Numerical techniques for FEM simulations of continuum models in biomathematics

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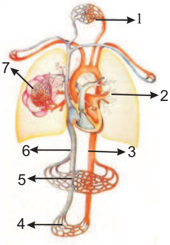
Motivation

- System of Blood flow



Picture taken from http://www.peacemotivate.com

1. Blood circulation in the head
2. Bronchial tree
3. Arterial blood circulation
4. Peripherial circulation
5. Circulation in body organs
6. Venous circulation
7. Pulmonary circulation

- Rheology of Blood flow
  - Blood behaves as Generalized Newtonian fluid in large vessels
    $\longrightarrow$ **Generalized Navier-stokes** equations
    $\longrightarrow$ coupled with further scalar equation (concentration, energy, ...)
  - Blood behaves as non-Newtonian fluid in small vessels
    $\longrightarrow$ coupled with **elastic stress tensor** equation

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**

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

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

Goal

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

$$\Downarrow$$

FeatFlow

Problem formulation

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

Typical saddle point problem

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

B and C are the gradient and divergence operator for the pressure and the stress respectively, and $\omega = \frac{\partial \mathbf{u}_2}{\partial x} - \frac{\partial \mathbf{u}_1}{\partial y}$

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

Usefull operator for spectral analysis !

Mathematical Challenges

The FEM techniques have to handle the following challenging points

- Stable FE spaces for velocity and pressure fields, and velocity and extra-stress fields: inf-sup condition has to be satisfied 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 "Johnson-Segalman" term $G_a(\mathbf{u})$ which is responsible for
  - no availability of a priori estimates
  - low Weissenberg number limitation
  - blow up phenomena for time dependent solution

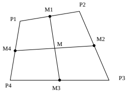
The nonliner solver has to deal with different source of nonlinearity

- nonlinear viscosities
- the strong coupling of equations

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**

Newton solver

The residual of nonlinear system of operator or of algebraic equations is obtained

$$\mathcal{R}(\mathbf{x}) = \mathbf{0}, \quad \mathbf{x} = (\mathbf{u}, \Theta, \boldsymbol{\sigma}, p)$$

Newton method with damping results in iterations of the form

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

- Continuous Newton: on variational level (before discretization)
  The continuous Jacobian operator can be calculated
- Inexact Newton: on matrix level (after discretization)
  The Jacobian matrix is **approximated** using finite differences as

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

New Edge-oriented FEM Stabilization

- **Based only on the "smoothness" of the discrete solution** we have proposed the following jump term

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

- 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

Multigrid solver

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

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

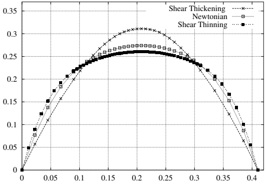
Coupled multigrid solver

  - 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 (tracer equation)
    - solve for $\boldsymbol{\sigma}$ (constitutive equation)

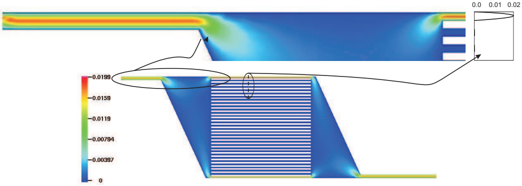
Decoupled multigrid solver

Numerical results

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

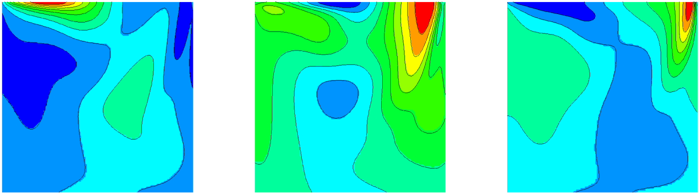


Velocity Profiles



Blocking of the flow

- **non-Newtonian flow:** Stress components $\boldsymbol{\sigma}_{11}, \boldsymbol{\sigma}_{12}$ and $\boldsymbol{\sigma}_{22}$



Reformulation of the constitutive equation

- Conformation tensor formulation
  - constitutive equation

$$\boldsymbol{\sigma}_c = \boldsymbol{\sigma} + \frac{\nu_p}{We}\mathbf{I}, \quad \boldsymbol{\sigma}_c + We\frac{D_a}{Dt}\boldsymbol{\sigma}_c = \frac{\nu_p}{We}\mathbf{I}$$

  - further expression

$$\boldsymbol{\sigma}_c(X,t) = \int_{\infty}^{t} \frac{\nu_p}{We^2} exp\left(\frac{-(t-s)}{We}\right) F(s,t)F(s,t)^T ds$$

- Emerging of log-conformation formulation
  - log-coformation tensor

$$\boldsymbol{\sigma}_c = exp(\mathbf{S})$$

  - consitutive equation

$$exp(\mathbf{S}) + We\frac{D_a}{Dt}exp(\mathbf{S}) = \frac{\nu_p}{We}\mathbf{I}$$

Simple change successfully helping to go beyond the HWNP

Summary

New numerical and algorithmic tools are available for nonlinear fluids using

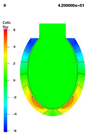
- Finite Element Method
- Flexible Newton Method
- Edge-oriented stabilization for
  - convective terms
  - same space approximation for velocity and extra-stress
- Fast multigrid solver with Global/Local MPSC smoother

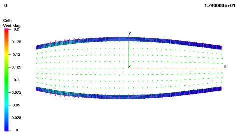
for the simulation of blood

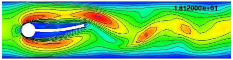
Outlook

The fluid part will be integrated with the solid part in

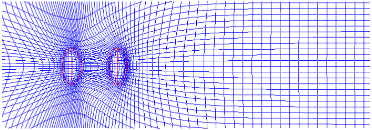
- Fluid structure interaction







- Particulate flow



To simulate a wide range of continuum models in biomathematics in realistic configurations