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An Adaptive Discrete Newton Method for Regularization-Free Bingham Model

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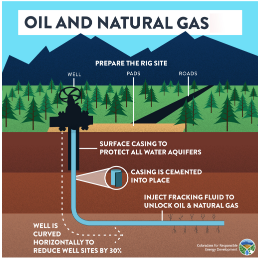
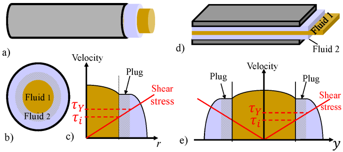
Motivation

- Viscoplastic lubrication in transport process
- Stabilization of interfaces in multi-layer flows
- Oil/gas fracking, site-specific drug delivery, medical imaging, food, cosmetic, and pharmaceutical product manufacturing, ...





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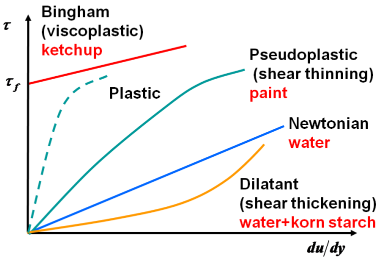
Classification of Fluids

Classification



- Linear relation $\rightarrow$ Newtonian
- Otherwise $\rightarrow$ Non-Newtonian

Bingham Constitutive Law

$$\begin{cases} \boldsymbol{\tau} = 2\eta \mathbf{D}(\boldsymbol{u}) + \tau_s \dfrac{\mathbf{D}(\boldsymbol{u})}{\|\mathbf{D}(\boldsymbol{u})\|} & \text{if } \|\mathbf{D}(\boldsymbol{u})\| \neq 0 \\ \|\boldsymbol{\tau}\| \leq \tau_s & \text{if } \|\mathbf{D}(\boldsymbol{u})\| = 0 \end{cases}$$

- Applied stress $\geq$ critical value of τ_s $\rightarrow$ Shear region
- Applied stress $\leq$ critical value of τ_s $\rightarrow$ Rigid or plug region

Primitive Variable Formulation

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- Viscosity model for Bingham flow

$$\eta(\|\mathbf{D}(\boldsymbol{u})\|) = 2\eta + \frac{\tau_s}{\|\mathbf{D}(\boldsymbol{u})\|}$$

- First, Shear region $\rightarrow \|\mathbf{D}(\boldsymbol{u})\| \neq 0$
- Second, Rigid or plug region $\rightarrow \|\mathbf{D}(\boldsymbol{u})\| = 0$
- Special treatment of plug zone: *Regularization*

$$\eta_\epsilon(\|\mathbf{D}(\boldsymbol{u})\|) = 2\eta + \frac{\tau_s}{\epsilon + \|\mathbf{D}(\boldsymbol{u})\|}$$ **Allouche et al. [1]**

$$\eta_\epsilon(\|\mathbf{D}(\boldsymbol{u})\|) = 2\eta + \frac{\tau_s(1 - exp(\frac{-\|\mathbf{D}(\boldsymbol{u})\|}{\epsilon}))}{\|\mathbf{D}(\boldsymbol{u})\|}$$ **Papanastasiou [2]**

$$\eta_\epsilon(\|\mathbf{D}(\boldsymbol{u})\|) = \begin{cases} 2\eta + \dfrac{\tau_s}{\|\mathbf{D}(\boldsymbol{u})\|} & \text{if } \|\mathbf{D}(\boldsymbol{u})\| \geq \epsilon\tau_s \\ \dfrac{2\eta}{\epsilon} & \text{if } \|\mathbf{D}(\boldsymbol{u})\| \leq \epsilon\tau_s \end{cases}$$

Tanner et al. [3]

$$\boxed{\eta_\epsilon(\|\mathbf{D}(\boldsymbol{u})\|) = 2\eta + \frac{\tau_s}{\sqrt{\mathbf{D} : \mathbf{D} + \epsilon^2}}}$$

Bercovier Engelman [4]

Two-Field Formulation:

$$\begin{cases} -\nabla \cdot \eta_\epsilon(\|\mathbf{D}(\boldsymbol{u})\|)\mathbf{D}(\boldsymbol{u}) + \nabla p = 0 & \text{in } \Omega \\ \nabla \cdot \boldsymbol{u} = 0 & \text{in } \Omega \\ \boldsymbol{u} = \boldsymbol{g}_D & \text{on } \Gamma_D \end{cases}$$

Three-Field Formulation

Two-Field $(\boldsymbol{u}, p)$

- Solve only for non vanishing regularization parameter $\epsilon \neq 0$
- Accuracy is compromised where yield properties are important

Three-Field $(\boldsymbol{u}, p, \boldsymbol{\sigma})$

- Introducing auxiliary stress tensor $\boldsymbol{\sigma}$
- Accurately solves regularization-free i.e $\epsilon = 0$ Bingham fluid flow

Three-Field Formulation

- Bingham model with additional symmetric viscoplastic stress tensor

$$\boldsymbol{\sigma} = \frac{\mathbf{D}(\boldsymbol{u})}{\|\mathbf{D}(\boldsymbol{u})\|_\epsilon}$$

$$\begin{aligned}
\|\mathbf{D}(\boldsymbol{u})\|_\epsilon \boldsymbol{\sigma} - \mathbf{D}(\boldsymbol{u}) &= 0 \quad && \text{in } \Omega \\
-\nabla \cdot (2\eta \mathbf{D}(\boldsymbol{u}) + \tau_s \boldsymbol{\sigma}) + \nabla p &= 0 \quad && \text{in } \Omega \\
\nabla \cdot \boldsymbol{u} &= 0 \quad && \text{in } \Omega \\
\boldsymbol{u} &= \boldsymbol{g}_D \quad && \text{on } \Gamma_D
\end{aligned}$$

- $\boldsymbol{\tau}_s$=yield stress
- $\mathbf{D}(\boldsymbol{u}) = \frac{1}{2}\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right)$
- η =viscosity
- $\boldsymbol{u}, p$= velocity, pressure

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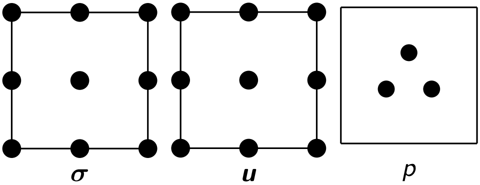
- $\mathbb{V} = \boldsymbol{H}_0^1(\Omega) := \left(H_0^1(\Omega)\right)^2$, $\mathbb{Q} = L_0^2(\Omega)$, and $\mathbb{M} = \left(L^2(\Omega)\right)_{\text{sym}}^{2\times 2}$ be the spaces for the velocity, pressure and stress
- Domain $\Omega \subset \mathbb{R}^d \longrightarrow$ grid $\mathcal{T}_h$ consisting of elements $K \in \mathcal{T}_h$
- Approximation spaces

$$\mathbb{V}^h = \left\{\boldsymbol{v}_h \in \mathbb{V}, \boldsymbol{v}_{h|K} \in (Q_2(K))^2\right\}$$
$$\mathbb{M}^h = \left\{\boldsymbol{\tau}_h \in \mathbb{M}, \boldsymbol{\sigma}_{h|K} \in (Q_2(K))^{2\times 2}\right\}$$
$$\mathbb{Q}^h = \left\{q_h \in \mathbb{Q}, q_{h|K} \in P_1^{\text{disc}}(K)\right\}$$



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Newton Method

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Algorithm

- Provide the input parameters, e.g. tolerance, parameters of the non-linear solver, initial guess and the iteration number n
- Repeat until the tolerance is achieved
- Calculate the residual $\mathcal{R}(\mathcal{U}^n) = A\,\mathcal{U}^n - b$
- Build the Jacobian $J(\mathcal{U}^n) = \frac{\partial \mathcal{R}(\mathcal{U}^n)}{\partial \mathcal{U}^n}$
- Solve $J(\mathcal{U}^n)\ \delta\mathcal{U}^n = \mathcal{R}(\mathcal{U}^n)$
- Find the optimal value of the damping factor $\omega^n \in (-1, 0]$
- Approximate $\mathcal{U}^{n+1} = \mathcal{U}^n - \omega^n\ \delta\mathcal{U}^n$

Sensitive parameters: initial guess, damping factor ω

Discrete Newton Method

$$J(\mathcal{U}^n)=\begin{bmatrix} \dfrac{\partial R_{\boldsymbol{u}}(\mathcal{U}^n)}{\partial \boldsymbol{u}} & \dfrac{\partial R_{\boldsymbol{u}}(\mathcal{U}^n)}{\partial \boldsymbol{\sigma}} & \dfrac{\partial R_{\boldsymbol{u}}(\mathcal{U}^n)}{\partial p} \\ \dfrac{\partial R_{\boldsymbol{\sigma}}(\mathcal{U}^n)}{\partial \boldsymbol{u}} & \dfrac{\partial R_{\boldsymbol{\sigma}}(\mathcal{U}^n)}{\partial \boldsymbol{\sigma}} & \dfrac{\partial R_{\boldsymbol{\sigma}}(\mathcal{U}^n)}{\partial p} \\ \dfrac{\partial R_{p}(\mathcal{U}^n)}{\partial \boldsymbol{u}} & \dfrac{\partial R_{p}(\mathcal{U}^n)}{\partial \boldsymbol{\sigma}} & \dfrac{\partial R_{p}(\mathcal{U}^n)}{\partial p} \end{bmatrix}$$

Jacobian calculation method

Analytical $\longrightarrow$ Knowledge of the Jacobian a priori

Approximation $\longrightarrow$ Black box manner

$$\left[\frac{\partial \mathcal{R}(\mathcal{U}^n)}{\partial \mathcal{U}^n}\right]_j \approx \frac{\mathcal{R}(\mathcal{U}^n + \chi\delta_j) - \mathcal{R}(\mathcal{U}^n - \chi\delta_j)}{2\chi}$$

$$\delta_j = \begin{cases} 1 & \text{j-index} \\ 0 & \text{otherwise} \end{cases}$$

Choice of the free parameter χ

- **Fixed constant:** Based on the perturbation analysis on the residum [5] selected as machine precision
- **Adaptive choice:** The sensitivity study of the nonlinear behavior of power law models w.r.t. the χ, *h* and strength of nonlinearity [6]
  - $\chi >> \rightarrow$ loss of the advantageous quasi-quadratic convergence
  - $\chi << \rightarrow$ divergence due to numerical instabilities

- Step size choice based on the current nonlinear reduction

$$\boxed{r_n = \frac{\|\mathcal{R}(\mathcal{U}^n)\|}{\|\mathcal{R}(\mathcal{U}^{n-1})\|}}$$

- Characteristic Function

$$\boxed{f(r_n) = 0.2 + \frac{0.4}{0.7 + \exp(1.5 r_n)}}$$

$$\boxed{\mathit{Adaptive} \quad \chi \longrightarrow \quad \chi_{n+1} = f^{-1}(r_n)\chi_n}$$

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Bingham Fluid Flow in Channel

- **Channel domain:** Unit square $\Omega = [0,1]^2$
- **Boundary conditions:** Dirichlet
- $u_y = 0$, $p = -x + c$ [7], $\eta = 1$

$$u_x = \begin{cases} \frac{1}{8}\left[(h-2\tau_s)^2 - (h-2\tau_s-2y)^2\right], & 0 \le y < \frac{h}{2} - \tau_s, \\ \frac{1}{8}(h-2\tau_s)^2, & \frac{h}{2} - \tau_s \le y \le \frac{h}{2} + \tau_s, \\ \frac{1}{8}\left[(h-2\tau_s)^2 - (2y-2\tau_s-h)^2\right], & \frac{h}{2} + \tau_s < y \le h. \end{cases}$$

Two-Field vs Three-Field

Table: **Two-field vs three-field formulation:** Number of iterations of the nonlinear solver in a channel flow at yield stress $\tau_s = 0.23$ for the two-field $(\boldsymbol{u}, p)$ and three-field formulation $(\boldsymbol{u}, p, \boldsymbol{\sigma})$

$\downarrow$ **L**$/\epsilon \rightarrow$	$\mathbf{10^{-1}}$	$\mathbf{10^{-2}}$	$\mathbf{10^{-3}}$	$\mathbf{10^{-4}}$	$\mathbf{10^{-5}}$	$\mathbf{10^{-1}}$	$\mathbf{10^{-2}}$	$\mathbf{10^{-3}}$	$\mathbf{10^{-4}}$	$\mathbf{10^{-5}}$	**0**
			Two-Field $(\boldsymbol{u}, p)$					**Three-Field**$(\boldsymbol{u}, p, \boldsymbol{\sigma})$			
3	2	3	-	-	-	2	3	4	6	9	1
4	2	3	-	-	-	2	3	4	8	9	1
5	2	3	-	-	-	1	2	3	9	5	2

Table: **Regularized viscosity approach in two-field variable $(\boldsymbol{u}, p)$:** Number of iterations of the nonlinear solver in a channel flow at yield stress $\tau_s = 0.23$ for the adaptive Newton and the classical Newton

$\downarrow$ **L**$/\epsilon \rightarrow$	$\mathbf{10^{-1}}$	$\mathbf{10^{-2}}$	$\mathbf{10^{-3}}$	$\mathbf{10^{-4}}$	$\mathbf{10^{-5}}$	$\mathbf{10^{-1}}$	$\mathbf{10^{-2}}$	$\mathbf{10^{-3}}$	$\mathbf{10^{-4}}$	$\mathbf{10^{-5}}$
			Newton					**Adaptive Newton**		
3	2	3	-	-	-	4	4	5	5	9
4	2	3	-	-	-	4	4	5	5	9
5	2	3	-	-	-	4	4	6	5	9

Table: **Regularization-free three-field formulation $(\boldsymbol{u}, p, \boldsymbol{\sigma})$:** Number of iterations of the nonlinear solver in a channel flow at yield stress $\tau_s = 0.23$ for the adaptive Newton and the classical Newton

$\downarrow$ **L**/ϵ $\rightarrow$	$\mathbf{10^{-1}}$	$\mathbf{10^{-2}}$	$\mathbf{10^{-3}}$	$\mathbf{10^{-4}}$	$\mathbf{10^{-5}}$	**0**	$\mathbf{10^{-1}}$	$\mathbf{10^{-2}}$	$\mathbf{10^{-3}}$	$\mathbf{10^{-4}}$	$\mathbf{10^{-5}}$	**0**
	Newton						**Adaptive Newton**					
3	2	3	4	6	9	1	2	2	2	5	1	2
4	2	3	4	8	9	1	1	2	2	4	2	2
5	1	2	3	9	5	2	1	1	1	1	3	1

$$\boxed{\quad Regularization - free \quad Bingham \quad \epsilon = \mathbf{0} \quad}$$

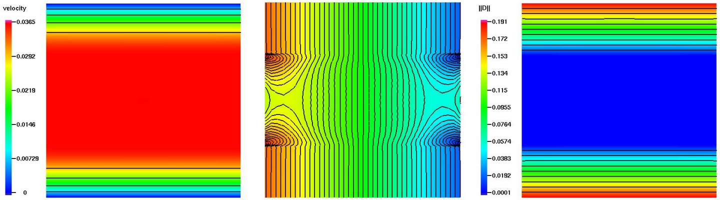


Figure: Visualization of the velocity contours, pressure and $\|\mathbf{D}(\boldsymbol{u})\|$ for the non-regularized Bingham fluid flow in a channel with $\tau_s = 0.23$ at refinement level L=5 ($h_x = 1/32$, $h_y = 1/96$).

Nonlinear convergence w.r.t χ for regularization-free Bingham

$\underline{\boldsymbol{\tau_s = 0.23}}$

- $h_x = \frac{1}{4}, h_y = \frac{1}{12}$
- $\chi_c = constant$

$\chi_{c_1} = 10^{-1}$

$\chi_{c_2} = 10^{-2}$

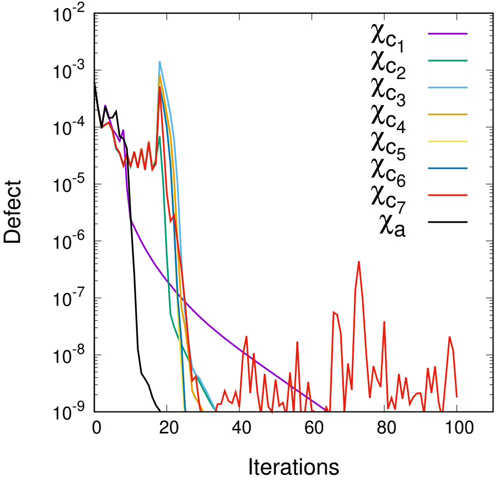
.

.

.

$\chi_{c_7} = 10^{-7}$

- $\chi_a = adaptive$



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Nonlinear convergence w.r.t χ for regularization-free Bingham

$\underline{\boldsymbol{\tau_s = 0.3}}$

- $h_x = \frac{1}{4}, h_y = \frac{1}{12}$
- $\chi_c = constant$

$\chi_{c_1} = 10^{-1}$

$\chi_{c_2} = 10^{-2}$

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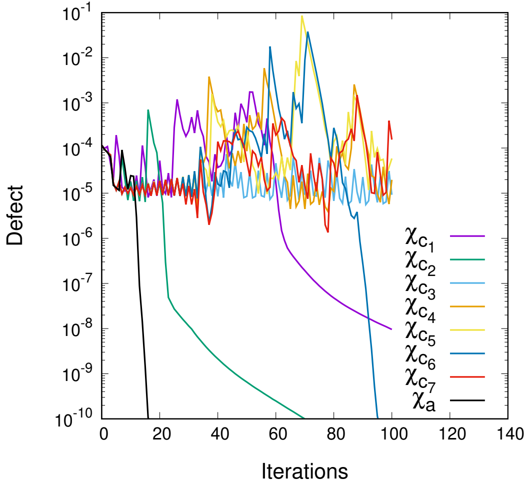
$\chi_{c_7} = 10^{-7}$

- $\chi_a = adaptive$



Nonlinear convergence w.r.t χ for regularization-free Bingham

$\underline{\tau_s = \mathbf{0.35}}$

- $h_x = \frac{1}{4}, h_y = \frac{1}{12}$
- $\chi_c = constant$

  $\chi_{c_1} = 10^{-1}$

  $\chi_{c_2} = 10^{-2}$

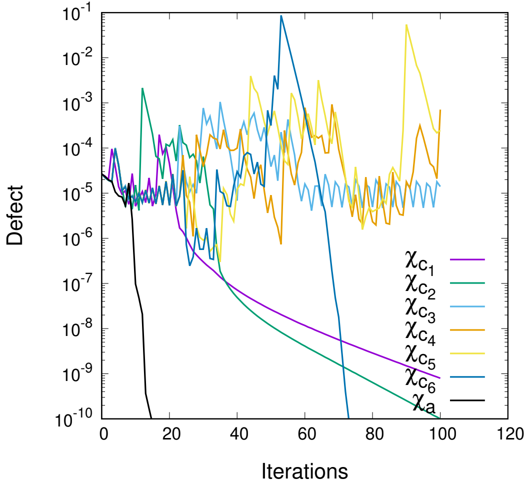
  .

  .

  .

  $\chi_{c_7} = 10^{-7}$

- $\chi_a = adaptive$



Nonlinear convergence w.r.t χ for regularization-free Bingham

$\underline{\boldsymbol{\tau_s = 0.4}}$

- $h_x = \frac{1}{4}, h_y = \frac{1}{12}$
- $\chi_c = constant$

$\chi_{c_1} = 10^{-1}$

$\chi_{c_2} = 10^{-2}$

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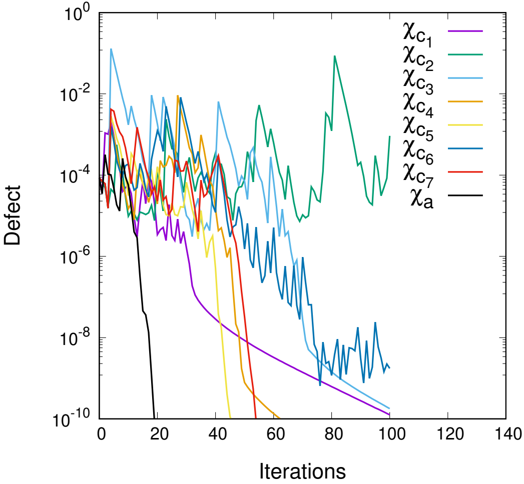
$\chi_{c_7} = 10^{-7}$

- $\chi_a = adaptive$



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Summary

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A new adaptive discrete Newton and regularization-free solver for yield stress fluids is developed

- Three-field formulation $\longrightarrow$ New auxiliary stress
- Adaptive step size $\longrightarrow$ Accurate and efficient

Advantages

- Accurate non-regularized viscoplastic solution $\longrightarrow \epsilon = 0$
- The method does not effect the shape of the yield surfaces
- Faster convergence ✓
- Significant reduction in nonlinear iterations ✓

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