Implicitly constituted materials: mixed formulations, numerical solutions and computations

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Governing equations

- 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

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

- boundary conditions

$$\mathbf{v} = \mathbf{v}_B$$

$$\mathbf{T}\mathbf{n} = \mathbf{g}$$

$$\mathbf{v} \cdot \mathbf{n} = 0, \quad \alpha \mathbf{v} \cdot \mathbf{t} = \mathbf{T}\mathbf{n} \cdot \mathbf{t}$$

Constitutive relation

- incompressible Newtonian fluid

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

- generalized Newtonian fluid

$$\mathbf{T} = -p\mathbf{I} + 2\mu(|\mathbf{D}|, \dots)\mathbf{D}$$

- general non-Newtonian simple viscous fluid, implicit constitutive law

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

- rate type models, visco-elastic models, ...

$$\mathcal{G}(\mathbf{T}, \frac{\mathrm{d}\mathbf{T}}{\mathrm{d}t}, \dots, \mathbf{D}, \frac{\mathrm{d}\mathbf{D}}{\mathrm{d}t}, \dots, \dots) = 0$$

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

K. R. Rajagopal, On implicit constitutive theories for fluids, 2006.

Málek: Mathematical properties of flows of incompressible power-law-like fluids that are described by implicit constitutive relations, 2008.

- discretization
  - in time fractional θ scheme (Rothe method)
  - in space mixed FEM stable pair (Q_2/P_1^{disc}) or equal order stabilized formulation (local projection, GLS, internal penalty)
- solving the discrete nonlinear system
  - Large scale Newton or quasi-Newton method
  - Linearization, Jacobian computation: analytical, automatic differentiation, finite differences approximation
- solving large linear system
  - direct sparse methods
  - iterative Krylov space based methods, multigrid methods, problem dependent smoothing operators, preconditioners
  - effective parallel implementation to use full current hardware potential
- error evaluation, adaptivity...

- time discretization by one step θ scheme: i.e. Crank-Nicholson scheme, implicit Euler scheme

$$\frac{\partial f}{\partial t} = A(f) \qquad \Rightarrow \qquad \frac{f^{n+1} - f^n}{\Delta t} = \theta A(f^{n+1}) + (1-\theta)A(f^n)$$

- time discretization in constitutive law

$$\mathcal{G}(\mathbf{T}, \frac{\mathrm{d}\mathbf{T}}{\mathrm{d}t}, \mathbf{D}, \frac{\mathrm{d}\mathbf{D}}{\mathrm{d}t}) \approx \mathcal{G}(\mathbf{T}^{n+1}, \mathbf{D}^{n+1}, \mathbf{v}^{n+1}, \mathbf{L}^{n+1}, \ldots)$$

☞ Stokes system - steady, slow flow, no inertial effects

Consider Stokes system with explicit constitutive law:

$$\begin{aligned} -\operatorname{div}\mathbf{T} &= \mathbf{f} && \text{in } \Omega \\ \operatorname{div}\mathbf{v} &= 0 && \text{in } \Omega \\ \mathbf{T} &= -p\mathbf{I} + \boldsymbol{\sigma} = -p\mathbf{I} + \mathcal{A}(\mathbf{D}) && \text{in } \Omega \\ \mathbf{v} &= 0 && \text{on } \partial\Omega \end{aligned}$$

- $\boldsymbol{\sigma} = \mathcal{A}(\mathbf{D})$, explicit constitutive law formulation: find $\mathbf{v} \in \mathbb{V}_{\mathrm{div}} = \{H^1(\Omega); \mathbf{v}|\Gamma = 0, \operatorname{div}\mathbf{v} = 0\}$ such that

$$\int_\Omega \mathcal{A}(\mathbf{D}(\mathbf{v})) : \mathbf{D}(\varphi) = \int_\Omega \mathbf{f}\cdot\varphi, \quad \forall\varphi \in \mathbb{V}_{\mathrm{div}}$$

$$[\tilde{\mathcal{A}}]\;[\mathbf{v}] = [\mathbf{f}]$$

Standard mixed formulation - velocity, pressure

Stokes like system:

$$-\operatorname{div}\mathbf{T} = \mathbf{f}, \qquad \operatorname{div}\mathbf{v} = 0, \qquad \mathbf{T} = -p\mathbf{I} + \boldsymbol{\sigma} = -p\mathbf{I} + \mathcal{A}(\mathbf{D}(\mathbf{v}))$$

- $\boldsymbol{\sigma} = \mathcal{A}(\mathbf{D})$, mixed formulation: find $(\mathbf{v}, p) \in \mathbb{V} \times \mathbb{P}$ such that

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

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

Standard mixed formulation - velocity, pressure

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

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

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

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

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

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

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

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

- 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
- discretely div-free solution: if $\mathrm{div}\, \mathbf{v}_h \in \mathbb{P}_h$ (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 $\mathbf{X}^{n+1} = \mathbf{X}^n + \omega \tilde{\mathbf{X}} \quad \omega \in [-1, 0)$
- continuation methods

- structure of the Jacobian

$$\frac{\partial \mathcal{R}}{\partial \mathbf{X}} = \begin{bmatrix} A & -B^T \\ B & 0 \end{bmatrix}$$

- finite difference approximation

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

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))

- ☞ direct sparse solver (umfpack, superLU)
- Krylov space based iterative solver with preconditioning (general ILU(k), special preconditioners?)
- multigrid geometric
  - standard geometric multigrid approach
  - smoother by overlapping block Gauss-Seidel (Vanka-like smoother)
  - full inverse of the local dense problems by standard LAPACK
  - full Q_2 and P_1^{disc} prolongation **P** by interpolation, restriction defined by $\mathbf{R} = \mathbf{P}^T$
- multigrid algebraic

Dual mixed formulation - stress, velocity

Consider again Stokes like system:

$$-\operatorname{div}\mathbf{T} = \mathbf{f}, \qquad \operatorname{div}\mathbf{v} = 0, \qquad \mathbf{T} = -p\mathbf{I} + \boldsymbol{\sigma} = -p\mathbf{I} + \mathcal{A}(\mathbf{D}(\mathbf{v}))$$

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

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

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

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 $(\mathbf{D}, \mathbf{v}, \mathbf{T}) \in \mathbb{D} \times \mathbb{V} \times \mathbb{S}$ such that

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

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

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

J.S. Howell, H.J. Walkington, Inf-Sup Conditions for Twofold Saddle Point Problems, *Numer. Math.*, 2010.

Generalized 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 [Howell et al. (2010)]:

- 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

Requirements on the finite elements for the cases $(\sigma, \boldsymbol{v}, p)$, $(\mathbf{T}, \boldsymbol{v})$ and $(\mathbf{D}, \boldsymbol{v}, \mathbf{T})$ - J. Stebel

Theorem

Let S_h, V_h, Q_h satisfy the following conditions:

(i) *There exists $c > 0$ such that:* $\sup_{\boldsymbol{\varphi} \in V_h} \frac{(p, \operatorname{div} \boldsymbol{\varphi})}{\|\boldsymbol{\varphi}\|_{1,2}} \geq c\,\|p\|_2 \;\; \forall p \in Q_h$;

(ii) $\{(\mathbf{D}\boldsymbol{\varphi})^{\delta};\ \boldsymbol{\varphi} \in V_h\} \subset S_h$.

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

Theorem

Let T_h, V_h satisfy the following conditions:

(i) $\{\mathbf{D}\boldsymbol{\varphi};\ \boldsymbol{\varphi} \in \boldsymbol{W}_h\} \subset T_h$;

(ii) *There exists $c > 0$ such that:* $\sup_{\boldsymbol{\varphi} \in V_h} \frac{(\operatorname{tr} \mathbf{T}, \operatorname{div} \boldsymbol{\varphi})}{\|\boldsymbol{\varphi}\|_{1,2}} \geq c\,\|\operatorname{tr} \mathbf{T}\|_2 \;\; \forall \mathbf{T} \in T_h$.

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

Theorem

Let D_h, V_h, T_h satisfy the following conditions:

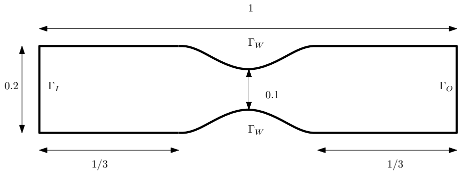
(i) $\{\mathbf{D}\boldsymbol{\varphi};\ \boldsymbol{\varphi} \in \boldsymbol{W}_h\} \subset T_h$;

(ii) $\{\mathbf{T}^{\delta};\ \mathbf{T} \in T_h\} \subset D_h$;

(iii) *There exists $c > 0$ such that:* $\sup_{\boldsymbol{\varphi} \in V_h} \frac{(\operatorname{tr} \mathbf{T}, \operatorname{div} \boldsymbol{\varphi})}{\|\boldsymbol{\varphi}\|_{1,2}} \geq c\,\|\operatorname{tr} \mathbf{T}\|_2 \;\; \forall \mathbf{T} \in T_h$.

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

Simulations of stress power-law model (with J. Stebel, K. Touška)



Boundary conditions

$$\mathbf{v} = (10^{-2} y(0.2 - y), 0) \quad \text{on } \Gamma_I, \tag{1}$$

$$\mathbf{v} = \mathbf{0} \quad \text{on } \Gamma_W, \tag{2}$$

$$\mathbf{Tn} \cdot \mathbf{n} = -p + \mathbf{Sn} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma_O, \tag{3}$$

$$\mathbf{v} \times \mathbf{n} = 0 \quad \text{on } \Gamma_O. \tag{4}$$

Simulations of stress power-law model

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

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

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}

- 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.
- All approximate formulations lead apparently to the same results.

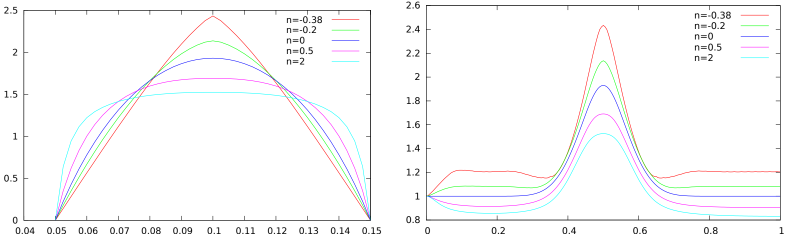


Figure : Velocity in the middle cross-section (left), along the channel (right).

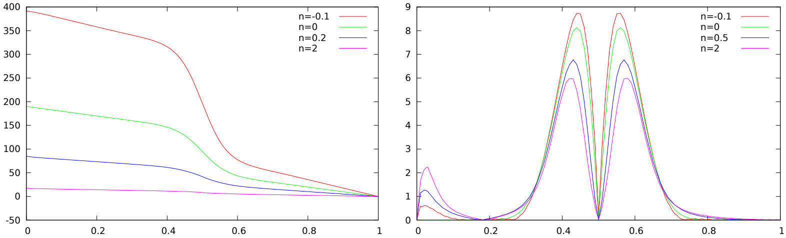


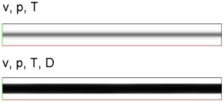
Figure : Pressure (left) and norm of $\mathbf{D}(\mathbf{v})$ (right) along the channel.

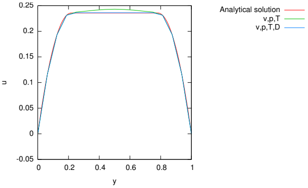
Numerical simulations of Bingham fluid (with K. Touška)

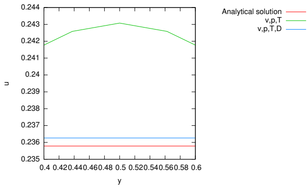
Stokes problem for regularized Bingham fluid in ”semi-implicit” formulation:

$$\begin{aligned} \operatorname{div} \mathbf{S} - \nabla p &= \mathbf{f}, \\ \operatorname{div} \mathbf{v} &= 0, \\ \mathbf{S}|\mathbf{D}_\varepsilon| - 2\mu \mathbf{D}|\mathbf{D}_\varepsilon| - \tau^* \mathbf{D} &= 0, \\ |\mathbf{D}_\varepsilon| &= \sqrt{|\mathbf{D}|^2 + \varepsilon^2}. \end{aligned}$$

- Dual-mixed formulation: unknowns $(\mathbf{v},\ p,\ \mathbf{T})$ - 5 equations (in 2 dimensions).
- It requires a series of computations with descending ε.
- ε stepping needs small steps or heuristic approach, both are time expensive.







Numerical simulations of Bingham fluid

- Lid driven cavity benchmark
- Unknowns ($\mathbf{D}, \boldsymbol{v}, \mathbf{T}$):

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

$$\mathbf{D} = 0 \Rightarrow |\mathbf{T}^\delta| \le \tau^*, \quad \mathbf{D} \ne 0 \Rightarrow \mathbf{T}^\delta = \tau^* \frac{\mathbf{D}}{|\mathbf{D}|} + 2\mu \mathbf{D},$$

$$\mathbf{D}\boldsymbol{v} = \mathbf{D}.$$

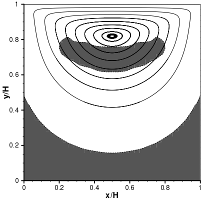
- Regularization:

$$\mathcal{G}(\mathbf{T}^\delta, \mathbf{D}) := \mathbf{T}^\delta |\mathbf{D}_\varepsilon| - \tau^* \mathbf{D} - 2\mu \mathbf{D} |\mathbf{D}_\varepsilon|, \quad |\mathbf{D}_\varepsilon| = \sqrt{\varepsilon^2 + |\mathbf{D}|^2}$$

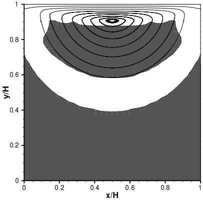
- The weak statement $\mathbf{D}\boldsymbol{v} = \mathbf{D}$ improves convergence for large τ^*

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

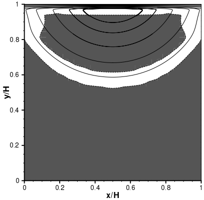
Lid driven cavity with Bingham fluid



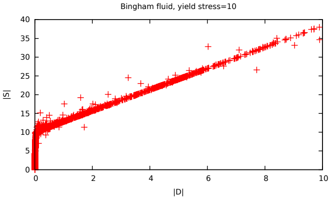
$\tau^* = 5$

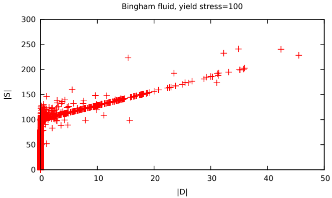


$\tau^* = 50$



$\tau^* = 500$

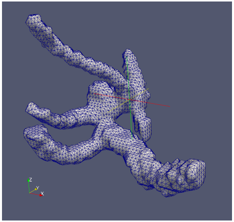


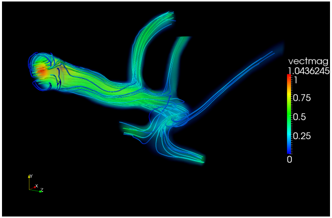


Satisfaction of the constitutive relation. Left: $\tau^* = 10$, right: $\tau^* = 100$.

Further developement - challanging problems

- Crystal plasticity $\rightarrow$ P. Minakowski
- Fluid-structure interaction in biomechanics





Spatial discretization: domain boundary incaurate; Material parameters: viscosity, wall stiffness inacurate; Boundary conditions: inflow/outflow location?, multiple inflow/outflows?, velocity/pressure values?...

- complete understanding of each step - from model equations, trough analysis and numerical solution
- efficient linear solver, preconditioners for block systems, as combination with iterative GMRES/BiCGStab/multigrid and direct methods...
- stopping criteria for nonlinear/linear solvers...