Computational results for flows of implicitly constituted fluids

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- balance equations

$$\varrho \frac{\partial \mathbf{v}}{\partial t} + \varrho [\nabla \mathbf{v}] \mathbf{v} = \operatorname{div} \mathbf{T} + \varrho \mathbf{f}$$
$$\operatorname{div} \mathbf{v} = 0$$

- constitutive equations

$$\mathcal{G}(\mathbf{T}^{\delta}, \mathbf{D}) = \mathbf{0}$$

- boundary conditions

$$\mathbf{v} \cdot \mathbf{n} = 0$$
$$\mathbf{g}((\mathbf{T}\mathbf{n})_t, \mathbf{v}_t) = \mathbf{0}$$

$$\mathbf{A}^{\delta} := \mathbf{A} - \frac{1}{d} (\operatorname{tr} \mathbf{A}) \mathbf{I} \qquad \mathbf{b}_t := (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \mathbf{b}$$

Constitutive relation

general non-Newtonian simple viscous fluid, implicit constitutive law

$$\mathcal{G}(\mathbf{S}, \mathbf{D}, \dots) = 0 \qquad \mathbf{T} = -p\mathbf{I} + \mathbf{S} \qquad \mathbf{D} = \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T)$$

- incompressible Newtonian fluid

$$\mathbf{T} = (-p\mathbf{I} + 2\mu\mathbf{D}) \qquad \Rightarrow \qquad \mathcal{G}(\mathbf{S}, \mathbf{D}) = \mathbf{S} - 2\mu\mathbf{D}$$

- generalized Newtonian fluid

$$\mathbf{T} = \left(-p\mathbf{I} + 2\mu(p, |\mathbf{D}|^2, \dots)\mathbf{D}\right) \quad \Rightarrow \quad \mathcal{G}(\mathbf{S}, \mathbf{D}) = \mathbf{S} - 2\mu(p, |\mathbf{D}|^2, \dots)\mathbf{D}$$

- more generalized, including stress power-law models

$$\mathcal{G}(\mathbf{S}, \mathbf{D}) = \alpha(|\mathbf{S}|^2, |\mathbf{D}|^2)\mathbf{S} - \beta(|\mathbf{S}|^2, |\mathbf{D}|^2)\mathbf{D}$$

Questions: Existence and qualitative properties of the solution...

K. R. Rajagopal ['06], Málek ['08]

M. Bulíček, P. Gwiazda, J. Málek, A. Świerczewska-Gwiazda ['09, '12, '12]

L. Diening, C. Kreuzer, E. Süli ['13]

J. Hron, J. Málek, J. Stebel, K. Touška [in preparation]

Standard mixed formulation - velocity, pressure

Stokes like system:

$$
\begin{aligned}
-\operatorname{div}\mathbf{S} + \nabla p &= \mathbf{f}, \\
\operatorname{div}\mathbf{v} &= 0, \\
\mathbf{S} &= \mathcal{A}(\mathbf{D}(\mathbf{v}))
\end{aligned}
$$

- primal formulation: eliminate $\mathbf{S}$, p and solve for $\mathbf{v}$ only
- dual formulation: eliminate $\mathbf{v}$ and solv for $\mathbf{T} = -p\mathbf{I} + \mathbf{S}$ only
- classical mixed formulation: find $(\mathbf{v}, p) \in \mathbb{V} \times \mathbb{P}$ such that

$$
\int_\Omega \mathcal{A}(\mathbf{D}(\mathbf{v})) : \mathbf{D}(\varphi) - p \operatorname{div}\varphi + \xi \operatorname{div}\mathbf{v} = \int_\Omega \mathbf{f}\cdot\varphi, \quad \forall(\varphi, \xi) \in \mathbb{V} \times \mathbb{P}
$$

$$
\begin{bmatrix} \tilde{\mathcal{A}} & -\operatorname{div}^T \\ \operatorname{div} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v} \\ p \end{bmatrix} = \begin{bmatrix} \cdot \\ \cdot \end{bmatrix}
$$

Standard mixed formulation - velocity, pressure

finite element formulation: find $(\mathbf{v}_h, p_h) \in \mathbb{V}_h \times \mathbb{P}_h$ such that

$$\int_\Omega \mathcal{A}(\mathbf{D}(\mathbf{v}_h)) : \mathbf{D}(\boldsymbol{\varphi}) - p_h \operatorname{div} \boldsymbol{\varphi} + \xi \operatorname{div} \mathbf{v_h} = \int_\Omega \mathbf{f} \cdot \boldsymbol{\varphi}, \quad \forall (\boldsymbol{\varphi}, \xi) \in \mathbb{V}_h \times \mathbb{P}_h$$

or if we define $\quad a(\mathbf{u}, \mathbf{v}) = \int_\Omega \mathcal{A}(\mathbf{D}(\mathbf{u})) : \mathbf{D}(\mathbf{v}), \quad b(p, \mathbf{u}) = \int_\Omega p \operatorname{div} \mathbf{u}$

$$\begin{aligned} a(\mathbf{v}_h, \boldsymbol{\varphi}) - b(p_h, \boldsymbol{\varphi}) &= (f, \boldsymbol{\varphi}) \\ b(\xi, \mathbf{v}_h) &= 0 \end{aligned}$$

let $\{\boldsymbol{\varphi}^i\}$ denote a basis for $\mathbb{V}_h$ and $\{\xi^i\}$ denote a basis for $\mathbb{P}_h$ then we look for

$$\mathbf{v}_h = \sum V_i \boldsymbol{\varphi}^i \qquad\qquad p_h = \sum P_i \xi^i$$

denoting $\mathbf{X} = (V, P)$ we can write the finite dimensional nonlinear system as

$$\mathcal{R}(\mathbf{X}) = \mathbf{0}$$

- solvability of the linear system $\Rightarrow$ inf-sup stability ($P_k/P_{k-1}, Q_k/Q_{k-1}, Q_k/P_{k-1}^{\mathrm{disc}}$)

$$\inf_{p_h \in \mathbb{P}_h} \sup_{\mathbf{v}_h \in \mathbb{V}_h} \frac{b(p_h, \mathbf{v}_h)}{||\mathbf{v}_h||_1 ||p_h||_0} = \beta_h \geq \beta > 0$$

Finite element selection

- equal order elements $\Rightarrow$ need for aditional stabilization
- inf-sup stability (P_k/P_{k-1}, Q_k/Q_{k-1}, $Q_k/P_{k-1}^{\mathrm{disc}}$)

$$\inf_{p_h \in \mathbb{P}_h} \sup_{\mathbf{v}_h \in \mathbb{V}_h} \frac{b(p_h, \mathbf{v}_h)}{||\mathbf{v}_h||_1 ||p_h||_0} = \beta_h \geq \beta > 0$$

- conforming vs. nonconforming: $\mathbf{v} \in \mathbf{H}^1, p \in L^2, \mathbf{T} \in \mathbf{H}(div, sym)$
- discretely div-free solution: if $\operatorname{div} \mathbf{v}_h \in \mathbb{P}_h$ (Scott, Vogelius)

vast existing literature for example: Babuška, Brezzi, Fortin, etc.
$\Rightarrow$ assures that the linear problem is solvable

Solution of the nonlinear problem - Newton method

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

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

- solve the linear system for $\tilde{\mathbf{X}}$

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

- adaptive line search strategy $\mathbf{X}^{n+1} = \mathbf{X}^n + \omega \tilde{\mathbf{X}} \quad \omega \in [-1, 0)$

Dual mixed formulation - stress, velocity

Stokes like system:

$$
\begin{aligned}
-\operatorname{div}\mathbf{T} &= \mathbf{f},\\
\operatorname{div}\mathbf{v} &= 0,\\
\mathbf{T}^{\delta} &= \mathcal{A}(\mathbf{D}(\mathbf{v}))
\end{aligned}
$$

- $\mathbf{D} = \mathcal{A}^{-1}(\mathbf{T})$, dual mixed formulation: find $(\mathbf{T}, \mathbf{v}) \in \mathbb{S} \times \mathbb{V}$ such that

$$
\int_\Omega \mathcal{A}^{-1}(\mathbf{T}) : \boldsymbol{\chi} + \mathbf{v} \cdot \operatorname{div}\boldsymbol{\chi} - \operatorname{div}\mathbf{T} \cdot \boldsymbol{\varphi} = \int_\Omega \mathbf{f} \cdot \boldsymbol{\varphi}, \quad \forall (\boldsymbol{\chi}, \boldsymbol{\varphi}) \in \mathbb{S} \times \mathbb{V}
$$

$$
\begin{bmatrix} \tilde{\mathcal{A}}^{-1} & \operatorname{div}^T \\ -\operatorname{div} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{T} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} \cdot \\ \cdot \end{bmatrix}
$$

General mixed formulation - stress, velocity, D

Stokes like system with general implicit constitutive law:

$$-\operatorname{div}\mathbf{T} = \mathbf{f}, \qquad \operatorname{div}\mathbf{v} = 0, \qquad \mathcal{G}(\mathbf{T}^\delta, \mathbf{D}) = 0, \qquad \mathbf{D} = \frac{1}{2}(\nabla\mathbf{v} + (\nabla\mathbf{v})^T)$$

- dual mixed formulation: find $(\mathbf{D}, \mathbf{v}, \mathbf{T}^\delta) \in \mathbb{D} \times \mathbb{V} \times \mathbb{S}$ such that

$$\int_\Omega \mathcal{G}(\mathbf{T}, \mathbf{D}) : \boldsymbol{\omega} - \operatorname{div}\mathbf{T} \cdot \boldsymbol{\varphi} + \mathbf{D} : \boldsymbol{\chi} + \mathbf{v} \cdot \operatorname{div}\boldsymbol{\chi} = \int_\Omega \mathbf{f} \cdot \boldsymbol{\varphi}, \ \forall(\boldsymbol{\omega}, \boldsymbol{\varphi}, \boldsymbol{\chi}) \in \mathbb{D} \times \mathbb{V} \times \mathbb{S}$$

$$\begin{bmatrix} \mathcal{G}_{\mathbf{D}} & 0 & \mathcal{G}_{\mathbf{T}} \\ 0 & 0 & -\operatorname{div} \\ I & \operatorname{div}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{D} \\ \mathbf{v} \\ \mathbf{T} \end{bmatrix} = \begin{bmatrix} . \\ . \\ . \end{bmatrix}$$

- classical inf-sup for velocity-pressure and velocity-stress
- double inf-sup for **D**-velocity-stress

J.S. Howell, H.J. Walkington ['10]

Generalized nonsymmetric saddle point problem

$$\begin{bmatrix} A & B_1^\top \\ B_2 & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

Sufficient and necessary conditions for well-posedness [Bernardi et al. (1988)]:

- A restricted to $\ker B_2$ is isomorphism onto $(\ker B_1)^*$
- B_1 and B_2 have full rank

Generalized twofold saddle point problem

$$\begin{bmatrix} A & 0 & B_1^\top \\ 0 & 0 & C_2 \\ B_2 & C_1^\top & 0 \end{bmatrix} \begin{bmatrix} u \\ p_1 \\ p_2 \end{bmatrix} = \begin{bmatrix} f \\ g_1 \\ g_2 \end{bmatrix}$$

Sufficient and necessary conditions for well-posedness:

- A restricted to $\ker B_2$ is isomorphism onto $(\ker B_1)^*$
- $B_1^\top$ and $B_2^\top$ restricted to $\ker C_2$, $\ker C_1$, respectively, have full rank
- C_1 and C_2 have full rank

J.S. Howell, H.J. Walkington ['10]

Requirements for the cases $(\mathbf{T}, \boldsymbol{v})$ and $(\mathbf{D}, \boldsymbol{v}, \mathbf{T})$

Theorem

Let $\mathbb{S}_h, \mathbb{V}_h$ satisfy the following conditions:

(i) $\{\mathbf{D}\boldsymbol{\varphi};\ \boldsymbol{\varphi} \in \mathbb{V}_h\} \subset \mathbb{S}_h$;

(ii) *There exists $c > 0$ such that:* $\sup_{\boldsymbol{\varphi}\in\mathbb{V}_h} \frac{(\mathrm{tr}\,\mathbf{T}, \operatorname{div}\boldsymbol{\varphi})}{\|\boldsymbol{\varphi}\|_{1,2}} \geq c\,\|\mathrm{tr}\,\mathbf{T}\|_2 \quad \forall \mathbf{T} \in \mathbb{S}_h$.

Then the linearized problem has a unique solution $(\mathbf{T}_h, \boldsymbol{v}_h)$.

Theorem

Let $\mathbb{D}_h, \mathbb{V}_h, \mathbb{S}_h$ satisfy the following conditions:

(i) $\{\mathbf{D}\boldsymbol{\varphi};\ \boldsymbol{\varphi} \in \mathbb{V}_h\} \subset \mathbb{S}_h$;

(ii) $\{\mathbf{T}^\delta;\ \mathbf{T} \in \mathbb{S}_h\} \subset \mathbb{D}_h$;

(iii) *There exists $c > 0$ such that:* $\sup_{\boldsymbol{\varphi}\in\mathbb{V}_h} \frac{(\mathrm{tr}\,\mathbf{T}, \operatorname{div}\boldsymbol{\varphi})}{\|\boldsymbol{\varphi}\|_{1,2}} \geq c\,\|\mathrm{tr}\,\mathbf{T}\|_2 \quad \forall \mathbf{T} \in \mathbb{S}_h$.

Then the linearized problem has a unique solution $(\mathbf{D}_h, \boldsymbol{v}_h, \mathbf{T}_h)$.

L. Diening, C. Kreuzer, E. Süli ['13]

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Finite element spaces selection

A. Unknowns $(\mathbf{S}, \mathbf{v}, p)$:

$$\operatorname{div}\mathbf{S} - \nabla p = \mathbf{f}$$
$$\operatorname{div}\mathbf{v} = 0$$

$$\mathbf{D}(\mathbf{v}) = (1 + |\mathbf{S}|^2)^n \mathbf{S}.$$

B. Unknowns $(\mathbf{T}, \mathbf{v})$:

$$\operatorname{div}\mathbf{T} = \mathbf{f}$$

$$\mathbf{D}(\mathbf{v}) = (1 + |\mathbf{T}^d|^2)^n \mathbf{T}^d$$

C. Unknowns $(\mathbf{T}, \mathbf{v}, \mathbf{D})$:

$$\operatorname{div}\mathbf{T} = \mathbf{f}$$
$$\mathbf{D}(\mathbf{v}) = \mathbf{D}$$

$$\mathbf{D} = (1 + |\mathbf{T}^d|^2)^n \mathbf{T}^d$$

Finite element approximation

triangular mesh

A		B		C	
$\mathbf{S}$	P_1^{disc}	$\mathbf{T}$	P_1^{disc}	$\mathbf{T}$	P_1^{disc}
$\mathbf{v}$	P_2	$\mathbf{v}$	P_2	$\mathbf{v}$	P_2
p	P_1			$\mathbf{D}$	P_1^{disc}

quadrilateral mesh

A		B		C	
$\mathbf{S}$	Q_2^{disc}	$\mathbf{T}$	Q_2^{disc}	$\mathbf{T}$	Q_2^{disc}
$\mathbf{v}$	Q_2	$\mathbf{v}$	Q_2	$\mathbf{v}$	Q_2
p	P_1^{disc}			$\mathbf{D}$	Q_2^{disc}

Observations:

- All approximate formulations lead apparently to the same results.
- In the cases B and C it is necessary to stabilize jumps of $\operatorname{tr}\mathbf{T}$ across edges in order to satisfy the inf-sup condition for the pressure on simplex mesh.

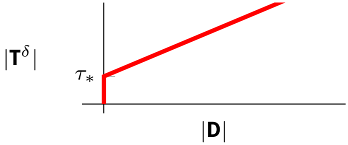
- Lid driven cavity benchmark

$$\begin{aligned} \operatorname{div} \mathbf{T} &= 0, \\ \operatorname{div} \boldsymbol{v} &= 0, \\ \mathbf{D} &= \frac{1}{2}(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T) \end{aligned}$$

- common formulation

$$\mathbf{D} = 0 \Rightarrow |\mathbf{T}^\delta| \leq \tau^*$$

$$\mathbf{D} \neq 0 \Rightarrow \mathbf{T}^\delta = \tau^* \frac{\mathbf{D}}{|\mathbf{D}|} + 2\mu \mathbf{D}$$



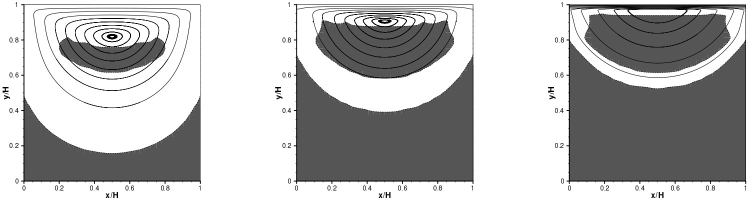
- implicit formulation

$$\mathcal{G}(\mathbf{T}^\delta, \mathbf{D}) = 2\mu\tau_* \mathbf{D} + (|\mathbf{T}^\delta| - \tau_*)^+ (2\mu\mathbf{D} - \mathbf{T}^\delta) \quad (1)$$

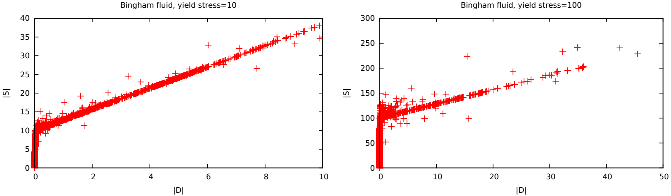
$$\mathcal{G}(\mathbf{T}^\delta, \mathbf{D}) = 2\mu\tau_* \mathbf{D} + (2\mu|\mathbf{D}|)^+ (2\mu\mathbf{D} - \mathbf{T}^\delta) \quad (2)$$

- regularization $|\mathbf{D}|_{\varepsilon_1} = \sqrt{\varepsilon_1^2 + |\mathbf{D}|^2}$, $(f)^+_{\varepsilon_2} = \max(f, \varepsilon_2)$

D. Vola, L. Boscardin, J.C. Latché: Laminar unsteady flows of Bingham fluids: a numerical strategy and some benchmark results, 2003.



$\tau^* = 5$ $\tau^* = 50$ $\tau^* = 500$



Satisfaction of the constitutive relation. Left: $\tau^* = 10$, right: $\tau^* = 100$.

- One can reach numerical solution with vanishing regularization in the $(\mathbf{D}, \boldsymbol{v}, \mathbf{T})$ formulation.

Imposing implicit boundary conditions

$$
\begin{aligned}
-\operatorname{div}\mathbf{T} &= \mathbf{f}\\
\operatorname{div}\mathbf{v} &= 0\\
\mathbf{T} + p\mathbf{I} - 2\mu\mathbf{D} &= 0
\end{aligned}
$$

$$
\begin{aligned}
\mathbf{v}\cdot\mathbf{n} &= 0\\
\mathbf{g}((\mathbf{Tn})_t, \mathbf{v}_t) &= \mathbf{0}
\end{aligned}
$$

How to impose such boundary conditions:

- Lagrange multiplier method
- as Dirichlet condition
- as natural boundary condition $\rightarrow$ Nitsche penalty method

$$
\mathbf{b}_t := (\mathbf{I} - \mathbf{n}\otimes\mathbf{n})\mathbf{b}
$$

Nitsche method for weakly imposing b.c.

$$-\operatorname{div}\mathbf{T} = \mathbf{f} \qquad \operatorname{div}\mathbf{v} = 0 \qquad \mathbf{T} + p\mathbf{I} - 2\mu\mathbf{D} = 0$$

$$\mathbf{v}\cdot\mathbf{n} = 0 \qquad \mathbf{g}((\mathbf{T}\mathbf{n})_t, \mathbf{v}_t) = \mathbf{0}$$

mixed formulation: find $(\mathbf{T}, \mathbf{v}, p) \in \mathbb{S}\times\mathbb{V}\times\mathbb{P}$ such that

$$\begin{aligned}\int_\Omega (\mathbf{T} : \nabla\boldsymbol{\varphi} - p\,\mathrm{tr}\,\boldsymbol{\sigma} + \xi\operatorname{div}\mathbf{v} + [\mathbf{T} + p\mathbf{I} - 2\mu\mathbf{D}(\mathbf{v})] : \boldsymbol{\sigma})dx \\ + \int_\Gamma (\mathbf{T}\mathbf{n}\cdot\boldsymbol{\varphi} + (\mathbf{v}\cdot\mathbf{n})(\boldsymbol{\sigma}\mathbf{n}\cdot\mathbf{n}) + \mathbf{g}((\mathbf{T}\mathbf{n})_t, \mathbf{v}_t)\cdot(\boldsymbol{\sigma}\mathbf{n})_t)ds \\ + \int_\Gamma \left(\frac{\beta}{h}((\mathbf{v}\cdot\mathbf{n})(\boldsymbol{\varphi}\cdot\mathbf{n}) + \mathbf{g}((\mathbf{T}\mathbf{n})_t, \mathbf{v}_t)\cdot\boldsymbol{\varphi}_t)\right) ds \\ = \int_\Omega \mathbf{f}\cdot\boldsymbol{\varphi}, \quad \forall(\boldsymbol{\sigma}, \boldsymbol{\varphi}, \xi) \in \mathbb{S}\times\mathbb{V}\times\mathbb{P}\end{aligned}$$

Nitsche, J. (1971). Uber ein Variationzprinzip zur Losung von Dirichlet Problemen bei Verwendung von Teilraumen, die kein Randbedingungen unterworfen sind.

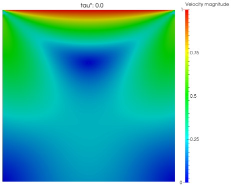
Juntunen, M., & Stenberg, R. (2009). Nitsche's method for general boundary conditions.

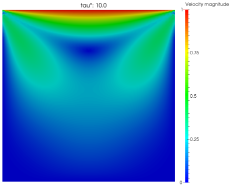
Vergara, C. (2010). Nitsche's Method for Defective Boundary Value Problems in Incompressibile Fluid-dynamics.

Burman, E. (2011). A penalty free non-symmetric Nitsche type method for the weak imposition of boundary conditions.

- Dirichlet condition at the top plate: $\mathbf{v} = (1,0)$
- Threshold condition on the walls:

$$|(\mathbf{Tn})_t| \leq \tau^* \Rightarrow \mathbf{v} = 0$$
$$|(\mathbf{Tn})_t| > \tau^* \Rightarrow \mathbf{g}((\mathbf{Tn})_t, \mathbf{v}_t) = |(\mathbf{Tn})_t|\mathbf{v} + \gamma(|(\mathbf{Tn})_t| - \tau^*)(\mathbf{Tn})_t = 0$$





Further development and goals

☞ Complete understanding of advantages and drawbacks - from model equations, trough analysis and numerical computations.

- Can we compensate for the larger systems by more efficient solution methods?
- Efficient linear solver, preconditioners for block systems, as combination with iterative GMRES/BiCGStab/multigrid and direct methods...
- Stopping criteria for nonlinear/linear solvers...