Simulations of flows of fluids characterized by a non-monotone implicit constitutive relation

Giordano Tierra Chica

Josef Málek

Mathematical Institute
Faculty of Mathematics and Physics
Charles University in Prague

Experiments for colloidal and surfactant suspensions:

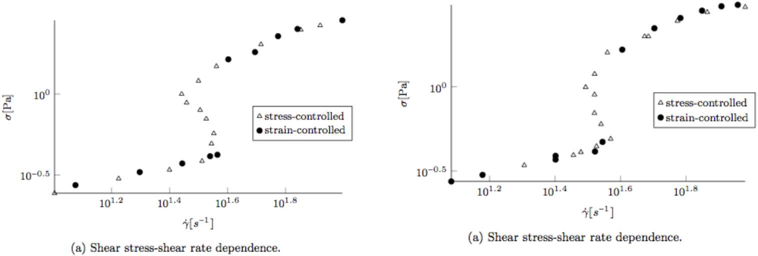


Figure: Extracted from T. Perlácová and V. Průsa. Tensorial implicit constitutive relations in mechanics of incompressible non-Newtonian fluids. J. Non-Newton. Fluid Mech. **216** (2015) 13-21

Non-Monotone Constitutive Relations.

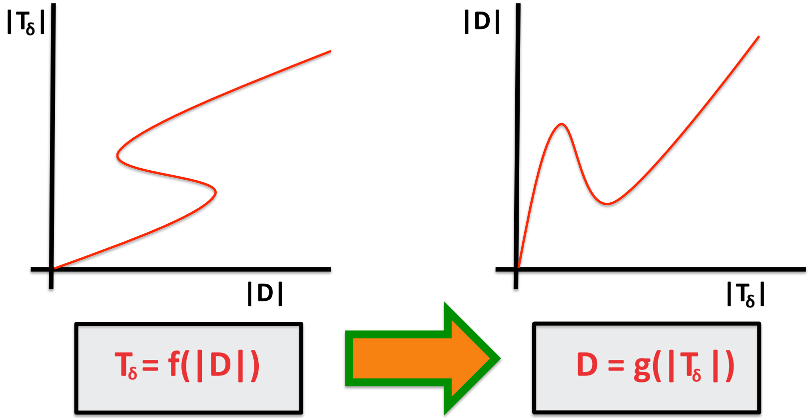


Figure: Idea: Instead of shear stress depending on shear rate, consider shear rate depending on shear stress

The model:

$$\left\{ \begin{aligned} \rho \frac{D\mathbf{v}}{Dt} &= \operatorname{div} \mathbb{T} + \rho \mathbf{b}\,, \\ \mathbb{D} &= \Big[\alpha(1+\beta|\mathbb{T}_\delta|^2)^s + \gamma\Big]\mathbb{T}_\delta\,, \\ \operatorname{div} \mathbf{v} &= 0\,. \end{aligned} \right. \qquad (1)$$

where $\frac{D\cdot}{Dt}$ denotes the material derivative, $\mathbb{D} := 1/2\Big(\nabla \mathbf{v} + (\nabla \mathbf{v})^t\Big)$ and $\mathbb{T}_\delta := \mathbb{T} - \frac{1}{3}(\mathrm{tr}\mathbb{T})\mathbb{I}$ (for simplicity $\rho = 1$).

Constants $\alpha, \beta > 0$, $\gamma \geq 0$ and $s \in R$ such that $s < -1/2$.

[C. Le Roux and K.R. Rajagopal. Shear flows of a new class of power-law fluids. Applications to Mathematics **58** (2013) 153-177]

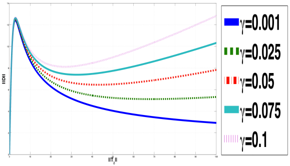


Figure: Examples of non-monotone constitutive relations given by $(1)_2$ with $\alpha = 10, \beta = 0.25, s = -0.75$ and $\gamma = 0.001, 0.025, 0.05, 0.075, 0.1$.

Idea: Rewrite the constitutive relation using a nonlinear viscosity dependent on the shear stress:

$$\mathbb{T}_\delta = \mu(|\mathbb{T}_\delta|)\mathbb{D}\,.$$

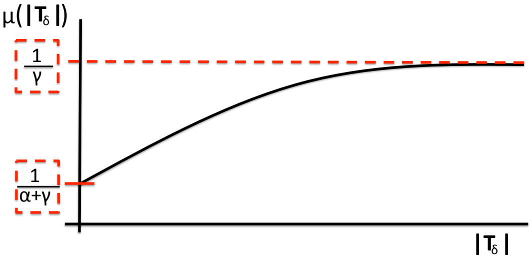
where

$$\mu = \mu(|\mathbb{T}_\delta|) := \left[\alpha(1 + \beta|\mathbb{T}_\delta|^2)^s + \gamma\right]^{-1}.$$

Q: What is the improvement of considering this nonlinear viscosity?

A: Viscosity μ is a monotone and bounded function !

Viscosity μ is a monotone and bounded function.



Remark

We have balance of energy ($0 < \frac{1}{\alpha+\gamma} \leq \mu \leq \frac{1}{\gamma}$)*:*

$$\frac{d}{dt}\left(\frac{1}{2}\int_\Omega |\boldsymbol{v}|^2\right) + 2\int_\Omega \mu|\mathbb{D}|^2 = 0\,,$$

and the following a priori estimates analogous to the Navier-Stokes system:

$$\boldsymbol{v} \in L^\infty(0,T;L^2(\Omega)^d) \cap L^2(0,T;H_0^1(\Omega)^d)\,,$$

Numerical scheme

For simplicity $\rho = cte = 1$ and we neglect the convective effects in the presentation of the scheme.

- Time - Finite Differences
- Space - Finite Elements

Compute $(\boldsymbol{v}^{n+1}, p^{n+1}, \mu^{n+1})$ as the solution of the following nonlinear scheme:

$$
\begin{aligned}
\left(\frac{\boldsymbol{v}^{n+1} - \boldsymbol{v}^{n}}{\Delta t}, \bar{\boldsymbol{v}}\right) + (2\mu^{n+1}\mathbb{D}^{n+1}, \overline{\mathbb{D}}) + (\nabla p^{n+1}, \bar{\boldsymbol{v}}) &= 0\,, \\
(\operatorname{div} \boldsymbol{v}^{n+1}, \bar{p}) &= 0\,, \\
(\mu^{n+1}, \bar{\mu}) - \left(\left[\alpha(1 + \beta\,|\mu^{n+1}|^2|\mathbb{D}^{n+1}|^2)^s + \gamma\right]^{-1}, \bar{\mu}\right) &= 0\,.
\end{aligned}
$$

We recover the discrete version of the balance of energy:

$$
\|\boldsymbol{v}^{n+1}\|^2_{L^2(\Omega)} + 2\,\Delta t \int_\Omega \mu^{n+1}|\mathbb{D}^{n+1}|^2 \le \|\boldsymbol{v}^{n}\|^2_{L^2(\Omega)}\,.
$$

Numerical scheme. Iterative algorithm.

Initialization:
Define $(\boldsymbol{v}^0, p^0, \mu^0) := (\boldsymbol{v}^n, p^n, \mu^n)$.
Step 1:
Given $(\boldsymbol{v}^l, p^l, \mu^l)$, to find $(\boldsymbol{v}^{l+1}, p^{l+1})$ such that $\forall\,(\bar{\boldsymbol{v}}, \bar{p}) \in \boldsymbol{V}_h \times P_h$:

$$\begin{aligned} \left(\frac{\boldsymbol{v}^{l+1} - \boldsymbol{v}^n}{\Delta t}, \bar{\boldsymbol{v}}\right) + (2\mu^l \mathbb{D}^{l+1}, \overline{\mathbb{D}}) + (\nabla p^{l+1}, \bar{\boldsymbol{v}}) &= 0\,, \\ (\operatorname{div} \boldsymbol{v}^{l+1}, \bar{p}) &= 0\,. \end{aligned} \tag{2}$$

Step 2:
Compute μ^{l+1}

$$\mu^{l+1} = \left[\alpha(1 + \beta|\mu^l|^2|\mathbb{D}^{l+1}|^2)^s + \gamma\right]^{-1}. \tag{3}$$

Step 3:

Compute the residual η

$$\eta = \|\mu^{l+1} - \mu^{l}\|_{L^2(\Omega)} + \|\boldsymbol{v}^{l+1} - \boldsymbol{v}^{l}\|_{L^2(\Omega)} \,.$$

Then check:

$$\begin{cases} \text{If } \eta > tol & \Rightarrow \quad \text{Go to } \textbf{Step 1} \text{ and iterate again}\,, \\ \text{If } \eta \leq tol & \Rightarrow \quad (\boldsymbol{v}^{n+1}, p^{n+1}, \mu^{n+1}) := (\boldsymbol{v}^{l+1}, p^{l+1}, \mu^{l+1})\,, \end{cases} \tag{4}$$

where $tol > 0$ represents a tolerance parameter.

Numerical simulations I. Reduced problem

Find (**q**-vector,u-scalar) such that

$$\begin{cases} u_t - \nabla \cdot \boldsymbol{q} \;=\; 0\,, \\ \nabla u = [\alpha(1+\beta|\boldsymbol{q}|^2)^s + \gamma]\boldsymbol{q}\,. \end{cases} \tag{5}$$

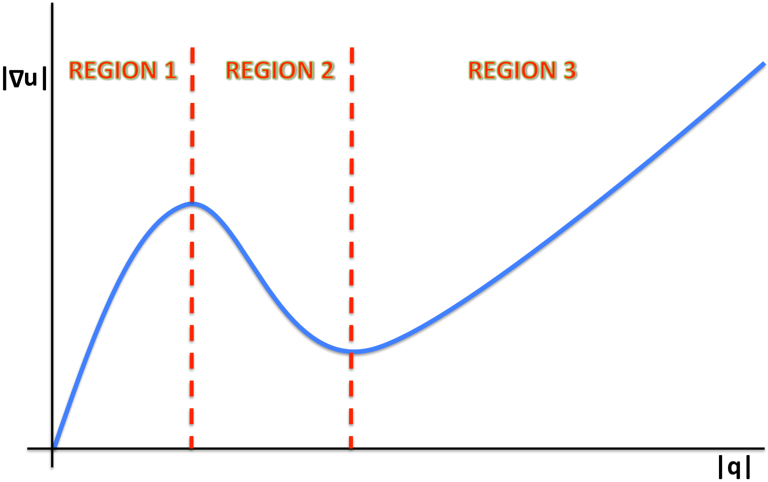
Constants $\alpha, \beta > 0$, $\gamma \geq 0$ and $s \in \boldsymbol{R}$ such that $s < -1/2$.

1. Rewrite the system with a nonlinear viscosity $\widetilde{\mu}$

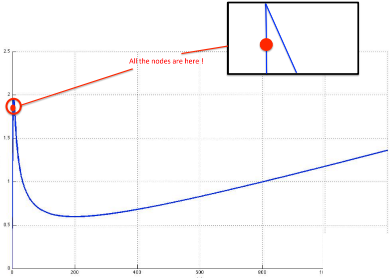
$$\widetilde{\mu} \;=\; \widetilde{\mu}(\boldsymbol{q}) \;:=\; [\alpha(1+\beta|\boldsymbol{q}|^2)^s + \gamma]^{-1}\,. \tag{6}$$

2. Design Iterative Numerical Scheme as before.

Numerical simulations I. Reduced problem

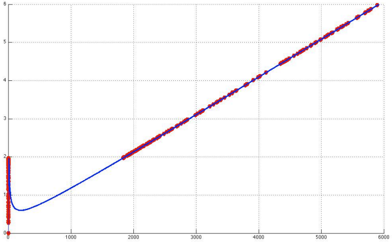


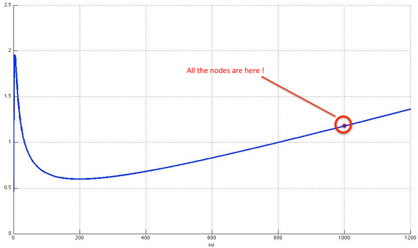
Numerical simulations I. Reduced problem



INITIALLY

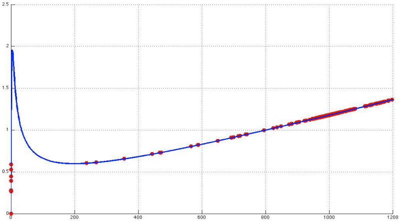
SIMULATIONS RESULTS



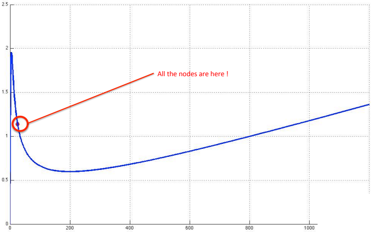


INITIALLY

SIMULATIONS RESULTS

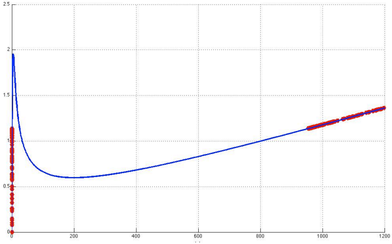


Numerical simulations I. Reduced problem

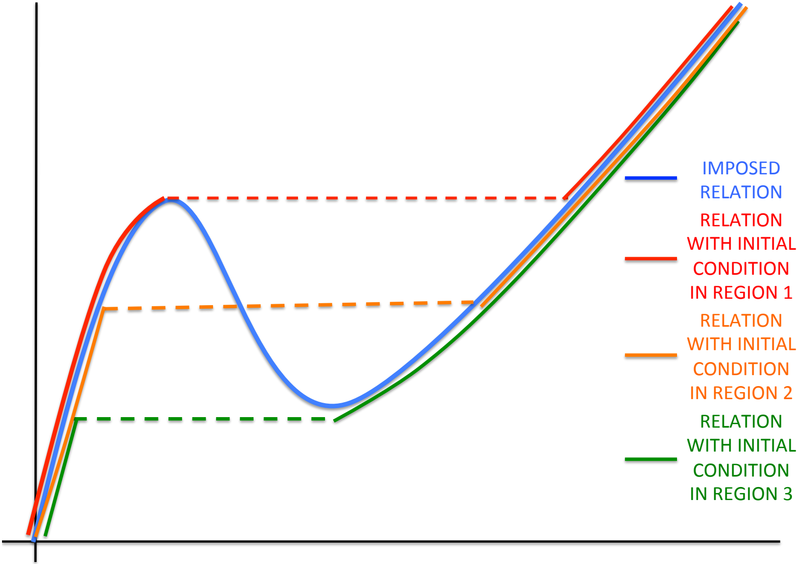


INITIALLY

SIMULATIONS RESULTS



Numerical simulations I. Reduced problem



Domain:

Boundary Conditions:

$$\begin{cases} \boldsymbol{v} = \boldsymbol{0} & \text{on } \Gamma_{top} \cup \Gamma_{bottom}\,, \\ (\mathbb{T}\boldsymbol{n})\boldsymbol{n} = \boldsymbol{0} & \text{on } \Gamma_{right}\,, \\ \boldsymbol{v} = \left(f_0(-y^2+y), 0\right) & \text{on } \Gamma_{left}\,, \end{cases}$$

Simulation Parameters:

Δt	α	β	s	γ	tol
1.0e-10	1.0	0.1	-0.75	1.0e-06	1.0e-05

Case 1: $f_0 = 0.1$

Case 1: $f_0 = 0.1$

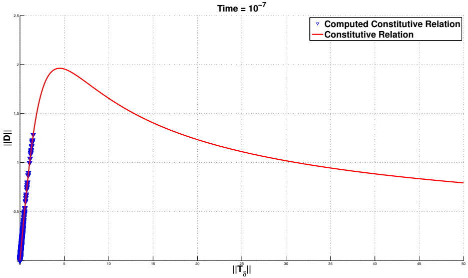


Figure: Approximation of the Constitutive Relation at time $t = 1.0e\text{-}07$ with $f_0 = 0.1$. In continuous red color the Constitutive Relation and in blue triangles the relations obtained in the simulations.

Case 2: $f_0 = 1.0$

Case 2: $f_0 = 1.0$

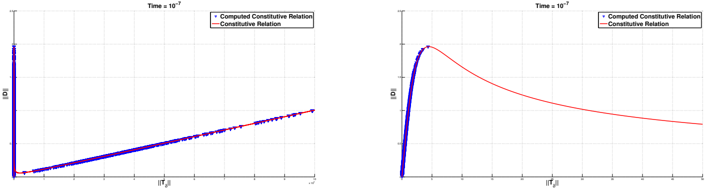


Figure: Approximation of the Constitutive Relation at time $t = 1.0e\text{-}07$ ($f_0 = 1$).

THANK YOU FOR YOUR ATTENTION!