FEM techniques and multigrid solvers for non-isothermal viscoelastic flows

S. Turek, H. Damanik and A. Ouazzi
(TP B3)

Institute for Applied Mathematics, LS III
University of Dortmund
Vogelpothsweg 87, D-44227 Dortmund, Germany

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

$$\Downarrow$$

FeatFlow

Governing equations

- **Momentum, mass and energy equations**

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \operatorname{div} \boldsymbol{\sigma} + \nabla p = \rho \mathbf{f}, \; \operatorname{div} \mathbf{u} = 0,$$

$$\frac{\partial \Theta}{\partial t} + \mathbf{u} \cdot \nabla \Theta - \operatorname{div} k \nabla \Theta - \mathbf{D} : \boldsymbol{\sigma} = 0,$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^s + \boldsymbol{\sigma}^p, \; \mathbf{D} = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

- **quasi-Newtonian model**

$$\boldsymbol{\sigma}^s = 2\nu_s(\mathbf{D}, \Theta)\mathbf{D}$$

- **Constitutive model**

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

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

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 $\mathbf{u} \cdot \nabla \boldsymbol{\sigma}$
- The presence of the "reactive" Johnson-Segalman term

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

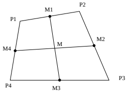
which is responsible for

  - 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 $\{F_\Gamma^{(a,b)}(\cdot), \Gamma \subset \partial \mathcal{T}_h\}$, with $F_\Gamma^a := |\Gamma|^{-1} \int_\Gamma v d\gamma$ or $F_\Gamma^b := v(m_\Gamma)$

$\rightarrow$ **High efficiency with minimal degrees of freedom**

- **The conforming Q_2/P_1^{disc}**

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

$\rightarrow$ **High accuracy with minimal numerical complexity**

Discrete nonlinear system

$$\begin{pmatrix} A_{\mathbf{u}}(\mathbf{u},\Theta) & 0 & C & B \\ 0 & A_{\Theta}(\mathbf{u}) & E & 0 \\ C^T & 0 & A_{\boldsymbol{\sigma}}(\mathbf{u}) & 0 \\ B^T & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \Theta \\ \boldsymbol{\sigma} \\ p \end{pmatrix} = \begin{pmatrix} \mathrm{rhs}_{\mathbf{u}} \\ \mathrm{rhs}_{\Theta} \\ \mathrm{rhs}_{\boldsymbol{\sigma}} \\ \mathrm{rhs}_{p} \end{pmatrix}$$

Typical discrete saddle point problem

$$\begin{aligned} A_{\mathbf{u}}(\mathbf{u},\Theta) &= L_{\mathbf{u}}(\mathbf{u},\Theta) + N(\mathbf{u}), & A_{\Theta}(\mathbf{u}) &= kL_{\Theta} + N(\mathbf{u}), \\ A_{\boldsymbol{\sigma}}(\mathbf{u}) &= \tfrac{1}{\lambda}M + N(\mathbf{u}) + G_a(\mathbf{u}), & E &= [-D_{11} - 2D_{12} - D_{22}] \end{aligned}$$

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

$$G_a(\mathbf{u}) = \begin{pmatrix} -2aD_{11} & W - 2aD_{12} & 0 \\ -\frac{1}{2}W - aD_{12} & 0 & \frac{1}{2}W - aD_{12} \\ 0 & -W - 2aD_{12} & -2aD_{22} \end{pmatrix}$$

Usefull matrix for spectral analysis !

Inexact Newton solver

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

$$\mathcal{R}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} = (\mathbf{u}_h, \boldsymbol{\sigma}_h, \Theta_h, p_h)$$

- Newton method with damping results in iterations of the form

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

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

$$\mathcal{R}(\mathbf{x}^{n+1}) \cdot \mathbf{x}^{n+1} \leq \mathcal{R}(\mathbf{x}^n) \cdot \mathbf{x}^n$$

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

$$\left[\frac{\partial \mathcal{R}(\mathbf{x}^n)}{\partial \mathbf{x}}\right]_{ij} \approx \frac{\mathcal{R}_i(\mathbf{x}^n + \varepsilon \mathbf{e}_j) - \mathcal{R}_i(\mathbf{x}^n - \varepsilon \mathbf{e}_j)}{2\varepsilon}$$

Multigrid solver

- Standard geometric multigrid approach
- Full $Q_2, \tilde{Q}_1, P_1^{\mathrm{disc}}$ and P_0 prolongation and restriction
- Smoother Local/Global MPSC
  - Local MPSC via Vanka-like smoother

$$\begin{bmatrix} \mathbf{u}^{l+1} \\ \boldsymbol{\sigma}^{l+1} \\ \Theta^{l+1} \\ p^{l+1} \end{bmatrix} = \begin{bmatrix} \mathbf{u}^{l} \\ \boldsymbol{\sigma}^{l} \\ \Theta^{l} \\ p^{l} \end{bmatrix} + \omega^l \sum_{T\in\mathcal{T}_h} [K_T]^{-1} \begin{bmatrix} \mathbf{Res_u} \\ \mathbf{Res}_{\boldsymbol{\sigma}} \\ \mathbf{Res}_{\Theta} \\ \mathbf{Res}_p \end{bmatrix}_{|T}$$

Coupled multigrid solver

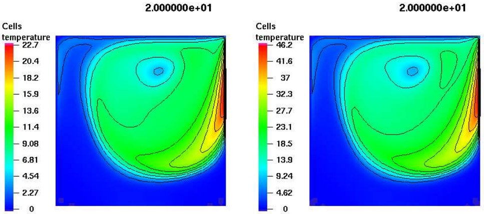
  - Global MPSC
    - solve for an intermediate $\tilde{\mathbf{u}}$ (generalized momentum equation)
    - solve for p (pressure poisson equation)
    - update of $\mathbf{u}$ and p
    - solve for Θ (energy equation)
    - solve for $\boldsymbol{\sigma}$ (constitutive equation)

Decoupled multigrid solver

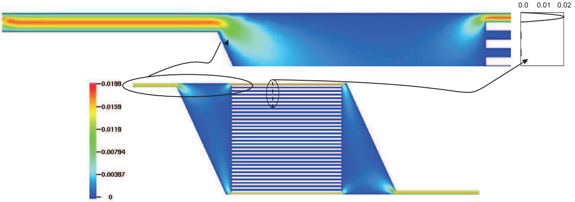
Numerical results: non-isothermal flow

- **energy equation with dissipation term**

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



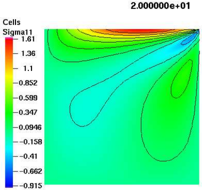
- **nonlinear viscosity:** $\nu_s(D, \Theta) = \nu_0 e^{\left(a_1 + \frac{a_2}{a_3 + T}\right)} (b_1 + b_2 |\mathbf{D}|)^{-b3}$

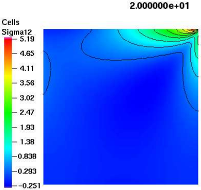


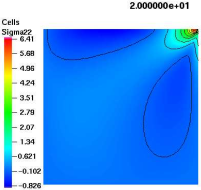
Blocking of the flow

Numerical results: visco-elastic flow

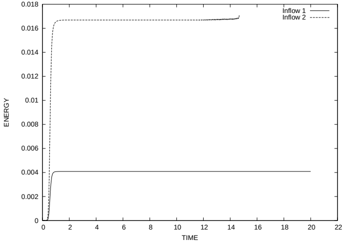
- Stress components for $Re = 0.5$, $We = 0.05$

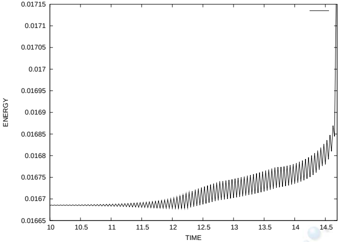






- Kinetic energy for two different velocity boundary values





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

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

- 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 !