FEM analysis and monolithic Newton-multigrid solver for thixo-viscoplastic flow problems

Naheed Begum, Abderrahim Ouazzi, Stefan Turek
Institute of Applied Mathematics, LS III,
TU Dortmund University, Dortmund, Germany

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German Association for Computational Mechanics

fakultät für mathematik

lehrstuhl für angewandte mathematik und numerik

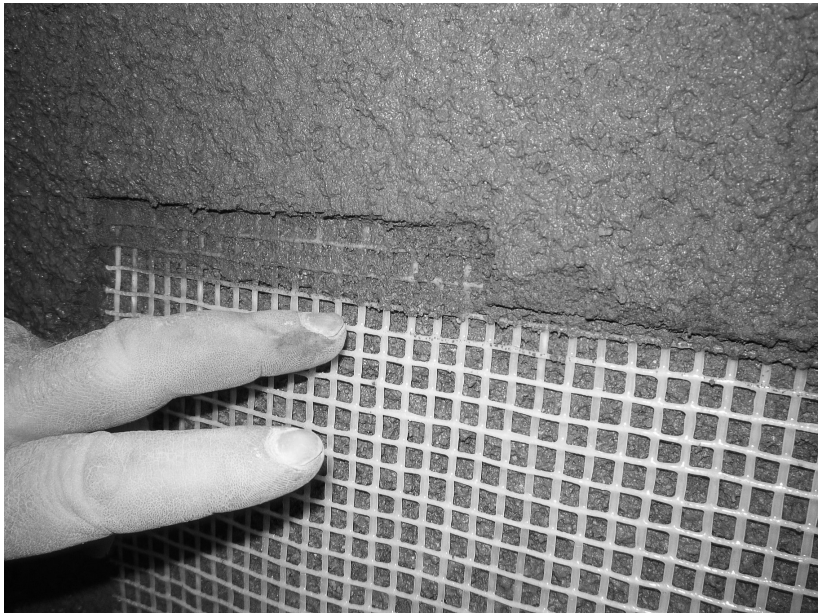
Motivation

Why "Thixotropic materials?

- **Processing of thixotropic materials relevant for industrial applications**

➡ **Lubrication, asphalt, self-compacting concrete…**

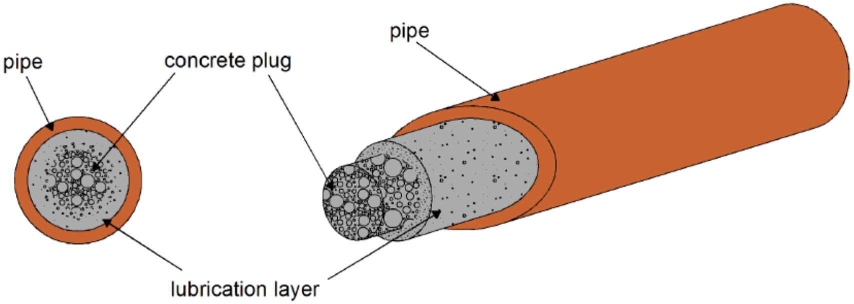
- **Physically fascinating due to improved mechanical properties**



Goal:

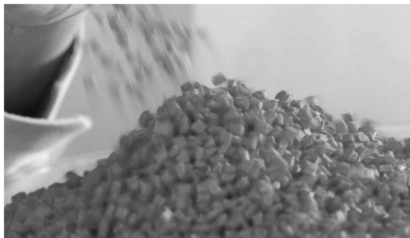
- **Modern CFD methods with high accuracy, robustness and efficiency for thixotropic materials**

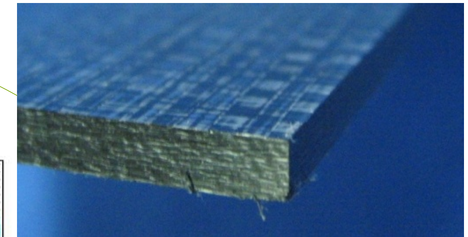
➡ **Saving time, money and resources**

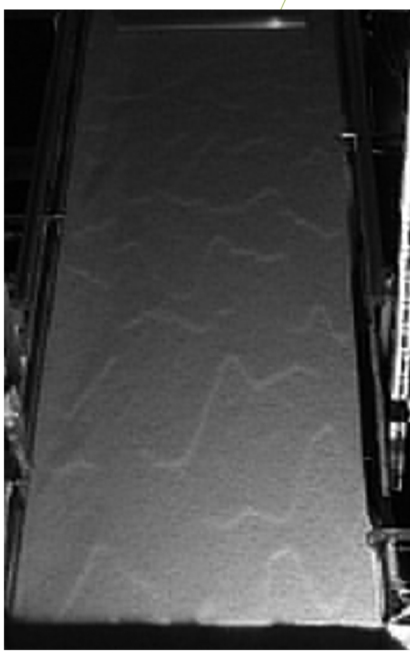


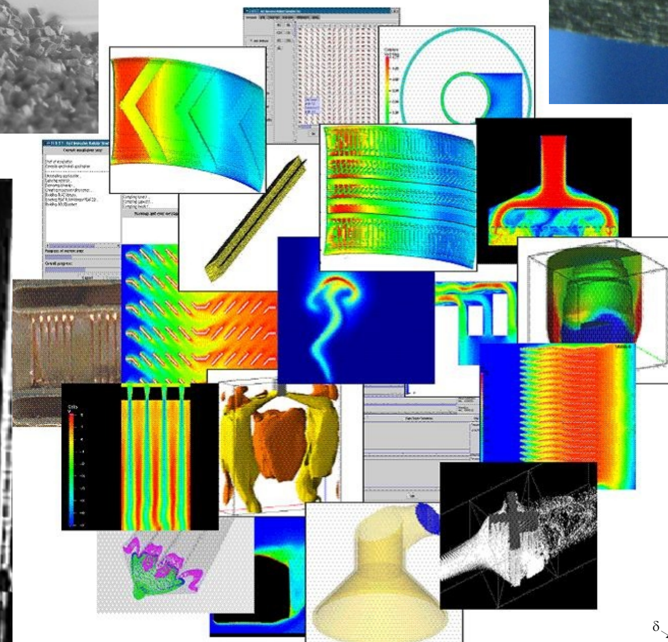
Investigation of solid/liquid and liquid/solid transitions based on micro-structure

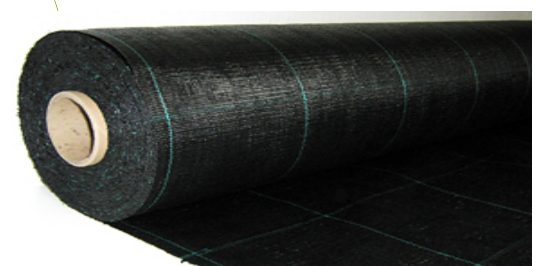
Thixotropy in complex fluidic process

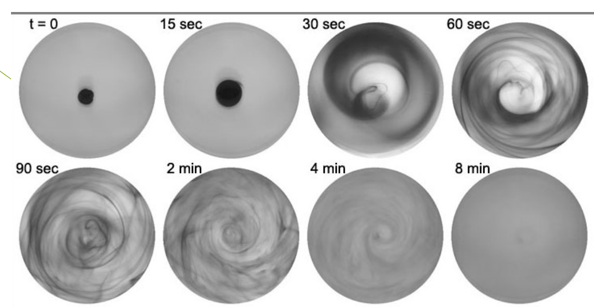


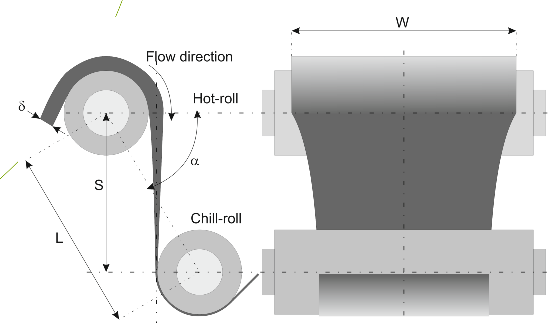












Archetypical thixotropic viscoplastic (TVP) models

$$\begin{cases} \boldsymbol{\sigma} = 2\,\eta(D_{\mathrm{II}},\lambda)\boldsymbol{D}(\boldsymbol{u}) + \sqrt{2}\,\tau(\lambda)\dfrac{\boldsymbol{D}(\boldsymbol{u})}{\sqrt{D_{\mathrm{II}}}} & \text{if } D_{\mathrm{II}} \neq 0 \\ \sigma_{\mathrm{II}} \leq \tau(\lambda) & \text{if } D_{\mathrm{II}} = 0 \end{cases}$$

Relations between rheological parameters and structural parameter

	$\eta(D_{\mathrm{II}},\lambda)$	$\tau(\lambda)$
Worrall and Tulliani[1]	$\lambda\eta_0$	τ_0
Coussot *et al.*[2]	$\lambda^a\eta_0$	–
Houska[3]	$(\eta_0+\eta_1\lambda)\,D_{\mathrm{II}}^{\frac{(n-1)}{2}}$	$(\tau_0+\tau_1\lambda)$
Mujumbar *et al.*[4]	$(\eta_0+\eta_1\lambda)\,D_{\mathrm{II}}^{\frac{(n-1)}{2}}$	$\lambda^{a+1}\mathrm{G}_0\Lambda_c{}^*$
Burgos *et al.*[5]	η_0	$\lambda\tau_0$
Dullaert & Mewis[6]	$\lambda\eta_0$	$\lambda\mathrm{G}_0\left(\lambda D_{\mathrm{II}}^{\frac{1}{2}}\right)\Lambda_c^*$

$*\Lambda_c$ is a constant/variable elastic strain.

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- **General format of evolution equation for structural parameter:**

$$\frac{\partial \lambda}{\partial t} + u \cdot \nabla \lambda = F_{buildup} - F_{breakdown}$$

- **Expressions for different thixotropic models:**

	$F_{buildup}$	$F_{breakdown}$
Worrall and Tulliani[1]	$c_1(1-\lambda)D_{\mathrm{II}}^{\frac{1}{2}}$	$c_2 \lambda D_{\mathrm{II}}^{\frac{1}{2}}$
Coussot *et al.*[2]	c_1	$c_2 \lambda D_{\mathrm{II}}^{\frac{1}{2}}$
Houska[3]	$c_1(1-\lambda)$	$c_2 \lambda^m D_{\mathrm{II}}^{\frac{1}{2}}$
Mujumbar *et al.*[4]	$c_1(1-\lambda)$	$c_2 \lambda D_{\mathrm{II}}^{\frac{1}{2}}$
Burgos *et al.*[5]	$c_1(1-\lambda)$	$c_2 \lambda D_{\mathrm{II}}^{\frac{1}{2}} \exp(a D_{\mathrm{II}}^{\frac{1}{2}})$
Dullaert & Mewis[6]	$(c_1 + c_3 D_{\mathrm{II}}^{\frac{1}{2}})(1-\lambda)t^{-b}$	$c_2 \lambda D_{\mathrm{II}}^{\frac{1}{2}} t^{-b}$

➢ Viscosity model for TVP flow

- **Classical approximations**

$$\begin{cases} I. & \dfrac{1}{\sqrt{D_{\mathrm{II},r}}} := \dfrac{1}{\sqrt{(D_{\mathrm{II}} + (k^{-1})^2)}} \\ II. & \dfrac{1}{\sqrt{D_{\mathrm{II},r}}} := \dfrac{1}{\sqrt{D_{\mathrm{II}}}}\left(1 - e^{-k\sqrt{D_{\mathrm{II}}}}\right) \end{cases}$$

- **Extended viscosity defined on all domain**

$$\mu(D_{\mathrm{II},r}, \lambda) = \eta(D_{\mathrm{II}}, \lambda) + \tau(D_{\mathrm{II}}, \lambda)\frac{\sqrt{2}}{2}\frac{1}{\sqrt{D_{\mathrm{II},r}}}$$

➢ Full set of equations

$$\begin{cases} \left(\dfrac{\partial}{\partial t} + \boldsymbol{u}\cdot\nabla\right)\boldsymbol{u} - \nabla\cdot\left(2\mu(\boldsymbol{D}_{\mathrm{II},r}, \lambda)\boldsymbol{D}(\boldsymbol{u})\right) + \nabla p = \boldsymbol{f}_{\boldsymbol{u}} & \text{in } \Omega \\ \nabla\cdot\boldsymbol{u} = 0 & \text{in } \Omega \\ \left(\dfrac{\partial}{\partial t} + \boldsymbol{u}\cdot\nabla\right)\lambda + \mathcal{M}(D_{\mathrm{II}}, \lambda) = f_\lambda & \text{in } \Omega \end{cases}$$

- **Flow variables** $(\lambda, \boldsymbol{u}, p)$
  - **Set** $\mathbb{T} := H^1_{\Gamma^-}(\Omega), \mathbb{V} := \left[H^1_0(\Omega)\right]^2, \mathbb{Q} := L^2(\Omega), \mathbb{W} := \mathbb{T} \times \mathbb{V}$
  - **Set** $\tilde{\boldsymbol{u}} := (\lambda, \boldsymbol{u})$
  - **Find** $(\lambda, \boldsymbol{u}, p) \in \mathbb{T} \times \mathbb{V} \times \mathbb{Q}$ **s.t.**

$$\left\langle \mathcal{K}(\lambda, \boldsymbol{u}, p), (\xi, \boldsymbol{v}, q) \right\rangle = \left\langle \mathcal{L}, (\xi, \boldsymbol{v}, q) \right\rangle, \quad \forall (\xi, \boldsymbol{v}, q) \in \mathbb{T} \times \mathbb{V} \times \mathbb{Q}$$

Theorem [Begum et. al 2022]

Let $\boldsymbol{f_u} \in (L^2(\Omega))^2$ and $f_\lambda \in L^2(\Omega)$, the thixo-viscoplastic problem has a unique solution $(\tilde{\boldsymbol{u}}, p) = (\lambda, \boldsymbol{u}, p) \in \mathbb{W} \times \mathbb{Q}$ with the following bound on data

$$\|\boldsymbol{u}\|_1 \leq \frac{1}{\eta_0 \mathcal{C}_K} \|\boldsymbol{f_u}\|_0$$

$$\mathcal{M}_a \|\lambda\|_0^2 + \frac{1}{2} \langle \lambda \rangle^2 \leq \frac{1}{\mathcal{M}_a} \|f_\lambda\|_0^2$$

$$\|p\|_0 \leq \frac{1}{\beta} \left(1 + \frac{2(\eta_\infty + k\tau_\infty) + |\boldsymbol{u}|_1}{\eta_0 \mathcal{C}_K}\right) \|\boldsymbol{f_u}\|_0$$

with $\mathcal{C}_K$ denotes Korn's inequality constant.

Coercivity in weaker norm for the microstructure !

Pressure is underdertmined in regid zone !

- **Conforming approximations**

$$\mathbb{T}_h \subset \mathbb{T},\ \mathbb{V}_h \subset \mathbb{V},\ \mathbb{Q}_h \subset \mathbb{Q},\ \mathbb{W}_h := \mathbb{T}_h \times \mathbb{V}_h \qquad \mathcal{A}_{\tilde{\boldsymbol{u}}h} = \mathcal{A}_{\tilde{\boldsymbol{u}}},\ \ \mathcal{B}_h = \mathcal{B}$$

  - **Find** $(\lambda_h, \boldsymbol{u}_h, p_h) \in \mathbb{T}_h \times \mathbb{V}_h \times \mathbb{Q}_h$ **s.t**

$$\Big\langle \mathcal{K}(\lambda_h, \boldsymbol{u}_h, p_h), (\xi_h, \boldsymbol{v}_h, q_h) \Big\rangle = \Big\langle \mathcal{L}, (\xi_h, \boldsymbol{v}_h, q_h) \Big\rangle,\ \ \forall (\xi_h, \boldsymbol{v}_h, q_h) \in \mathbb{T}_h \times \mathbb{V}_h \times \mathbb{Q}_h$$

Theorem

Let $\boldsymbol{f}_{\boldsymbol{u}} \in (L^2(\Omega))^2$ *and* $f_\lambda \in L^2(\Omega)$, *the approximate thixo-viscoplastic problem has a unique solution* $(\tilde{\boldsymbol{u}}_h, p_h) = (\lambda_h, \boldsymbol{u}_h, p_h) \in \mathbb{W}_h \times \mathbb{Q}_h$ *with the following a priori best approximation*

$$\|\lambda - \lambda_h\|_0^2 \ \le\ (2 + 2\tilde{\mathcal{C}}_{\lambda,\lambda}) \inf_{\xi_h \in \mathbb{T}_h} \|\lambda - \xi_h\|_1^2 + \tilde{\mathcal{C}}_{\lambda,\boldsymbol{u}} \inf_{\boldsymbol{v}_h \in \mathbb{V}_h} |\boldsymbol{u} - \boldsymbol{v}_h|_{1,\infty}^2$$

$$|\boldsymbol{u} - \boldsymbol{u}_h{}_{1,\infty}^2 \le \tilde{\mathcal{C}}_{\boldsymbol{u},\lambda} \inf_{\xi_h \in \mathbb{T}_h} \|\lambda - \xi_h\|_1^2 + (2 + 2\tilde{\mathcal{C}}_{\boldsymbol{u},\boldsymbol{u}}) \inf_{\boldsymbol{v}_h \in \mathbb{V}_h} |\boldsymbol{u} - \boldsymbol{v}_h|_{1,\infty}^2$$
$$+ \mathcal{C}_{\boldsymbol{u},p} \inf_{q_h \in \mathbb{Q}_h} \|p - q_h\|_0^2$$

Remark (Finite element approximation)

- **Regularization**

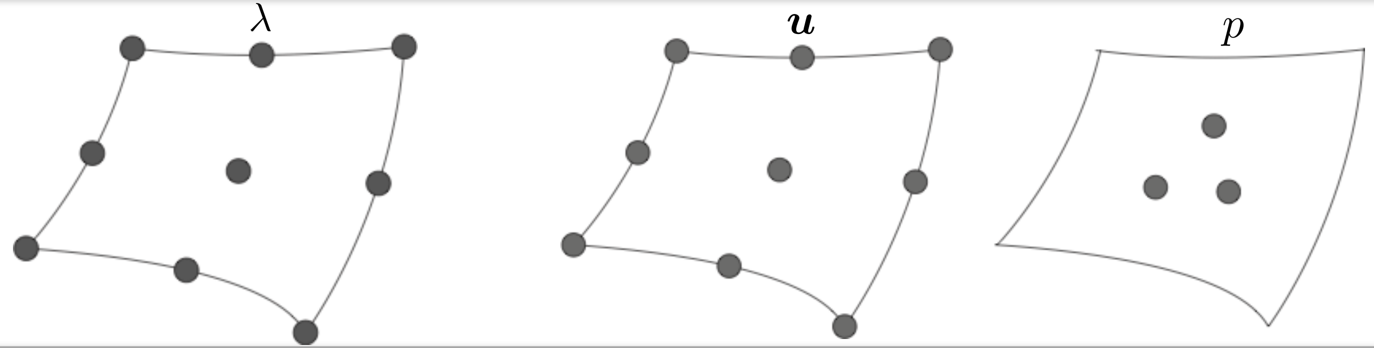
$$|\boldsymbol{u} - \boldsymbol{u}_h|_1^2 \equiv \tilde{\mathcal{C}}_{\boldsymbol{u},\lambda} h^{2r} |\lambda|_{r+1} + (2 + 2\tilde{\mathcal{C}}_{\boldsymbol{u},\boldsymbol{u}}) h^{2r} |\boldsymbol{u}|_{r+1}^2 + \mathcal{C}_{\boldsymbol{u},p} h^{2r} \|p\|_r^2 \equiv \mathcal{O}(k^2 h^{2r})$$

- **Coercivity in a weaker norm**

$$\|\lambda - \lambda_h\|_0 \equiv \mathcal{O}(h^r)$$

Higher order conforming FEM

✓ **The family of conforming FEM $Q_r/Q_r/P_{r-1}^{\text{disc}},\ r \geq 2$ for $(\lambda, \boldsymbol{u}, p)$ with stabilization**



- ➢ **Inf-sup conditions is satisfied**
- ➢ **Discontinuous pressure**
  - ➢ **Practical w.r.t. monolithic approach**
  - ➢ **Element-wise mass conservation**

✓ **Highly consistent and symmetric stabilization**

$$j_\lambda(\lambda_h, \xi_h) = \sum_{e \in \mathcal{E}_h} h^2 \gamma_\lambda \int_e [\nabla \lambda_h] : [\nabla \xi_h] \, d\Omega, \quad j_{\lambda,l} := j_\lambda \text{ for } \gamma_\lambda = \text{cst.}$$

- ➢ **Coercivity in a strong norm for the microstructure eq.**
- ➢ **Reduces the regularity requirement for velocity**
- ➢ **Efficient and robust w.r.t. multigrid solver**

Stabilized FEM for TVP problem

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- **Coercivity in a stronger norm**

$$|||\lambda||| = \left(\mathcal{M}_a \|\lambda\|_0 + \frac{1}{2} \langle \lambda \rangle^2 + j_\lambda(\lambda, \lambda) \right)^{\frac{1}{2}}$$

Theorem

Let $\boldsymbol{f_u} \in (L^2(\Omega))^2$ *and* $f_\lambda \in L^2(\Omega)$*, the approximate thixo-viscoplastic problem has a unique solution* $(\tilde{\boldsymbol{u}}_h, p_h) = (\lambda_h, \boldsymbol{u}_h, p_h) \in \mathbb{W}_h \times \mathbb{Q}_h$ *with the following a priori best approximation*

$$|||\lambda - \lambda_h|||^2 \le (2 + 2\tilde{\mathcal{C}}_{\lambda,\lambda}) \inf_{\xi_h \in \mathbb{T}_h} \|\lambda - \xi_h\|_1^2 + \tilde{\mathcal{C}}_{\lambda,\boldsymbol{u}} \inf_{\boldsymbol{v}_h \in \mathbb{V}_h} |\boldsymbol{u} - \boldsymbol{v}_h|_1^2 + \inf_{\xi_h \in \mathbb{T}_h} \frac{1}{2} j_{\lambda,l}(\lambda - \xi_h, \lambda - \xi_h)$$

$$|\boldsymbol{u} - \boldsymbol{u}_h|_1^2 \le \tilde{\mathcal{C}}_{\boldsymbol{u},\lambda} \inf_{\xi_h \in \mathbb{T}_h} \|\lambda - \xi_h\|_1^2 + (2 + 2\tilde{\mathcal{C}}_{\boldsymbol{u},\boldsymbol{u}}) \inf_{\boldsymbol{v}_h \in \mathbb{V}_h} |\boldsymbol{u} - \boldsymbol{v}_h|_1^2 + \mathcal{C}_{\boldsymbol{u},p} \inf_{q_h \in \mathbb{Q}_h} \|p - q_h\|_0^2$$

Remark

- **Regularization:** ***Higher order FEM counterbalance the regularization coarseness***

$$|\boldsymbol{u} - \boldsymbol{u}_h|_1 \equiv \mathcal{O}(k^{-1}) \implies h \le \mathcal{O}(k^{-\frac{2}{r}})$$

- **Coercivity in a stronger norm:** ***The optimal order and regularity is recovered***

$$\|\lambda - \lambda_h\|_0 \equiv \mathcal{O}(h^{r+\frac{1}{2}})$$

Global discrete Newton's method

Let $\{\varphi_i, i=1,2,\ldots,\mathtt{dim}\mathbb{W}_h\}$ and $\{\psi_i,\ i=1,\ldots,\mathtt{dim}\mathbb{Q}_h\}$ denote the basis of spaces $\mathbb{W}_h$ and $\mathbb{Q}_h$, respectively. The solution $\mathcal{U}=(\lambda,\boldsymbol{u},p)=(\tilde{\boldsymbol{u}},p)\in\mathbb{W}_h\times\mathbb{Q}_h$

$$\mathcal{U}=\sum_{i=1}^{\mathtt{dim}\mathbb{W}_h}\tilde{\boldsymbol{u}}_i\varphi_i+\sum_{i=1}^{\mathtt{dim}\mathbb{Q}_h}p_i\psi_i$$

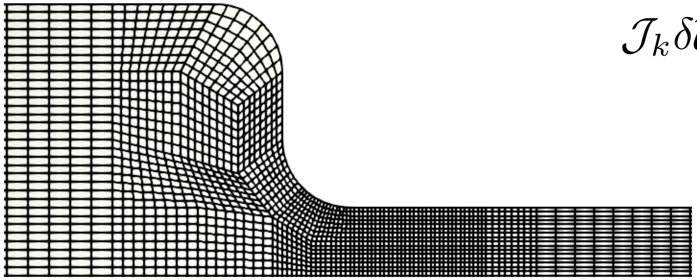
The residuals of discrete TVP problem $\mathcal{R}(\mathcal{U})\in\mathbb{R}^{\mathtt{dim}\mathbb{W}_h+\mathtt{dim}\mathbb{Q}_h}$

$$\mathcal{R}(\mathcal{U})=(\mathcal{R}_\lambda(\lambda,\boldsymbol{u}),\mathcal{R}_{\boldsymbol{u}}(\lambda,\boldsymbol{u},p),\mathcal{R}_p(\boldsymbol{u}))=(\mathcal{R}_{\tilde{\boldsymbol{u}}}(\tilde{\boldsymbol{u}},p),\mathcal{R}_p(\boldsymbol{u}))$$

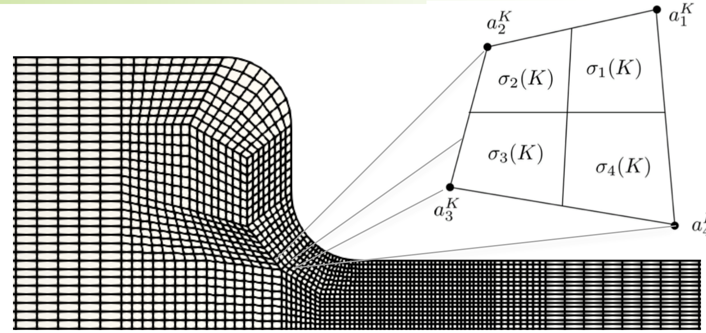
- **Residuum rate convergence** $r_l:=\|\mathcal{R}(\mathcal{U}^l)\|/\|\mathcal{R}(\mathcal{U}^{l-1})\|$
- **Adaptive step length** $\epsilon_{l+1}=g(r_l)\epsilon_l,$
  $g(r_l)=1/f(r_l),\ \ f(r_l)=0.2+4/(0.7+e^{1.5r_l})$
- **Discrete Jacobian** $\left[\dfrac{\partial\mathcal{R}(\mathcal{U}^l)}{\partial\mathcal{U}}\right]_{ij}\approx\dfrac{\mathcal{R}_i(\mathcal{U}^l+\varepsilon_l\boldsymbol{e}_j)-\mathcal{R}_i(\mathcal{U}^l-\varepsilon_l\boldsymbol{e}_j)}{2\varepsilon_l}$
- **Newton's update** $\mathcal{U}^{l+1}=\mathcal{U}^l-\omega_l\left(\dfrac{\partial\mathcal{R}(\mathcal{U}^l)}{\partial\mathcal{U}}\right)^{-1}\mathcal{R}(\mathcal{U}^l),\ \ \omega_l\in]0,1]$

Global and blackbox !
Robustness and efficiency: Coupled Geometric-MG

- **Two-level algorithm**



$$\mathcal{J}_k \delta\mathcal{U} = \mathcal{R}$$



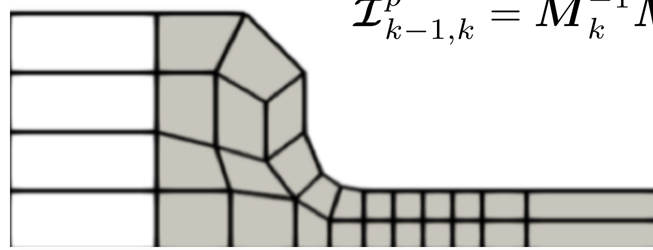
$$\delta\mathcal{U}_l = \delta\mathcal{U}_{l-1} + \mathcal{C}_k^{-1}(\mathcal{R} - \mathcal{J}_k \delta\mathcal{U}_{l-1}), l \leq \nu_1$$
$$\mathcal{Z}_1 = MG_F(k-1, \mathbf{0}, \boldsymbol{\mathcal{I}}_k^{k-1}(\mathcal{R} - \mathcal{J}_k \delta\mathcal{U}_{\nu_1}))$$

$$\delta\mathcal{U}_l = \delta\mathcal{U}_{l-1} + \mathcal{C}_k^{-1}(\mathcal{R} - \mathcal{J}_k \delta\mathcal{U}_{l-1}), l \leq \nu_2$$
$$MG(k, \delta\mathcal{U}_0, \boldsymbol{\mathcal{R}}) = \delta\mathcal{U}_{\nu_1} + \boldsymbol{\mathcal{I}}_{k-1}^k \mathcal{Z}_2$$

- **Geometric transfer between FE spaces**

$$\boldsymbol{\mathcal{I}}^{\tilde{\boldsymbol{u}}}_{k,k-1} = \boldsymbol{M}_{k-1}^{-1} \left(\boldsymbol{\mathcal{I}}^{\tilde{\boldsymbol{u}}}_{k-1,k}\right)^T \boldsymbol{M}_k$$
$$\boldsymbol{\mathcal{I}}^p_{k-1,k} = \boldsymbol{M}_k^{-1} \boldsymbol{M}_{k-1}$$

$$\left[\boldsymbol{\mathcal{I}}^{\tilde{\boldsymbol{u}}}_{k-1,k}\right]_{ij} = \mathcal{N}_j^k(\varphi_i^{k-1})$$
$$\boldsymbol{\mathcal{I}}^p_{k-1,k} = \boldsymbol{M}_k^{-1} \boldsymbol{M}_{k-1}$$



- **Coarse grid solver**

$$\mathcal{R}_{k-1} = \left(\boldsymbol{\mathcal{I}}^{\tilde{\boldsymbol{u}}}_{k-1,k}\right)^T \mathcal{R}_k$$
$$\mathcal{J}^{\tilde{\boldsymbol{u}}}_{k-1} = \left(\boldsymbol{\mathcal{I}}^{\tilde{\boldsymbol{u}}}_{k-1,k}\right)^T \mathcal{J}^{\tilde{\boldsymbol{u}}}_k \boldsymbol{\mathcal{I}}^{\tilde{\boldsymbol{u}}}_{k,k-1}$$

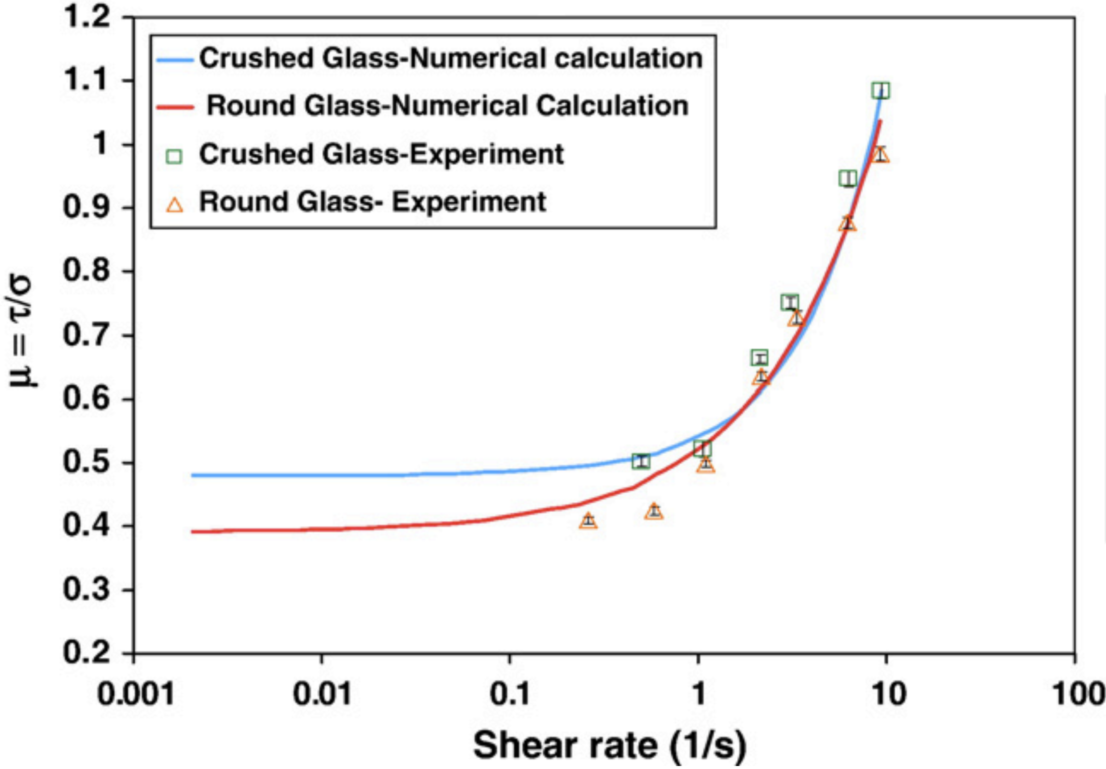
$$MG\,(1, \delta\mathcal{U}_0, \mathcal{R}) = \mathcal{J}_1^{-1}\mathcal{R}$$

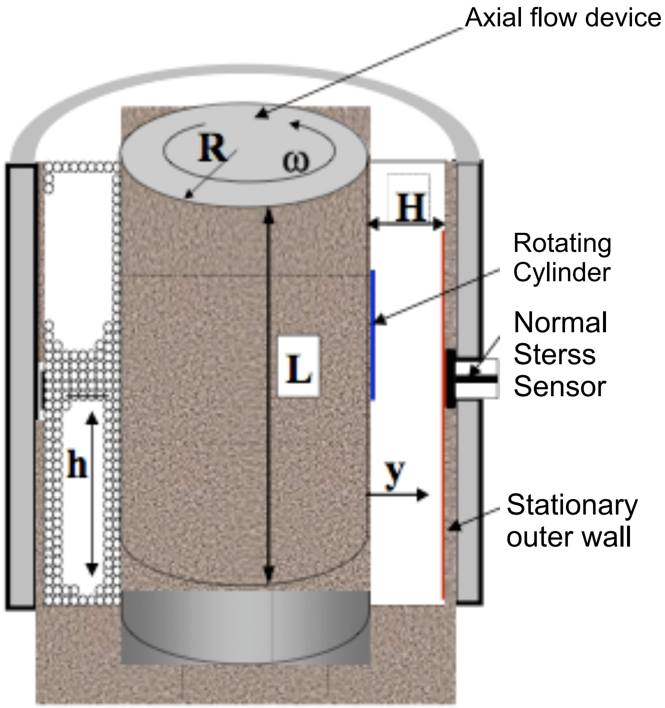
- **Block Gauß-Seidel iteration reads: Local Multilevel Pressure Schur Complement**

$$\mathcal{U}^{k+1} = \mathcal{U}^k - \omega_k \sum_{K \in \mathcal{T}_h} \boldsymbol{\mathcal{P}}_K \left(\boldsymbol{\mathcal{P}}_K^{\mathrm{T}} \left(\frac{\partial \mathcal{R}(\mathcal{U}^k)}{\partial \mathcal{U}}\right) \boldsymbol{\mathcal{P}}_K\right)^{-1} \boldsymbol{\mathcal{P}}_K^{\mathrm{T}} \mathcal{R}(\mathcal{U}^k).$$

Type-transitions investigation

Axial flow experiment and numerical simulations in the Couette device





- **The material can transit from the quasi-static to the intermediate regime as the shearing rate is increased**

Solid / Liquid & liquid / solid type-transitions investigation w.r.t. to thixotropy !

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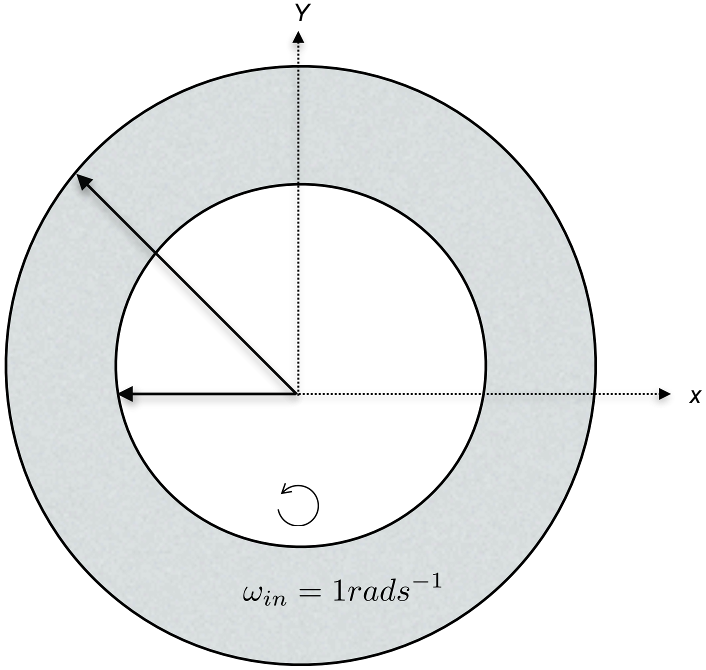
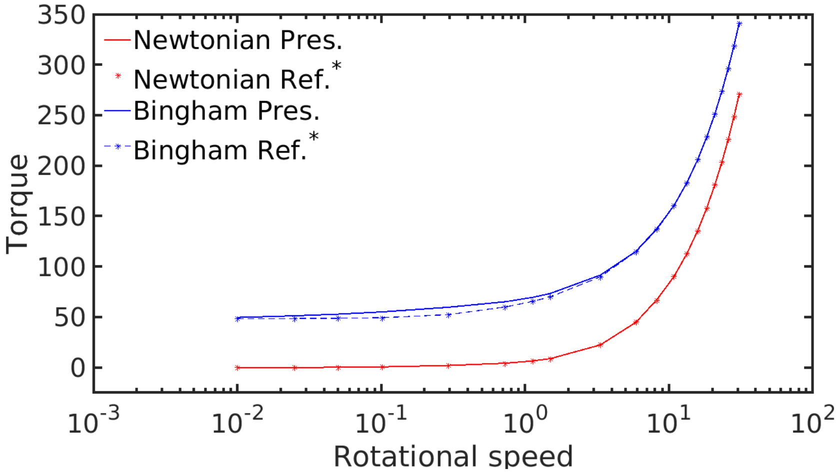
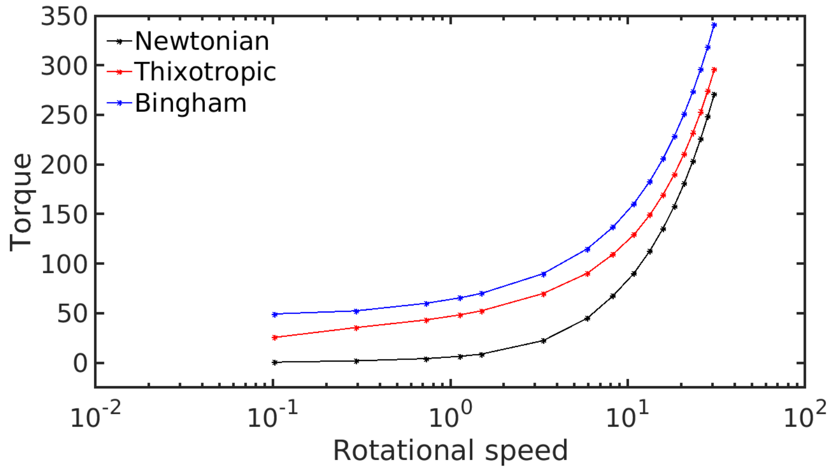
- **Torque calculation**



$$M = -\oint_S (X - X_0) T_{ij} \vec{n} dS$$

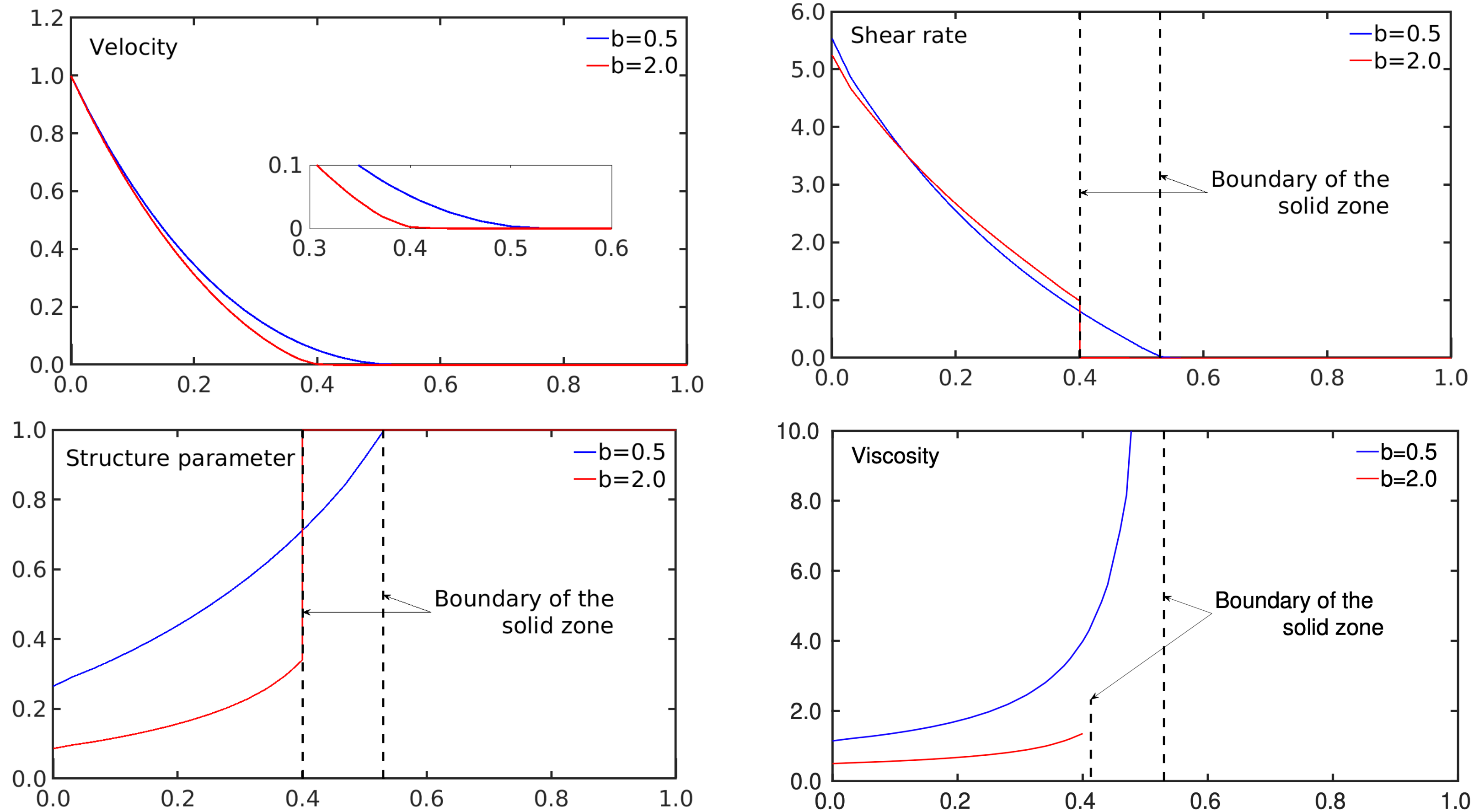




- ✓ **Torque calculation for Non-thixotropic flow**
- ✓ **Thixotropic flow is encompassed between Newtonian flow and Bingham plastic flow, as predicted by the Houska's model, allowing for type-transitions study**

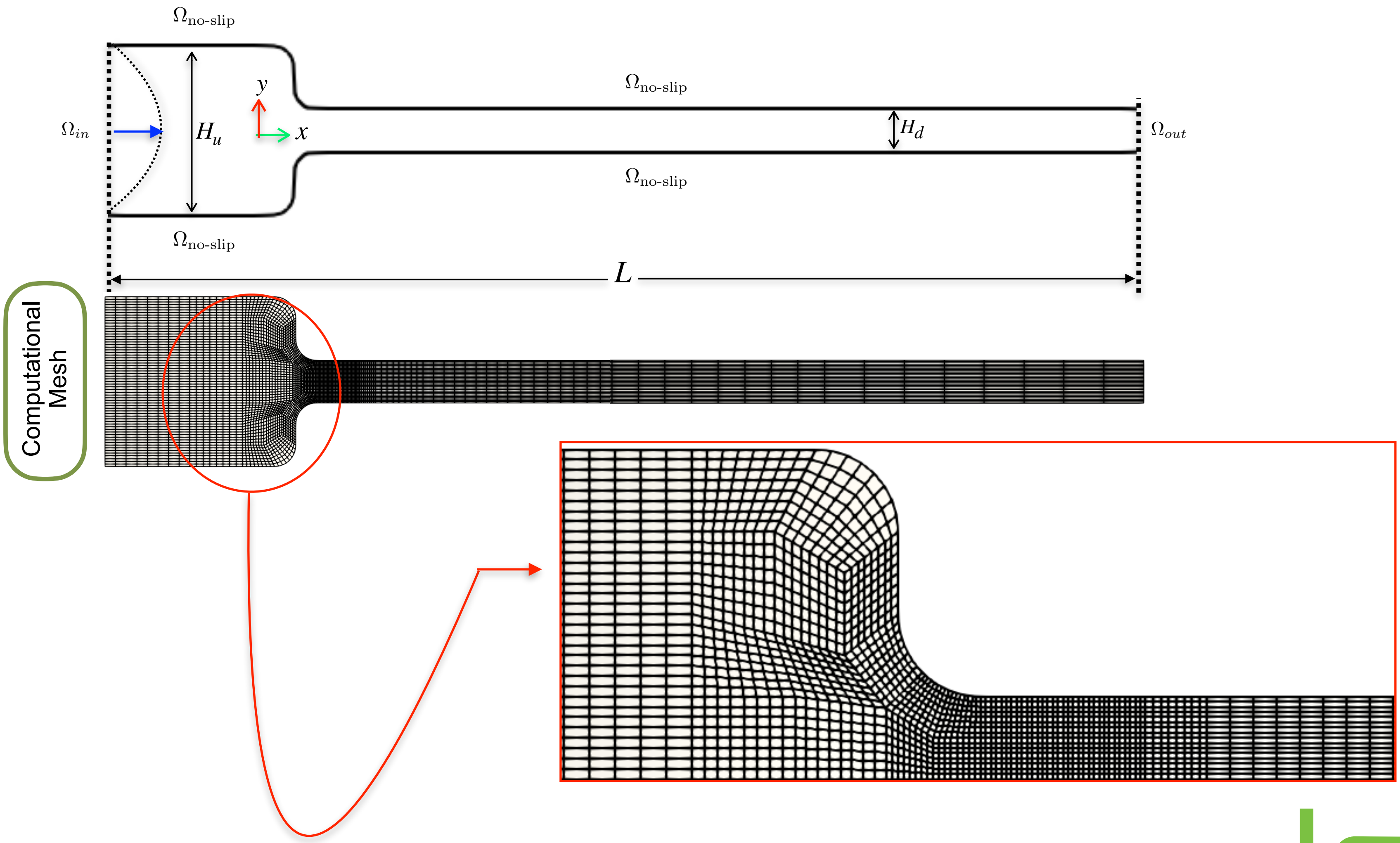
Thixo-viscoplastic flow in Couette

- **Cut-line positions $c; c \in [0, 2\pi]$ in a Couette device w.r.t breakdown parameter**

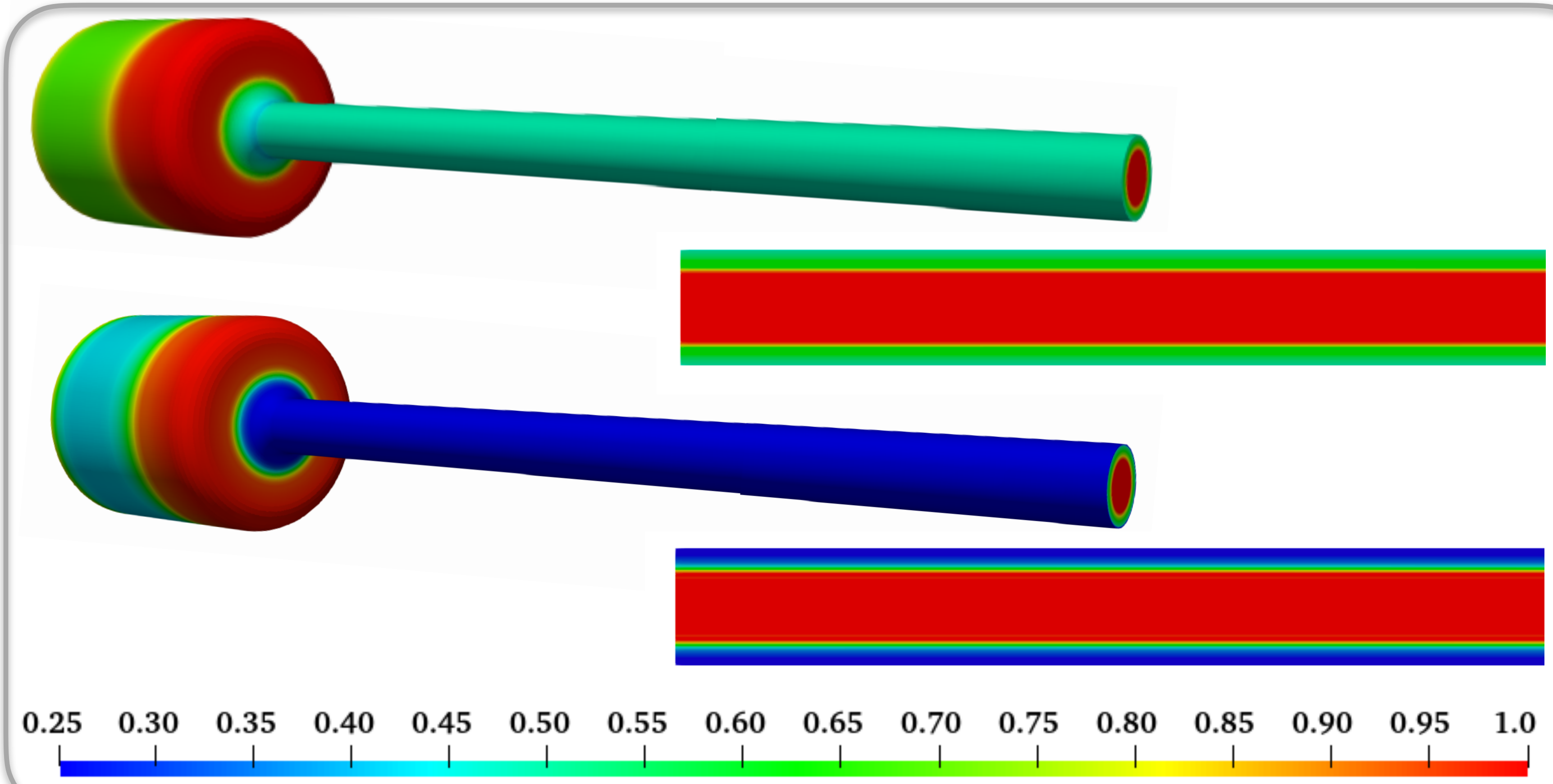


- ✓ **Shear Localization & shear banding transition types w.r.t breakdown parameter**
- ✓ **Transition point for shear-rate and structure parameter match with velocity**
- ✓ **Structure parameter predicts the shape and extent of rigid zones**

- **2D-FEM simulation results for thixotrpic flow- validation of 1D tool**
- **Specifying the "1D-profiles as boundary Data" in 2D simulations for contraction domain**



- Material micro-structural level w.r.t. breakdown



- Inherent thixotropy speed-up the breakdown

✓ Appearance of more breakdown layers
✓ Applications: restart pressure in pipelines is optimised

Summary

Coupled geometric-multigrid FEM solver for thixo-viscoplastic flows is developed based on

- ✓ **Quasi-Newtonian modelling approach**
- ✓ **Higher order finite element method**
- ✓ **Monolithic Newton-multigrid solver using**
  - **Global adaptive discrete Newton's method**
  - **Geometric multigrid with local MPSC**

To analyze the thixo-viscoplastic flow behavior in different circumstance

- ✓ **TVP flow in Couette devices**
- ✓ **TVP flow in contractions**

With the goal to incorporate the thixotropy inhabited in materials for complex fluidic processes.

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[1] Begum, N., Ouazzi, A., Turek, S., *FEM simulation of thixo-viscoplastic flow problems;* Wellposedness results, Ergebnisberichte des Instituts für Angewandte Mathematik Nummer 653, Fakultät für Mathematik, TU Dortmund, 653, 2022.

[2] Begum, N., Ouazzi, A., Turek, S., Monolithic Newton-multigrid FEM for the simulation of thixotropic flow problems, *Kaliske, M., 21, 1, 92nd Annual Meeting of the International Association of Applied Mathematics and Mechanics (Gamm), Wiley-Interscience*, https://doi.org/10.1002/pamm.202100019, 2021.

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Realization in FeatFlow

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HPC features:
- Moderately parallel
- GPU computing
- Open source


Hardware -oriented Numerics

Numerical features:
- Higher order FEM in space & (semi-) Implicit FD/FEM in time
- Semi-(un)structured meshes with dynamic adaptive grid deformation
- Fictitious Boundary (FBM) methods
- Newton-Multigrid-type solvers

Non-Newtonian flow module:
•generalized Newtonian model (Power-law, Carreau,Houska,…)
•viscoelastic differential model (Giesekus, FENE, Oldroyd,...)

Multiphase flow module (resolved interfaces):
•l/l – interface capturing (Level Set)
•s/l – interface tracking (FBM)
•s/l/l – combination of l/l and s/l

Engineering aspects:
•Geometrical design
•Modulation strategy
•Optimization

FEM-based tools for the accurate simulation of (thixotropic) flow problems

For details, please visit: www.featflow.de

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