FEM techniques and multigrid solvers for non-isothermal viscoelastic flows

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SFB/TR TRR 30 meeting, Paderborn: November 9th, 2007
Goal of the project (Dortmund)

- FEM-techniques for the numerical simulation of flow problems with non-isothermal nonlinear material models
- Implicit, monolithic CFD methods with high accuracy, robustness and efficiency
- Grid adaptation and error control

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FeatFlow
Governing equations

- **Momentum, mass and energy equations**

\[
\rho \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \text{div } \mathbf{\sigma} + \nabla \rho = \rho \mathbf{f}, \quad \text{div } \mathbf{u} = 0,
\]

\[
\frac{\partial \Theta}{\partial t} + \mathbf{u} \cdot \nabla \Theta - \text{div } k \nabla \Theta - \mathbf{D} : \mathbf{\sigma} = 0,
\]

\[
\mathbf{\sigma} = \mathbf{\sigma}^s + \mathbf{\sigma}^p, \quad \mathbf{D} = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)
\]

- **quasi-Newtonian model**

\[
\mathbf{\sigma}^s = 2\nu_s(\mathbf{D}, \Theta)\mathbf{D}
\]

- **Constitutive model**

\[
\mathbf{\sigma}^p + \lambda \frac{D_a \mathbf{\sigma}^p}{Dt} = 2\nu_p \mathbf{D},
\]

\[
\frac{D_a \mathbf{\sigma}}{Dt} = \left( \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{\sigma} + \frac{1 - a}{2} \left( \mathbf{\sigma} \nabla \mathbf{u} + \nabla \mathbf{u}^T \mathbf{\sigma} \right) - \frac{1 + a}{2} \left( \nabla \mathbf{u} \mathbf{\sigma} + \mathbf{\sigma} \nabla \mathbf{u}^T \right)
\]
Mathematical Challenges

The FEM techniques have to handle the following challenging points

- Stable FE spaces for velocity and pressure fields: inf-sup condition has to be satisfied
- Stable FE spaces for the velocity and extra-stress fields or adequate stabilization procedure
- Special treatment of the convective terms $\mathbf{u} \cdot \nabla \mathbf{u}$, $\mathbf{u} \cdot \nabla \Theta$ and $\mathbf{u} \cdot \nabla \sigma$
- The presence of the “reactive” Johnson-Segalman term

$$
\frac{1 - a}{2} (\sigma \nabla \mathbf{u} + \nabla \mathbf{u}^T \sigma) - \frac{1 + a}{2} (\nabla \mathbf{u} \sigma + \sigma \nabla \mathbf{u}^T)
$$

which is responsible for

- no availability of a priori estimates
- low Weissenberg number limitation
- blow up phenomena for time dependent solution
Finite Element Discretization

**The nonconforming \( \tilde{Q}_1/P_0 \)**

\[
\tilde{Q}_1 := \{ q \circ \psi_T^{-1} : q \in \text{span} < 1, x, y, x^2 - y^2 > \}
\]

The degree of freedom are determined by the nodal functionals \( \{ F_{\Gamma}^{(a,b)}(\cdot), \Gamma \subset \partial T_h \} \), with \( F_{\Gamma}^a := |\Gamma|^{-1} \int_{\Gamma} \mathbf{v} d\gamma \) or \( F_{\Gamma}^b := \mathbf{v}(m_{\Gamma}) \)

→ **High efficiency with minimal degrees of freedom**

**The conforming \( Q_2/P_1^{\text{disc}} \)**

\[
Q_2(T) := \{ q \circ \psi_T^{-1} : q \in \text{span} < 1, x, y, xy, x^2, y^2, x^2y, y^2x, x^2y^2 > \}
\]
\[
P_1(T) := \{ q \circ \psi_T^{-1} : q \in \text{span} < 1, x, y > \}
\]

→ **High accuracy with minimal numerical complexity**
Discrete nonlinear system

\[
\begin{pmatrix}
A_u(u, \Theta) & 0 & C & B \\
0 & A_\Theta(u) & E & 0 \\
C^T & 0 & A_\sigma(u) & 0 \\
B^T & 0 & 0 & 0 \\
\end{pmatrix}
\begin{pmatrix}
u \\
\Theta \\
\sigma \\
p \\
\end{pmatrix}
=
\begin{pmatrix}
\text{rhs}_u \\
\text{rhs}_\Theta \\
\text{rhs}_\sigma \\
\text{rhs}_p \\
\end{pmatrix}
\]

Typical discrete saddle point problem

\[
A_u(u, \Theta) = L_u(u, \Theta) + N(u), \quad A_\Theta(u) = kL_\Theta + N(u),
\]
\[
A_\sigma(u) = \frac{1}{\lambda} M + N(u) + G_a(u), \quad E = [-D_{11} - 2D_{12} - D_{22}]
\]

\[
B \text{ and } C \text{ are the discrete gradient operator applied to the pressure and velocity spaces respectively, } M \text{ is the mass matrix, } \omega = \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2},
\]
\[
d_{ij} = \frac{1}{2} (\sum_{i,j=1}^{2} \frac{\partial u_i}{\partial x_j}), \quad [W]_{k,l} = \omega [M]_{k,l} \text{ and } [D_{ij}]_{k,l} = d_{ij} [M]_{k,l}
\]

\[
G_a(u) = \begin{pmatrix}
-2ad_{11} & W - 2ad_{12} & 0 \\
-\frac{1}{2}W - ad_{12} & 0 & \frac{1}{2}W - ad_{12} \\
0 & -W - 2ad_{12} & -2ad_{22} \\
\end{pmatrix}
\]

Usefull matrix for spectral analysis!
Inexact Newton solver

- A system for the residual of nonlinear algebraic equations is obtained

\[ \mathcal{R}(x) = 0, \quad x = (u_h, \sigma_h, \Theta_h, p_h) \]

- Newton method with damping results in iterations of the form

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

- The damping parameter \( \omega^n \in (-1, 0) \) is chosen such that

\[ \mathcal{R}(x^{n+1}) \cdot x^{n+1} \leq \mathcal{R}(x^n) \cdot x^n \]

- The Jacobian matrix \( \left[ \frac{\partial \mathcal{R}(x^n)}{\partial x} \right] \) is approximated using finite differences as

\[ \left[ \frac{\partial \mathcal{R}(x^n)}{\partial x} \right]_{ij} \approx \frac{\mathcal{R}_i(x^n + \varepsilon e_j) - \mathcal{R}_i(x^n - \varepsilon e_j)}{2\varepsilon} \]
Multigrid solver

- Standard geometric multigrid approach
- Full $Q_2$, $Q_1$, $P_1^{\text{disc}}$ and $P_0$ prolongation and restriction
- Smoother Local/Global MPSC
  - Local MPSC via Vanka-like smoother
    \[
    \begin{bmatrix}
    u^{l+1} \\
    \sigma^{l+1} \\
    \Theta^{l+1} \\
    p^{l+1}
    \end{bmatrix}
    =
    \begin{bmatrix}
    u^l \\
    \sigma^l \\
    \Theta^l \\
    p^l
    \end{bmatrix}
    + \omega^l \sum_{T \in \mathcal{T}_h} [K_T]^{-1}
    \begin{bmatrix}
    \text{Res}_u \\
    \text{Res}_\sigma \\
    \text{Res}_\Theta \\
    \text{Res}_p
    \end{bmatrix}
    \bigg|_T
    \]

  - Global MPSC
    - solve for an intermediate $\tilde{u}$ (generalized momentum equation)
    - solve for $p$ (pressure poisson equation)
    - update of $u$ and $p$
    - solve for $\Theta$ (energy equation)
    - solve for $\sigma$ (constitutive equation)

Coupoleled multigrid solver

Decoupled multigrid solver
Numerical results: non-isothermal flow

- **energy equation with dissipation term**

  production of heat in absence of the source term
decoupled (left)/coupled (right) with constitutive equation

- **nonlinear viscosity:** \( \nu_s(D, \Theta) = \nu_0 e^{(a_1 + \frac{a_2}{a_3 + T})}(b_1 + b_2|D|)^{-b_3} \)

Blockage of the flow
Numerical results: visco-elastic flow

Stress components for $Re = 0.5$, $We = 0.05$

Kinetic energy for two different velocity boundary values

Blow up phenomena!

What should be the reason behind this limitation?
New Edge-oriented FEM Stabilization

- Based only on the “smoothness” of the discrete solution, we have proposed the following jump term:

\[ \sum_{\text{edge } E} \max(\gamma \nu h_E, \gamma^* h_E^2, \gamma_{\text{dist}} f(\text{dist}(\Gamma); h_E)) h_E \int_E [\nabla u][\nabla v] d\sigma \]

- only one generic stabilization takes care of all instabilities
  - Insatisfaction of Korn’s inequality in the case of low order FE approximation; Ouazzi, PhD Dortmund University (2005)
  - Convection dominated flow for medium and high Reynolds number, even for pure transport; Turek and Ouazzi, Unified edge-oriented stabilization of nonconforming finite element methods for incompressible flow problems: Numerical investigation, JNM (2007)
  - Spurious velocity due to the interface for flow with interfaces; Turek et. all, On pressure Separation Algorithms (PSepA) for improving the accuracy of incompressible flow simulation (2007)

Only the compatibility condition between velocity and pressure FE spaces is required
Outlook

- Use EO-FEM stabilization for
  - convective terms
  - same space approximation for velocity and extra-stress
- Reformulation of the constitutive equation
  - log-conformation formulation "Kupferman trick" (2004)
  - Lee and Xu formulation (2006)

Hope: make the HWNP mysterium a history!