Monolithic FEM techniques for flows with temperature, pressure and/or shear-dependent viscosity

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Non-Newtonian fluids

☞ important areas of mathematical modeling and applications

- polymer, food, paper processing
- bioengineering, blood flow, synovial fluids
- lubrication, asphalt, granular materials, ...

mathematical models

- viscous fluid flow
- non-constant viscosity
- nonlinear dependence of the viscosity

numerical tasks involved

- space and time discretization
- nonlinear system
- solution of large linear system

testing and validation

- benchmarking
- accuracy, efficiency, robustnes

Governing equations

balance equations

$$\varrho \frac{\partial \mathbf{v}}{\partial t} + \varrho(\nabla \mathbf{v})\mathbf{v} = \operatorname{div} \boldsymbol{\sigma} + \mathbf{f} \qquad \text{in } \Omega$$

$$\operatorname{div} \mathbf{v} = 0 \qquad \text{in } \Omega$$

boundary conditions

$$\mathbf{v} = \mathbf{v}_B \qquad \text{on } \Gamma^0$$

$$\boldsymbol{\sigma}\mathbf{n} = \mathbf{g} \qquad \text{on } \Gamma^1$$

additional quantities

$$\frac{\partial \theta}{\partial t} + (\nabla \mathbf{v})\theta = \operatorname{div}(k\nabla\theta) + \boldsymbol{\sigma} : \mathbf{D} + r \qquad \text{in } \Omega$$

Constitutive equations

☞ incompressible Newtonian fluid

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\nu\mathbf{D} \qquad \mathbf{D} = \frac{1}{2}(\nabla\mathbf{v} + \nabla\mathbf{v}^T)$$

☞ generalized Newtonian fluid

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\nu(\|\mathbf{D}\|, p, \theta, ...)\mathbf{D}$$

☞ general non-Newtonian viscous fluid

$$g(\boldsymbol{\sigma}, \mathbf{D}, \theta, ...) = 0$$

Discretization in time

The time interval $(0, T)$

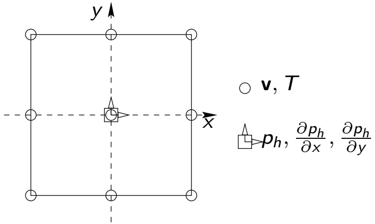
- divide it into n subintervals $I_n = [t^n, t^{n+1}]$
- time step $k_n = t^{n+1} - t^n$.
- for time interval $[t^n, t^{n+1}]$ approximate by central differences

$$\frac{df}{dt} \approx \frac{f^{n+1} - f^n}{k_n}$$

- Crank-Nicholson scheme (2^{nd} order) or fractional θ scheme (2^{nd} order, better stability) with adaptive time-step selection

Discretization in space

FEM $Q_2/P_1^{disc}/Q_2$



$$V_h = \{\mathbf{v}_h \in [C(\Omega_h)]^2, \mathbf{v}_h|_T \in [Q_2(T)]^2 \forall T \in \mathcal{T}_h, \mathbf{v}_h = \mathbf{0} \text{ on } \Gamma_D\},$$
$$P_h = \{p_h \in L^2(\Omega_h), p_h|_T \in P_1(T) \forall T \in \mathcal{T}_h\},$$
$$Q_h = \{Q_h \in C(\Omega_h), Q_h|_T \in Q_2(T) \forall T \in \mathcal{T}_h, Q_h = 0 \text{ on } \Gamma_D\}.$$

Discrete nonlinear system

$$\mathcal{R}(\mathbf{X}) = \mathbf{0}, \qquad \mathbf{X} = (\mathbf{v}_h, p_h, q_h) \in V_h \times P_h \times Q_h$$

$$\begin{aligned} Mv_h + \frac{k}{2}N(v_h, v_h) + \frac{k}{2}S(v_h, p_h, q_h) - kBp_h &= \mathrm{rhs}(v_h^n, p_h^n, q_h^n) \\ B^T v_h &= 0 \\ Mq_h + \frac{k}{2}N(v_h, q_h) + \frac{k}{2}S(v_h, p_h, q_h) &= \mathrm{rhs} \end{aligned}$$

$$\Downarrow$$

$$\frac{\partial \mathcal{R}}{\partial \mathbf{X}}(\mathbf{X}) = \begin{pmatrix} A_{vv} & kB + A_{vp} & A_{vq} \\ B^T & 0 & 0 \\ A_{qv} & A_{qp} & A_{qq} \end{pmatrix}$$

☞ compute the Jacobian matrix (analytic, automatic differentiation, divided differences)

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

☞ solve the linear system for $\tilde{\mathbf{X}}$ (BiCGStab or GMRes(m)/ILU(k), MG, direct solver)

$$\left[\frac{\partial \boldsymbol{\mathcal{R}}}{\partial \mathbf{X}}(\mathbf{X}^n)\right]\tilde{\mathbf{X}} = \boldsymbol{\mathcal{R}}(\mathbf{X}^n)$$

☞ adaptive line search strategy

$$\mathbf{X}^{n+1} = \mathbf{X}^n + \omega\tilde{\mathbf{X}} \qquad \omega \in [-1, 0) \text{ such that } f(\omega) = \boldsymbol{\mathcal{R}}(\mathbf{X} + \omega\tilde{\mathbf{X}}) \cdot \mathbf{X} \searrow$$

Jacobian approximation

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

ε / TOL	10^{-8}	10^{-4}	10^{-2}	10^{-1}
10^{-8}	7 /107.57 [21.52]	12 /57.08 [26.52]	12 /47.00 [23.75]	17 /33.06 [27.38]
10^{-4}	7 /108.71 [24.57]	**8 /62.75 [17.77]**	**10 /42.20 [18.95]**	18 /31.33 [29.05]
10^{-2}	16 /109.75 [51.65]	20 /47.35 [38.28]	25 /29.80 [38.58]	56 /16.98 [73.83]
10^{-1}	44 /116.11 [141.30]	48 /35.79 [81.72]	49 /17.92 [65.77]	–

nonlinear solver it. / avg. linear solver it. [CPU time] for BiCGStab(ILU(0))

Multigrid solver

- standard geometric multigrid approach
- smoother by local MPSC-Ansatz (Vanka-like smoother)

$$\begin{bmatrix} \mathbf{v}^{l+1} \\ q^{l+1} \\ p^{l+1} \end{bmatrix} = \begin{bmatrix} \mathbf{u}^{l} \\ q^{l} \\ p^{l} \end{bmatrix} - \omega \sum_{\text{Patch } \Omega_i} \begin{bmatrix} A_{\mathbf{vv}|\Omega_i} & A_{\mathbf{v}q|\Omega_i} & kB_{|\Omega_i} + C_{\mathbf{v}p|\Omega_i} \\ A_{q\mathbf{v}|\Omega_i} & A_{qq|\Omega_i} & C_{qp|\Omega_i} \\ B^T_{|\Omega_i} & 0 & 0 \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{def}^l_{\mathbf{v}} \\ def^l_q \\ def^l_p \end{bmatrix}$$

- full inverse of the local dense problems by standard LAPACK
- alternatives: simplified local problems
- full Q_2 and P_1^{disc} prolongation $\mathbf{P}$, restriction by $\mathbf{R} = \mathbf{P}^T$

Examples: natural convection flow in enclosure

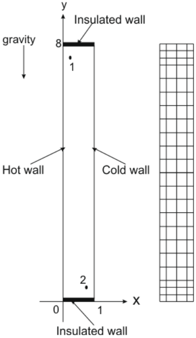
Oberbeck-Boussinesq equation, constant viscosity

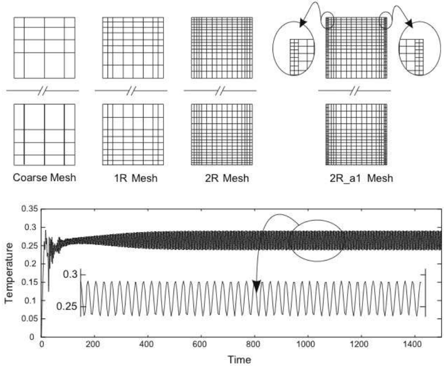
$$\frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v})\mathbf{v} = \operatorname{div} \boldsymbol{\sigma} + \mathbf{e}_j \theta \qquad \text{in } \Omega$$

$$\operatorname{div} \mathbf{v} = 0 \qquad \text{in } \Omega$$

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\mu \mathbf{D}$$

$$\frac{\partial \theta}{\partial t} + (\nabla \mathbf{v})\theta = \operatorname{div}(k \nabla \theta) \qquad \text{in } \Omega$$





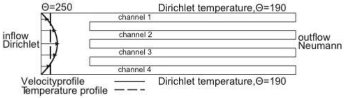
MIT benchmark (M.A. Christon, P.M. Gresho, S.B. Sutton, 2001)

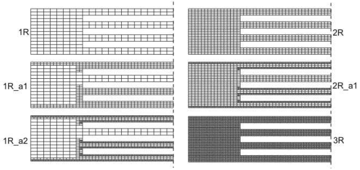
Example: heat exchanger

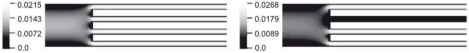
temperature and shear dependent viscosity

$$
\begin{aligned}
\frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v})\mathbf{v} &= \operatorname{div} \boldsymbol{\sigma} && \text{in } \Omega \\
\operatorname{div} \mathbf{v} &= 0 && \text{in } \Omega \\
\frac{\partial \theta}{\partial t} + (\nabla \mathbf{v})\theta &= \operatorname{div}(k \nabla \theta) && \text{in } \Omega \\
\boldsymbol{\sigma} &= -p\mathbf{I} + 2\mu \mathbf{D}
\end{aligned}
$$

$$
\mu(\|\mathbf{D}\|, \theta) = \mu_0 \exp\left(\frac{a_1}{a_2 + a_3\theta}\right)(\epsilon + \|\mathbf{D}\|)^{-\beta}
$$







Example: viscous heat dissipation

power-law model, heat equation with viscous dissipation term

$$\frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v})\mathbf{v} = \operatorname{div} \boldsymbol{\sigma} + \mathbf{e}_j \theta \qquad \text{in } \Omega$$

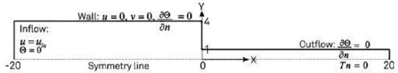
$$\operatorname{div} \mathbf{v} = 0 \qquad \text{in } \Omega$$

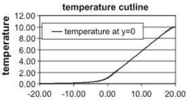
$$\frac{\partial \theta}{\partial t} + (\nabla \mathbf{v})\theta = \operatorname{div}(k \nabla \theta) + \boldsymbol{\sigma} : \mathbf{D} \qquad \text{in } \Omega$$

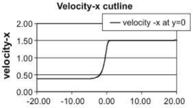
$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\mu \mathbf{D}$$

$$\mu(\|\mathbf{D}\|, \theta) = \mu_0(\epsilon + \|\mathbf{D}\|)^{-\alpha}$$

	mesh level					
linear tolerance	1R	2R	3R	1Ra1	1Ra2	2Ra1
10^{-1}	11/1	12/2	12/2	13/1	12/1	11/1
10^{-2}	9/2	10/3	10/4	9/2	9/2	9/2
10^{-3}	9/4	9/5	9/6	9/2	9/3	9/3
10^{-8}	9/13	9/17	9/19	9/7	9/7	9/9
exact	9/-	9/-	9/-	9/-	9/-	9/-







Examples: synovial fluids

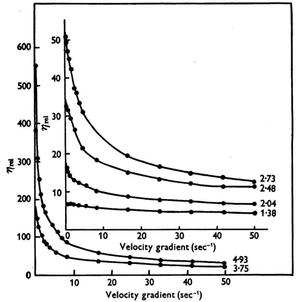
$$\frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v})\mathbf{v} = \operatorname{div} \boldsymbol{\sigma} \qquad \text{in } \Omega$$

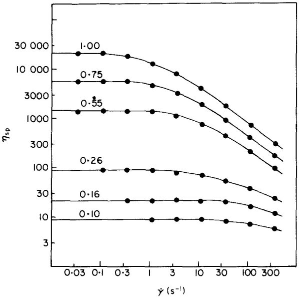
$$\operatorname{div} \mathbf{v} = 0 \qquad \text{in } \Omega$$

$$\frac{\partial c}{\partial t} + (\nabla \mathbf{v})c = \operatorname{div}(k \nabla c) \qquad \text{in } \Omega$$

$$\boldsymbol{\sigma} = -p\mathbf{I} + 2\mu \mathbf{D}$$

$$\mu(\|\mathbf{D}\|, c) = (\epsilon + \gamma \|\mathbf{D}\|^2)^{\exp(-\alpha c) - 1}$$





for increasing shear the breakdown of molecular network of hyaluronan acid molecules results in decrease in viscosity

Examples: synovial fluids

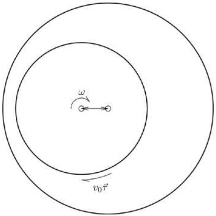
simple example flow

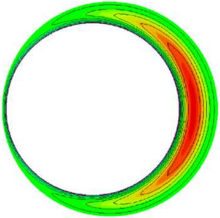
mbox_mu_v50_t04.avi

Examples: pressure dependent viscosity

- lubrication - journal bearing flow

$$\mu(\|\mathbf{D}\|, p) = exp(\alpha p)$$





- continuum models of granular flow

$$\mu(\|\mathbf{D}\|, p) = \frac{\alpha p}{\|\mathbf{D}\|}$$

Examples: numerical fluid-structure interaction benchmarking

☞ based on the DFG *flow around cylinder* (Turek, Schäfer , 1996)

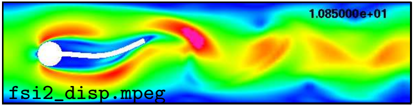
☞ realistic materials

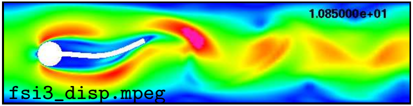
- **incompressible Newtonian fluid**, laminar flow regime
- **elastic solid**, large deformations

☞ setup with simple periodic oscillations + reasonable deformations

☞ computable configuration ⇒ laminar flow, reasonable aspect ratios

☞ results collection, see
`http://fsw.informatik.tu-muenchen.de/intern/wiki/index.php/Benchmark`





Examples: model of aneurysm with stents

- 2D approximation
- acurate material model for the wall and fluid

pul_elastic_vecm.avi

pul_elastic_stent_vecm.avi

Example: pulsative flow in elastic tube

10^6 equations, 1 week comput. time (4 CPUs, direct solver MUMPS)

test1.avi

test3.avi

test5.avi

- ☞ monolithic, fully coupled FEM (Q_2/P_1^{disc}, P_2/P_1^{disc}) for **viscous incompressible fluid** with wide range of viscosities
- ☞ *direct* steady calculation fully implicit 2nd order discretization in time, adaptive timestep selection
- ☞ Newton-like method for the coupled system (Jacobian matrix via divided differences)
- ☞ MG-solver, problems with mesh anisotropy
- ☞ combination with GMRES/BiCGStab methods
- ☞ a priori space-adapted mesh