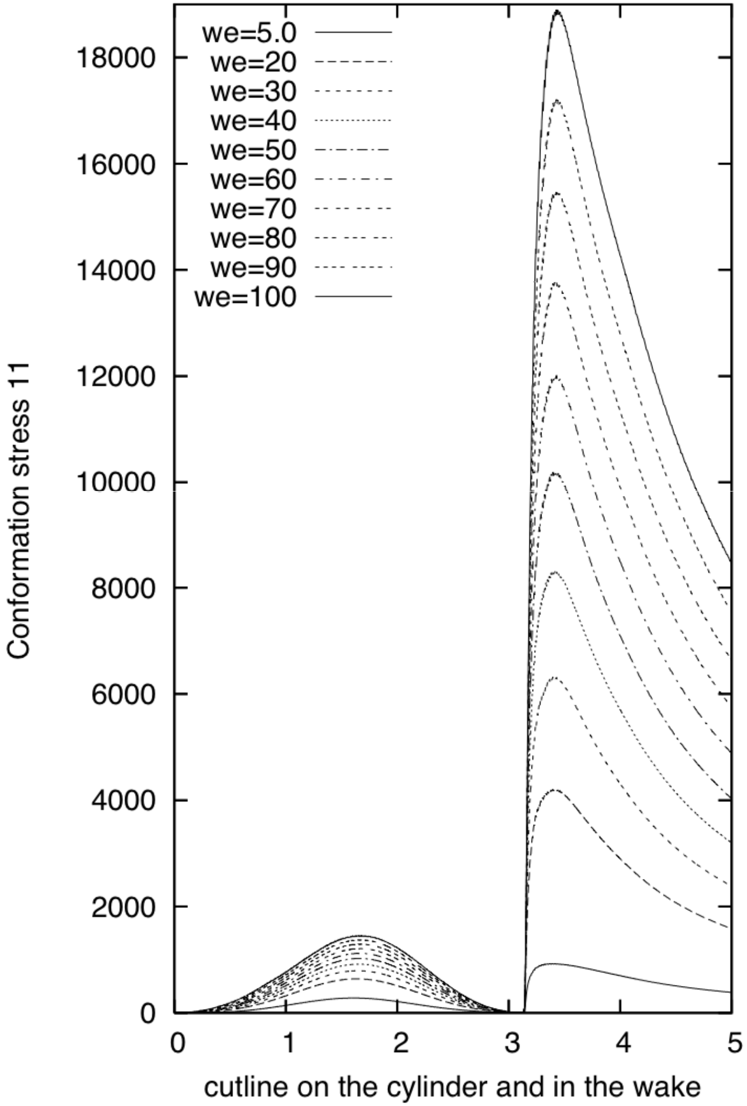
Cutline of Stress_11 component at y = 1.0

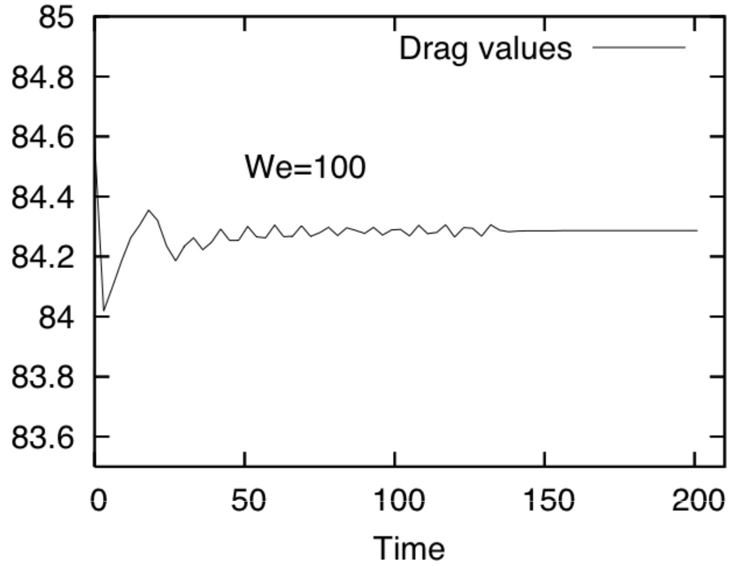


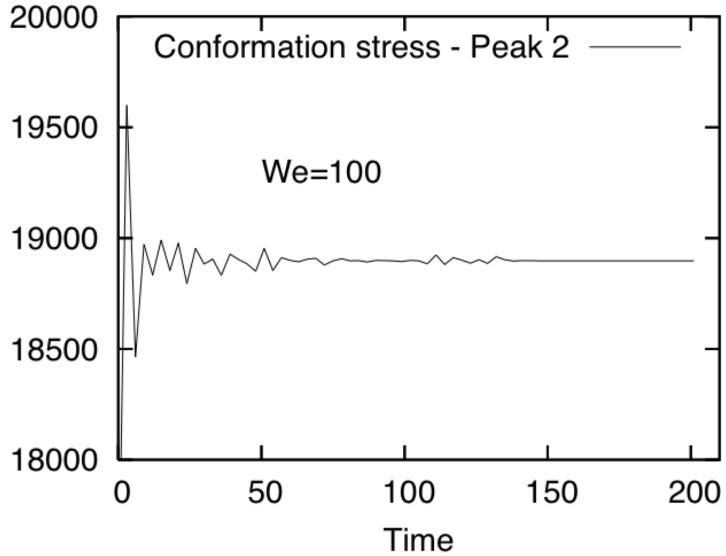


Solvers

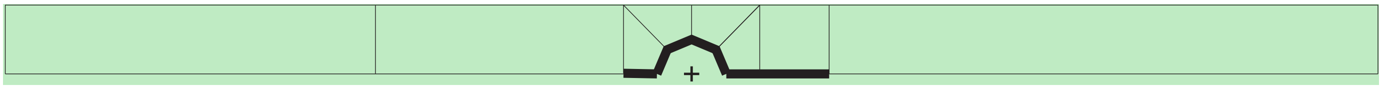
- **Direct steady vs. non-steady approach for Giesekus**







Planar Flow around Cylinder



We	0.01		0.1		1.0	
Linear Tol	0.1	0.01	0.1	0.01	0.1	0.01
R1	9/2	5/3	10/1	7/3	14/1	10/3
R2	9/3	5/5	10/2	7/4	16/2	10/5
R3	9/3	5/6	10/3	7/5	16/2	11/5
R4	9/3	5/6	10/3	9/5	13/3	11/5

Stable Newton and multigrid solver !