Monolithic FEM Techniques for Viscoelastic Flow

S. Turek, A. Ouazzi, H. Damanik
Institute of Applied Mathematics, LS III, TU Dortmund
http://www.featflow.de

ECCOMAS CFD 2010, Lissabon
• **Generalized Navier-Stokes equations**

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

\[
D(u) = \frac{1}{2} (\nabla u + (\nabla u)^T)
\]

\[
\sigma = \sigma^s + \sigma^p
\]

• **Viscous stress**

\[
\sigma^s = 2\eta_s (D_\Pi, p) D, \quad D_\Pi = \text{tr}(D(u)^2).
\]

• **Elastic stress**

\[
\sigma^p + \text{We} \frac{\partial \varepsilon^T \sigma^p}{\partial t} = 2\eta_p D(u).
\]
Constitutive Models (I)

- **Viscous stress**

\[ \sigma^s = 2 \eta_s (D_{11}, p) D_1, \quad D_1 = \text{tr}(D(u)^2). \]

- **Power law model**

\[ \eta_s(z, p) = \eta_0 z^2 \quad , \quad (\eta_0 > 0, r > 1) \]

- **Carreau model**

\[ \eta_s(z, p) = \eta_\infty + (\eta_0 - \eta_\infty)(1 + \lambda z)^{-1} \]

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

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

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

\[ (\phi \text{ is angle of internal friction, } r > 1) \]
Constitutive Models (II)

- Elastic stress

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

- Upper/Lower convective derivative

\[
\frac{\delta_a \sigma}{\delta l} = \left( \frac{\partial}{\partial l} + u \cdot \nabla \right) \sigma + g_u(\sigma, \nabla u)
\]

\[
g_u(\sigma, \nabla u) = \frac{1 - a}{2} \left( \sigma \nabla u + (\nabla u)^T \sigma \right) - \frac{1 + a}{2} \left( \nabla u \sigma + \sigma (\nabla u)^T \right) \quad (a = \pm 1)
\]
Constitutive Models (III)

- **Generalized differential constitutive model**

\[
\sigma \mid \mathcal{W} \frac{\delta_{\alpha} \sigma}{\delta t} \mid \mathbf{G}(\sigma, D) \mid \mathbf{H}(\sigma) = 2\eta_p D(u)
\]

- **Oldroyd**

\[
\mathbf{G} = 0, \quad \mathbf{H} = 0
\]

- **Giesekus**

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

- **Phan-Thien and Tanner**

\[
\mathbf{G} = 0, \quad \mathbf{H} = [\exp(\alpha \text{tr}(\sigma)) \quad 1] \sigma
\]

- **White and Metzner**

\[
\mathbf{G} = \alpha (2D : D)^{1/2}, \quad \mathbf{H} = 0
\]
Problem Reformulation

Old $\Rightarrow (u, p, \sigma^p)$

\[
\begin{align*}
\rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) &= -\nabla p + 2\eta_s \nabla \cdot D + \nabla \cdot \sigma^p, \\
\nabla \cdot u &= 0, \\
\Lambda \frac{\delta_a \sigma^p}{\delta t} + \sigma^p - 2\eta_p D &= 0
\end{align*}
\]

Conformation tensor $\Rightarrow (u, p, \tau) \text{ which is positive definite by design}$

Replace $\sigma^p$ in (1) with $\sigma^p = \frac{\eta_p}{\Lambda} (\tau - I) \Rightarrow \text{special discretization: TVD}$

\[
\begin{align*}
\rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) &= -\nabla p + 2\eta_s \nabla \cdot D + \frac{\eta_p}{\Lambda} \nabla \cdot \tau, \\
\nabla \cdot u &= 0, \\
\frac{\delta_a \tau}{\delta t} + \frac{1}{\Lambda} (\tau - I) &= 0
\end{align*}
\]
Conformation Tensor Properties

\[ \tau(t) = \int_0^t \frac{1}{\text{We}} \exp \left( -\frac{(t - s)}{\text{We}} \right) F(s, t) F(s, t)^T ds \]

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

\[
\rho \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) = -\nabla p + 2\eta_s \nabla \cdot D + \frac{\eta_p}{\text{We}} \nabla \cdot (\exp \psi),
\]

$\nabla \cdot u = 0,$

\[
\frac{\delta_a (\exp \psi)}{\delta t} + \frac{1}{\text{We}} (\exp \psi - 1) = 0
\]

Gradient of exponential of $\psi \rightarrow ???$

Solvers $\rightarrow ???$
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

\[
\psi = R \log(\lambda) R^T
\]
LCR for Oldroyd-B Model

\[ \tau(t) = \int_0^t \frac{1}{\text{We}} \exp \left(-\frac{(t-s)}{\text{We}}\right) F(s, t) F(s, t)^T \, ds \]

Oldroyd-B

\[ \text{We} \frac{\delta \sigma^p}{\delta t} + \sigma^p - 2\eta_p D = 0, \]

\[ \sigma^p = \frac{\eta_p}{\text{We}} (\tau - I) \]

\[ \frac{\delta_a \tau}{\delta t} + \frac{1}{\text{We}} (\tau - I) = 0, \]

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

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

\[ \tau = \exp \psi \quad \psi = R \log(\lambda_t) R^T \]

LCR

\[ \partial_t \psi + (\nabla u) \psi - (\Omega \psi - \psi \cdot \Omega) + 2B = \frac{1}{\text{We}} (\exp(-\psi) - I) \]
LCR Equations for Different Models

- LCR equations

\[
\rho \frac{d}{dt} (u \cdot \nabla) u = -\nabla p + \nabla \cdot (2\eta_s (D_{II}, p) D(u)) + \frac{\eta_p}{\text{We}} \nabla \cdot e^\psi, \\
\nabla \cdot u = 0,
\]

\[
\frac{d}{dt} (\psi \cdot \nabla) \psi - (\Omega \psi - \psi \Omega) - 2B = \frac{1}{\text{We}} f(\psi).
\]

- Oldroyd-B model

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

- Giesekus model

\[
f(\psi) = (e^{-\psi} - I) - \alpha e^\psi (e^{-\psi} - I)^2.
\]
Numerical Techniques

- 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 $u \cdot \nabla u$, $u \cdot \nabla \sigma$
    → 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 $Q_2/Q_2/P_1^{\text{disc}}$ for velocity-stress-pressure

- Advantages:
  - Inf-sup stable for velocity and pressure
    \[ \sup_{u \in [H^1_0(\Omega)]^2} \frac{\int_{\Omega} \nabla \cdot u \, q \, dx}{\|u\|_{1, \Omega}} \geq \beta_1 \|q\|_{0, \Omega} \quad \forall q \in L^2_0(\Omega) \]
  - 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

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

• Inexact Newton: Jacobian is approximated using finite differences

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

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

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

Typical saddle point problem!
• **Monolithic multgrid solver**

- **Standard geometric multigrid approach**

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

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

\[
\begin{bmatrix}
\begin{array}{c}
\mathbf{u}^{l+1} \\
\mathbf{\sigma}^{l+1} \\
\mathbf{p}^{l+1}
\end{array}
\end{bmatrix} = \begin{bmatrix}
\begin{array}{c}
\mathbf{u}^{l} \\
\mathbf{\sigma}^{l} \\
\mathbf{p}^{l}
\end{array}
\end{bmatrix} + \omega^{l} \sum_{T \in h} \left[ (\widetilde{\mathbf{K}} - J)_{|T} \right]^{-1} \begin{bmatrix}
\begin{array}{c}
\text{Res}_u \\
\text{Res}_\sigma \\
\text{Res}_p
\end{array}
\end{bmatrix}_{|T}
\]

**Coupled Monolithic Multigrid Solver !**
Viscoelastic Benchmark

- Planar flow around cylinder (Oldroyd-B)

The numerical method is quantitatively validated.

S. Turek | FEM for LCR of viscoelastic
Viscoelastic Benchmark

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

\[ \text{WC} = 0.7 \]

\[ \text{WC} = 5.0 \]

Lack of pointwise mesh convergence!
Viscoelastic Benchmark

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

Lack of pointwise mesh convergence!

S. Turek | FEM for LCR of viscoelastic
- **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 | 126.666 | 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 | 8  | 80  | 84.987 | 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!*
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 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)

→ 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...

![Kinetic Energy for two different velocity inflow](Image)

**Zoom shows oscillation...!!**
Our Numerical Approach

Fully implicit monolithic FEM
Multigrid solver for LCR formulation!
Exponential Behaviour

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

Old Formulation Vs Lcr

\[ \text{We} = 0.5 \quad \text{We} = 1.5 \]

Cutline of Stress_11 component at y = 1.0
• Direct steady vs. non-steady approach for Giesekus
### Planar Flow around Cylinder

<table>
<thead>
<tr>
<th>We</th>
<th>Linear Tol</th>
<th>0.01</th>
<th>0.1</th>
<th>1.0</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0.1</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>R1</td>
<td></td>
<td>9/2</td>
<td>10/1</td>
<td>14/1</td>
</tr>
<tr>
<td>R2</td>
<td></td>
<td>9/3</td>
<td>10/2</td>
<td>16/2</td>
</tr>
<tr>
<td>R3</td>
<td></td>
<td>9/3</td>
<td>10/3</td>
<td>16/2</td>
</tr>
<tr>
<td>R4</td>
<td></td>
<td>9/3</td>
<td>10/3</td>
<td>13/3</td>
</tr>
</tbody>
</table>

**Stable Newton and multigrid solver!**