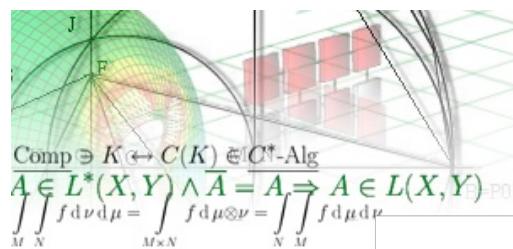


# Monolithic Newton-multigrid FEM for the simulation of thixotropic flow problems

N. Begum, A. Ouazzi, S. Turek  
Institute of Applied Mathematics, LS III,  
TU Dortmund University, Dortmund, Germany

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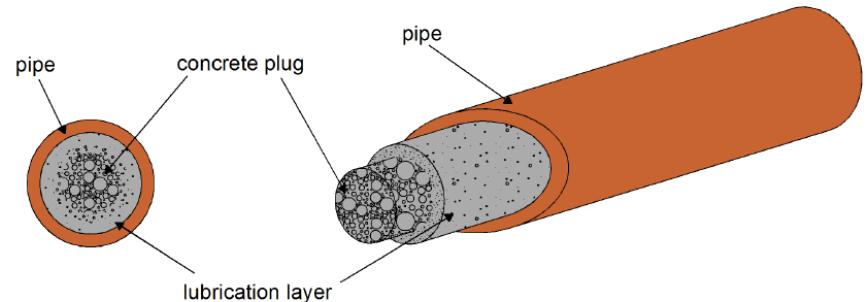
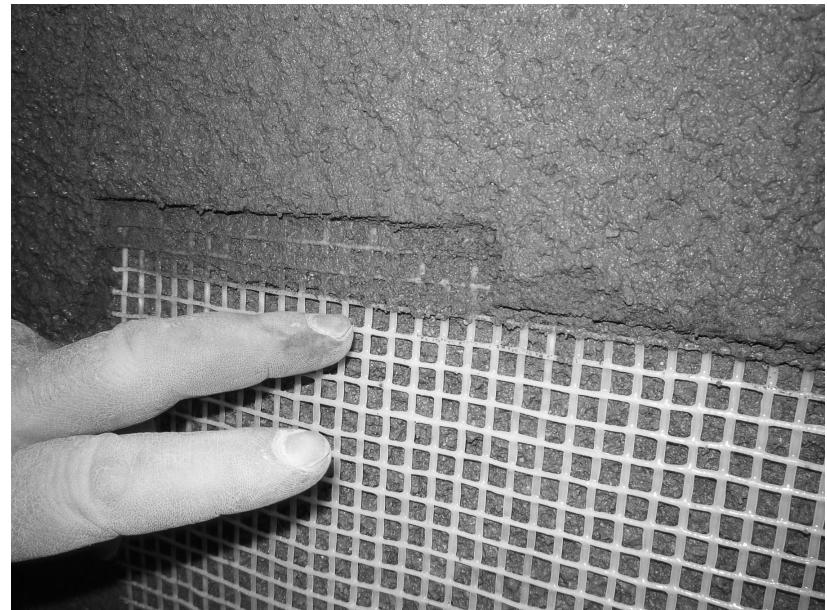
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## Why “Thixotropic materials?

- 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 means
  - combination of two greek words
  - Thixis: shaking/stirring
  - trepo: turning/changing
- Thixotropy concept
  - Based on viscosity
  - Flow induced by time-dependent decrease of viscosity
  - The phenomena is reversible
- Rejuvenation / Breakdown
  - “Faster” flow: fluid rejuvenates
  - Decreases of viscosity with acceleration of the flow
- Aging / Build-up
  - At rest or under slow flow: fluid ages
  - Increases of the viscosity in time



## 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

**Here: FEM-based tools for the accurate simulation of (thixotropic) flow problems, particularly with complex rheology**



For details, please visit: [www.featflow.de](http://www.featflow.de)

→ starting point: Generalized Navier-Stokes equations (+initial and boundary conditions)

$$\rho \left( \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} - \nabla \cdot \boldsymbol{\sigma} + \nabla p = \rho f,$$
$$\nabla \cdot \mathbf{u} = 0,$$

- velocity- and pressure field  $\mathbf{u}$  and  $p$
- stress tensor  $\boldsymbol{\sigma}$
- linear material behaviour - Newtonian fluids

$$\boldsymbol{\sigma} = 2\eta_s \mathbf{D}(\mathbf{u}) \quad : \eta_s \text{ is constant viscosity}$$

- non-linear material behaviour- structurally viscous / viscoplastic

$$\boldsymbol{\sigma} = 2\eta_s(D_{\mathbb{II}}, p, \Theta, \lambda) \mathbf{D}(\mathbf{u}), \quad D_{\mathbb{II}} = \text{tr} \left( \frac{1}{2} \mathbf{D}(\mathbf{u})^2 \right)$$


- Power-law, Carreau, Bingham, Herschel-Bulkley, Houska, ...

- structure parameter  $\lambda$

- Archetypical yield-stress driven thixotropic models

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

- Relations between rheological parameters and structural parameter

	$\eta(D_{\text{II}}, \lambda)$	$\tau(\lambda)$
Worrall and Tulliani <sup>1</sup>	$\lambda\eta_0$	$\tau_0$
Coussot <i>et al.</i> <sup>2</sup>	$\lambda^a\eta_0$	—
Houska <sup>3</sup>	$(\eta_0 + \eta_1\lambda)D_{\text{II}}^{\frac{(n-1)}{2}}$	$(\tau_0 + \tau_1\lambda)$
Mujumbar <i>et al.</i> <sup>4</sup>	$(\eta_0 + \eta_1\lambda)D_{\text{II}}^{\frac{(n-1)}{2}}$	$\lambda^{a+1}G_0\Lambda_c^*$
Burgos <i>et al.</i> <sup>5</sup>	$\eta_0$	$\lambda\tau_0$
Dullaert & Mewis <sup>6</sup>	$\lambda\eta_0$	$\lambda G_0 \left( \lambda D_{\text{II}}^{\frac{1}{2}} \right) \Lambda_c^*$

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



- 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 <sup>1</sup>	$c_1(1 - \lambda)D_{II}^{\frac{1}{2}}$	$c_2\lambda D_{II}^{\frac{1}{2}}$
Coussot <i>et al.</i> <sup>2</sup>	$c_1$	$c_2\lambda D_{II}^{\frac{1}{2}}$
Houska <sup>3</sup>	$c_1(1 - \lambda)$	$c_2\lambda^m D_{II}^{\frac{1}{2}}$
Mujumbar <i>et al.</i> <sup>4</sup>	$c_1(1 - \lambda)$	$c_2\lambda D_{II}^{\frac{1}{2}}$
Burgos <i>et al.</i> <sup>5</sup>	$c_1(1 - \lambda)$	$c_2\lambda D_{II}^{\frac{1}{2}} \exp(aD_{II}^{\frac{1}{2}})$
Dullaert & Mewis <sup>6</sup>	$(c_1 + c_3 D_{II}^{\frac{1}{2}})(1 - \lambda)t^{-b}$	$c_2\lambda D_{II}^{\frac{1}{2}}t^{-b}$

## ● Viscoplastic model

$$\begin{cases} \eta_s(D_{\text{II}}) = \eta_0 + \frac{\sqrt{2}}{2} \tau_0 D_{\text{II}}^{-\frac{1}{2}} & \text{if } D_{\text{II}} \neq 0 \\ \|\boldsymbol{\sigma}\| \leq \tau_0 & \text{else} \end{cases}$$

(  $\tau_0$  : yield stress )

## ● Thixotropic model

$$\begin{cases} \eta_s(D_{\text{II}}, \lambda) = \eta(\lambda) + \frac{\sqrt{2}}{2} \tau(\lambda) D_{\text{II}}^{-\frac{1}{2}} & \text{if } D_{\text{II}} \neq 0 \\ \|\boldsymbol{\sigma}\| \leq \tau(\lambda) & \text{else} \end{cases}$$

(  $\lambda$  : structure parameter )

## → Structure evolution equation

$$\frac{\partial \lambda}{\partial t} + \mathbf{u} \cdot \nabla \lambda = a(1 - \lambda) - b\lambda D_{\text{II}}^{\frac{1}{2}}$$

(  $a, b$  are structure parameters )

- **Viscosity model for thixotropic flow i.e. extended viscosity defined on all domains s.t.**

$$\begin{cases} \eta_s(D_{\text{II}}, \lambda) = \eta(\lambda) + \frac{\sqrt{2}}{2} \tau(\lambda) D_{\text{II}}^{-\frac{1}{2}} & \text{if } D_{\text{II}} \neq 0 \\ & \|\boldsymbol{\sigma}\| \leq \tau(\lambda) \\ & \text{else} \end{cases}$$

- **Examples:**

$$\begin{cases} I. \quad \eta_s(D_{\text{II}}, \lambda) = \eta(\lambda) + \frac{\sqrt{2}}{2} \tau(\lambda) \frac{1}{\sqrt{(D_{\text{II}} + (k^{-1})^2)}} \\ II. \quad \eta_s(D_{\text{II}}, \lambda) = \eta(\lambda) + \frac{\sqrt{2}}{2} \tau(\lambda) \frac{1}{D_{\text{II}}^{\frac{1}{2}}} (1 - e^{-k D_{\text{II}}^{\frac{1}{2}}}) \end{cases}$$

( $k$  : regularization parameter)

- **Full set of equations**

$$\begin{cases} \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) u - \nabla \cdot \left( 2\eta_s(D_{\text{II}}, \lambda) D(u) \right) + \nabla p = 0 & \text{in } \Omega \\ \nabla \cdot u = 0 & \text{in } \Omega \\ \frac{\partial \lambda}{\partial t} + u \cdot \nabla \lambda - a(1 - \lambda) + b\lambda D_{\text{II}}^{\frac{1}{2}} = 0 & \text{in } \Omega \end{cases}$$

Let  $\mathcal{U} = (\lambda, \mathbf{u}, p)$ , and  $\mathcal{R}_{\mathcal{U}}(\mathcal{U})$  be the continuous or the discrete corresponding system's residuum.

- Update of the nonlinear iteration with the correction  $\delta\mathcal{U}$  i.e.

$$\mathcal{U}^N = \mathcal{U} + \delta\mathcal{U}$$

- The linearization of the residual provides

$$\begin{aligned}\mathcal{R}_{\mathcal{U}}(\mathcal{U}^N) &= \mathcal{R}_{\mathcal{U}}(\mathcal{U} + \delta\mathcal{U}) \\ &= \mathcal{R}_{\mathcal{U}}(\mathcal{U}) + \mathcal{J}(\mathcal{U}) \cdot \delta\mathcal{U}\end{aligned}$$

- The Newton's method assuming invertible Jacobian

$$\mathcal{U}^N = \mathcal{U} - \mathcal{J}^{-1}(\mathcal{U}) \mathcal{R}_{\mathcal{U}}(\mathcal{U})$$



## Jacobian calculations

$$\mathcal{J}(\mathcal{U}) = \left( \frac{\partial \mathcal{R}_u(\mathcal{U})}{\partial \mathcal{U}} \right)$$

- Continuous Adaptive Newton based on a priori study of Jacobian's properties and decompositions

$$\mathcal{J}(\mathcal{U}) = \left( \frac{\partial \hat{\mathcal{R}}_u(\mathcal{U})}{\partial \mathcal{U}} \right) + \delta \left( \frac{\partial \tilde{\mathcal{R}}_u(\mathcal{U})}{\partial \mathcal{U}} \right)$$

- Discrete Adaptive Newton based on the rate of residuum's convergence

$$\left( \frac{\partial \mathcal{R}}{\partial \mathcal{U}} \right)_{ij} \approx \left( \frac{\mathcal{R}_i(\mathcal{U} + \epsilon e_j) - \mathcal{R}_i(\mathcal{U} - \epsilon e_j)}{2\epsilon} \right)$$



- **Flow variables**  $(\lambda, \mathbf{u}, p)$

- **Set**  $\mathbb{T} := L^2(\Omega), \mathbb{V} := [H_0^1(\Omega)]^2, \mathbb{Q} := L_0^2(\Omega)$
- **Set**  $\tilde{\mathbf{u}} := (\lambda, \mathbf{u})$
- **Find**  $(\lambda, \mathbf{u}, p) \in (\mathbb{T} \cap H^1(\Omega)) \times \mathbb{V} \times \mathbb{Q}$  **s.t.**

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

$$\mathcal{K} = \begin{bmatrix} \mathcal{A}_{\tilde{\mathbf{u}}} & \mathcal{B}^T \\ \mathcal{B} & 0 \end{bmatrix}$$

- **Compatibility constraints**

$$\sup_{\mathbf{v} \in \mathbb{V}} \frac{\langle \mathcal{B}\mathbf{v}, q \rangle}{\|\mathbf{v}\|_{\mathbb{V}}} \geq \beta \|q\|_{\mathbb{Q}/Ker \mathcal{B}^T}, \quad \forall q \in \mathbb{Q}$$



- Discretizations have to handle the following challenges

- Stable FEM spaces
- Non-symmetric, non-coercive and ill-posedness
- Convection and positivity preserving
- Locally adapted meshes for steep gradients

- Solvers have to deal with

- Different source of nonlinearities
- Strong coupling of equations
- Robustness and efficiency

- **Conforming approximations**

$$\mathbb{T}_h \subset \mathbb{T}, \quad \mathbb{V}_h \subset \mathbb{V}, \quad \mathbb{Q}_h \subset \mathbb{Q}$$

$$\mathcal{A}_{\tilde{\mathbf{u}}_h} = \mathcal{A}_{\tilde{\mathbf{u}}}, \mathcal{B}_h = \mathcal{B}$$

- **Discrete inf-sup condition**

$$\sup_{\mathbf{v}_h \in \mathbb{V}_h} \frac{\langle \mathcal{B}_h \mathbf{v}_h, q_h \rangle}{\|\mathbf{v}_h\|_{\tilde{\mathbb{V}}}} \geq \beta_h \|q_h\|_{\mathbb{Q}/Ker \mathcal{B}_h^T}, \quad \forall q_h \in \mathbb{Q}_h$$

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

$$J_\lambda(\lambda_h, \xi_h) = \gamma_\lambda \sum_{e \in \mathcal{E}_h} h \int_e [\nabla \lambda_h] : [\nabla \xi_h] d\Omega$$

- Inf-sup conditions is satisfied
- Discontinuous pressure
  - Good for the solver
  - Element-wise mass conservation
- Discrete problem is well-posed
- Highly consistent and symmetric stabilization
- Robust solver w.r.t. the monolithic approach
- Efficient solver w.r.t. multigrid solver

- Standard geometric multigrid solver for linearized system
- Full  $Q_r$  and  $P_{r-1}^{\text{disc}}$  restriction and prolongation
- Local Multilevel Pressure Schur Complement via Vanka-like smoother

$$\begin{pmatrix} \lambda^{l+1} \\ u^{l+1} \\ p^{l+1} \end{pmatrix} = \begin{pmatrix} \lambda^l \\ u^l \\ p^l \end{pmatrix} + \omega^l \sum_{T \in \mathcal{T}_h} \left( (\mathcal{K}_h + \mathcal{J}_\lambda)_{|T} \right)^{-1} \begin{pmatrix} \mathcal{R}_{\lambda^l} \\ \mathcal{R}_{u^l} \\ \mathcal{R}_{p^l} \end{pmatrix}_{|T}$$

**Coupled Monolithic Multigrid Solver !**



- “Validation”: manufactured exact solution for Bingham flow in a unit channel domain

→ Dirichlet boundary conditions

→ analytical solution for velocity  $u_{exact} = (u, 0)^T$ , such that  $u$

$$u = \begin{cases} \frac{1}{8} \left( (1 - 2\tau_0)^2 - (1 - 2\tau_0 - 2y)^2 \right) & \text{if } y \in [0, \frac{1}{2} - \tau_0) \\ \frac{1}{8}(1 - 2\tau_0)^2 & \text{if } y \in [\frac{1}{2} - \tau_0, \frac{1}{2} + \tau_0] \\ \frac{1}{8} \left( (1 - 2\tau_0)^2 - (2y - 2\tau_0 - 1)^2 \right) & \text{if } y \in (\frac{1}{2} + \tau_0, 1] \end{cases}$$

→ solution show that the plug zone,  $y \in [\frac{1}{2} - \tau_0, \frac{1}{2} + \tau_0]$ , is a moving rigid body with a constant velocity.

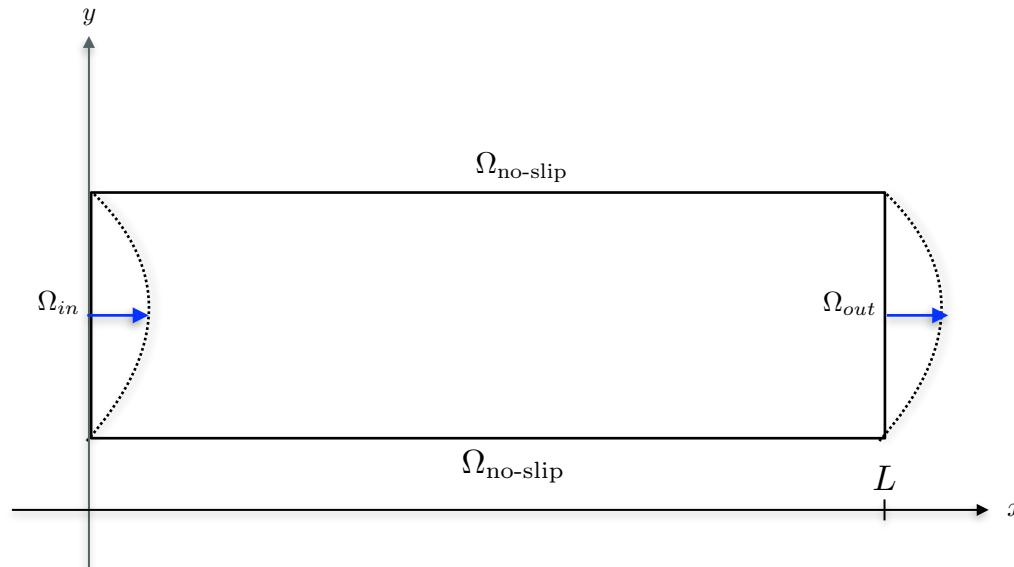




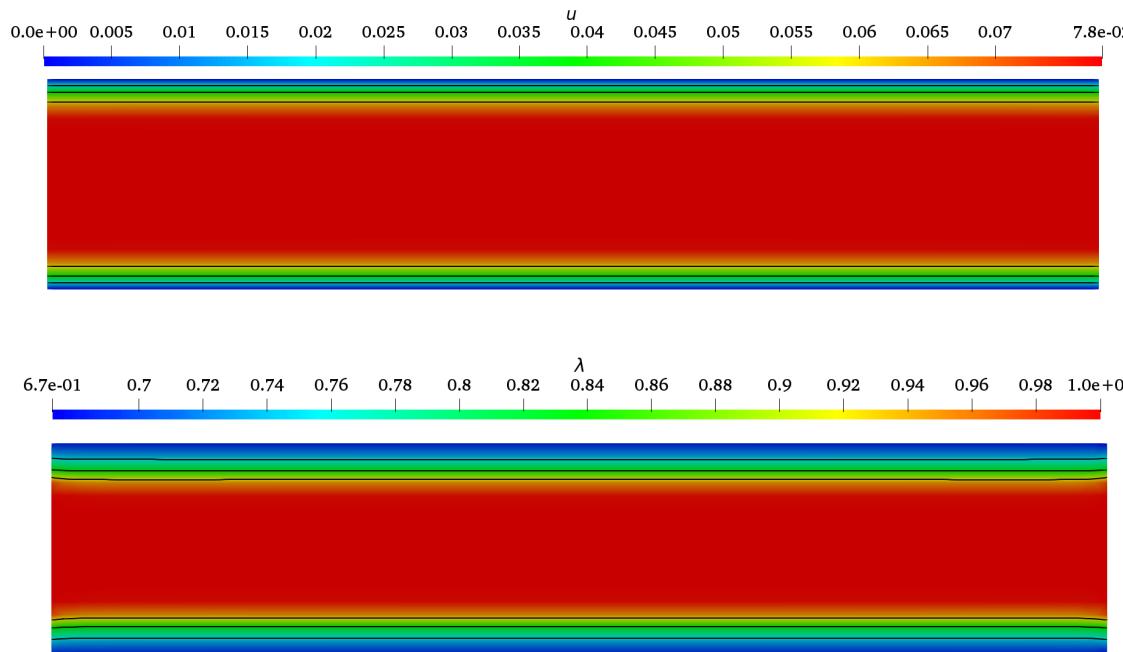
- Starting point : consider the flow in infinitely long channel
- Flow variables varies only w.r.t 'y' i.e., no change in  $x$ -direction

$$\mathbf{u} = \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u(y) \\ 0 \end{pmatrix}, \quad \mathbf{D}(\mathbf{u}) = \frac{1}{2} \begin{pmatrix} 0 & \frac{\partial u}{\partial y} \\ \frac{\partial u}{\partial y} & 0 \end{pmatrix}, \quad \frac{\partial u}{\partial x} = \frac{\partial \lambda}{\partial x} = 0$$

- Reduction of complete flow model in 1D problem
- Fast , efficient, high resolutions calculations possible for fully developed flow



- Prototypical simulation results for thixotropic flow- validation of 1D tool
- Specifying the “1D-profiles as boundary Data” in 2D simulations of channel flow
- Parameters:  $\eta_0 = 1.0, \tau_1 = 0.25, \eta_1 = \tau_0 = 0.0, a = b = 1.0, k = 10^4$



- ✓ Horizontal isolines w.r.t. each flow variable
- ✓ Same flow profiles over  $y$  at each  $x$ -position

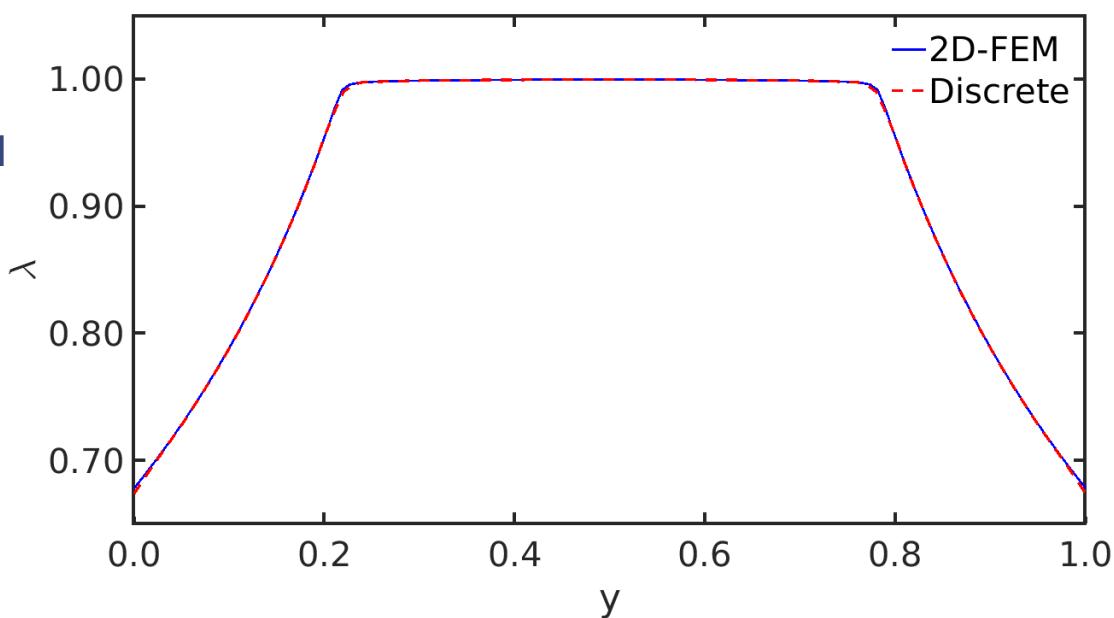
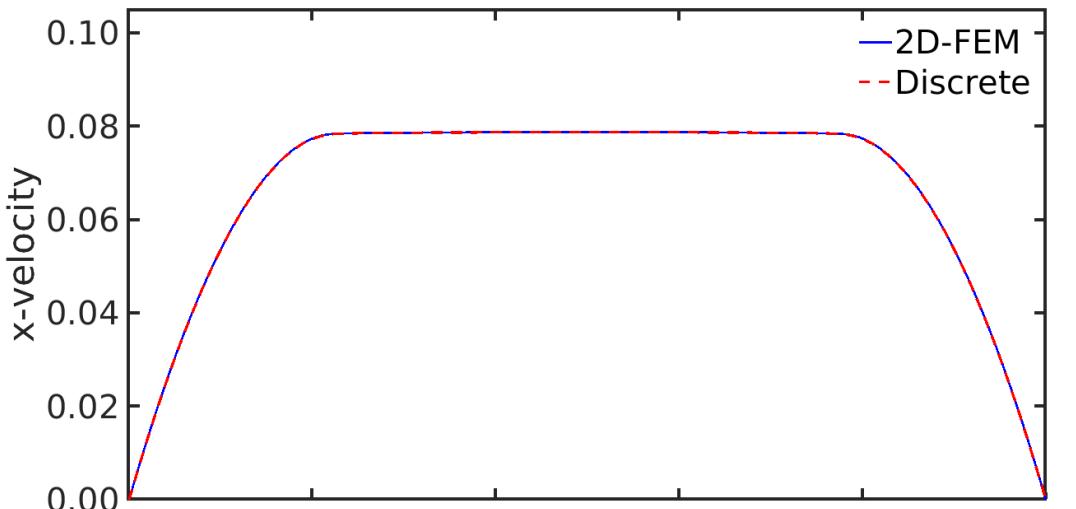
- Comparison of velocity and structure parameter profiles at middle  $x$ -position for thixotropic material

✓ 1D and 2D-FEM simulations leads to same results

✓ Detailed validation for varying the parameters ( $k, \eta(\lambda), \tau(\lambda), \dots$ )

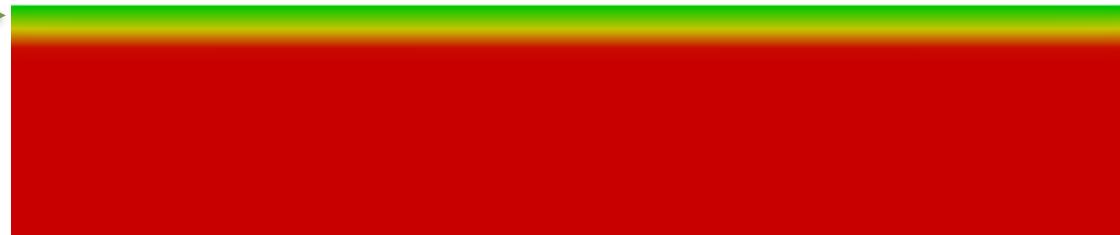
✓ Validated to recover the analytical Bingham profiles in unit channel

→ In principle, this approach can be analogously applied to any thixotropic elasto-viscoplastic model

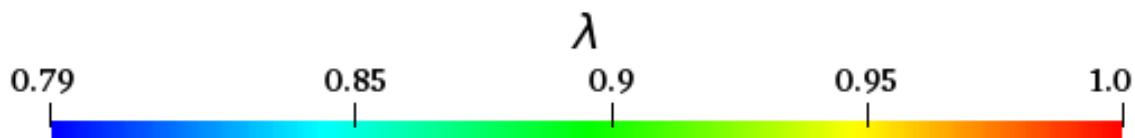


- Impact of thixotropic viscosity and yield-stress on structural parameter

Without thixotropy



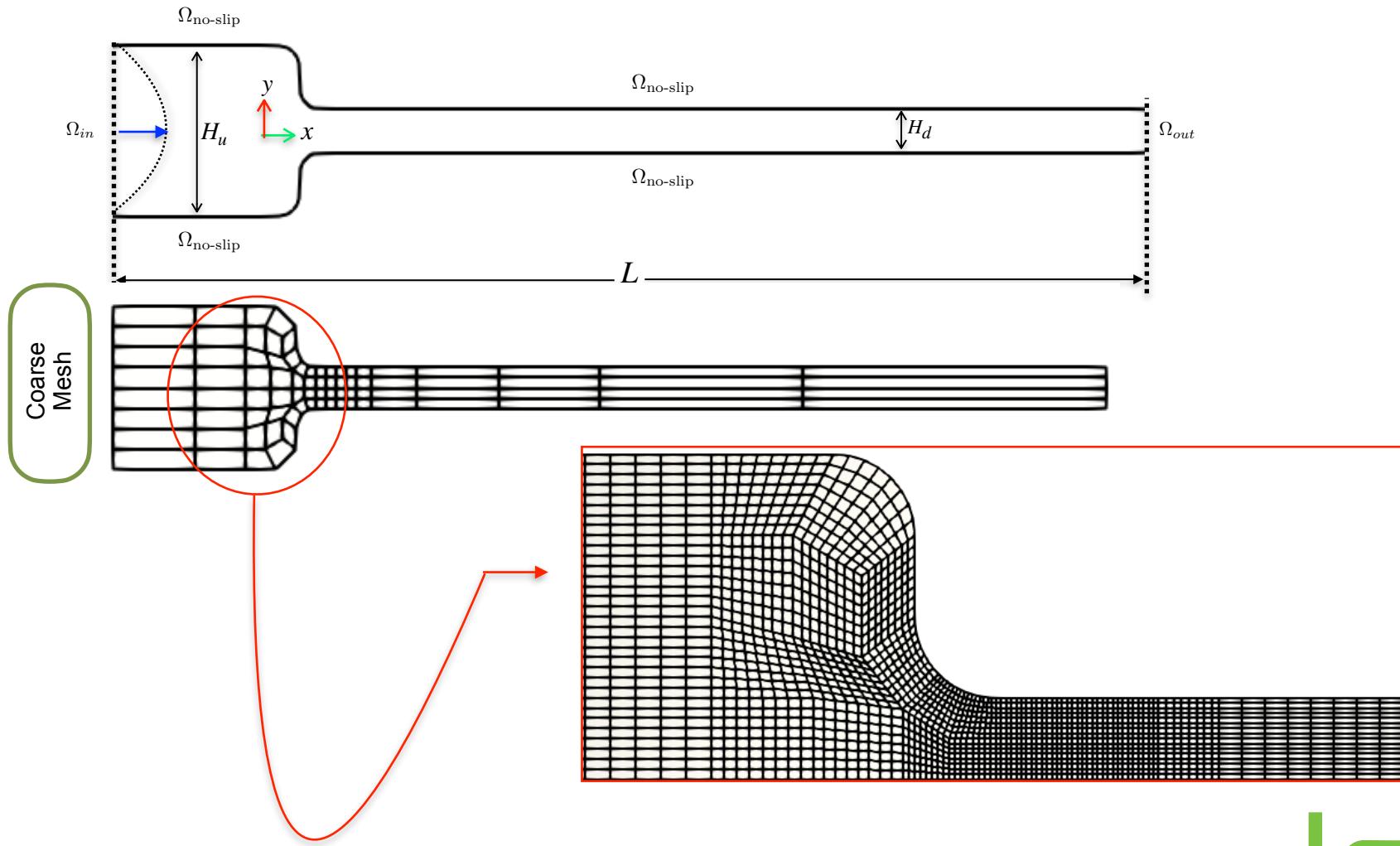
With thixotropy



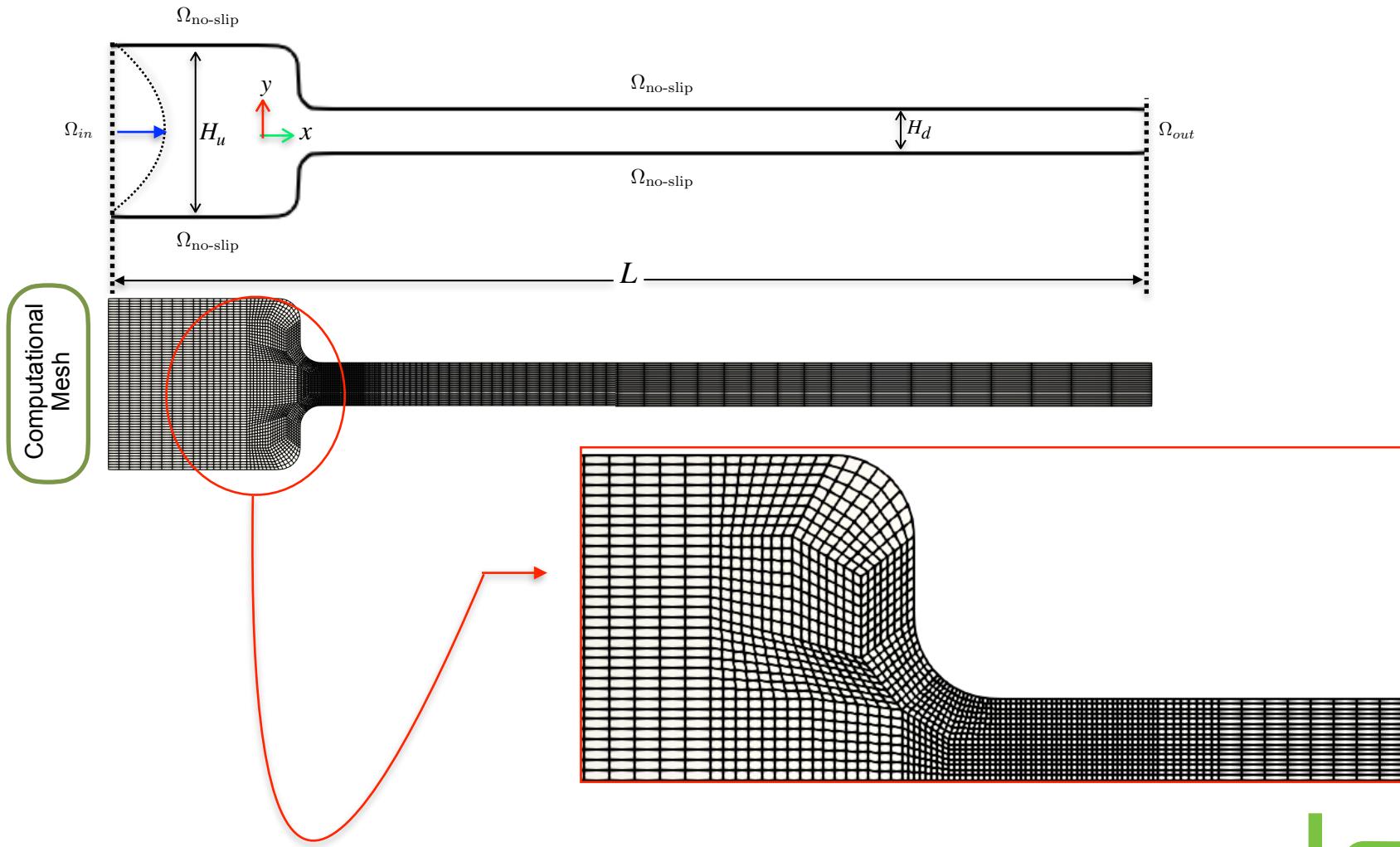
- Inherent thixotropy speed-up the breakdown

- ✓ Appearance of breakdown layer
- ✓ Restart pipelines pressure should not be over-estimated

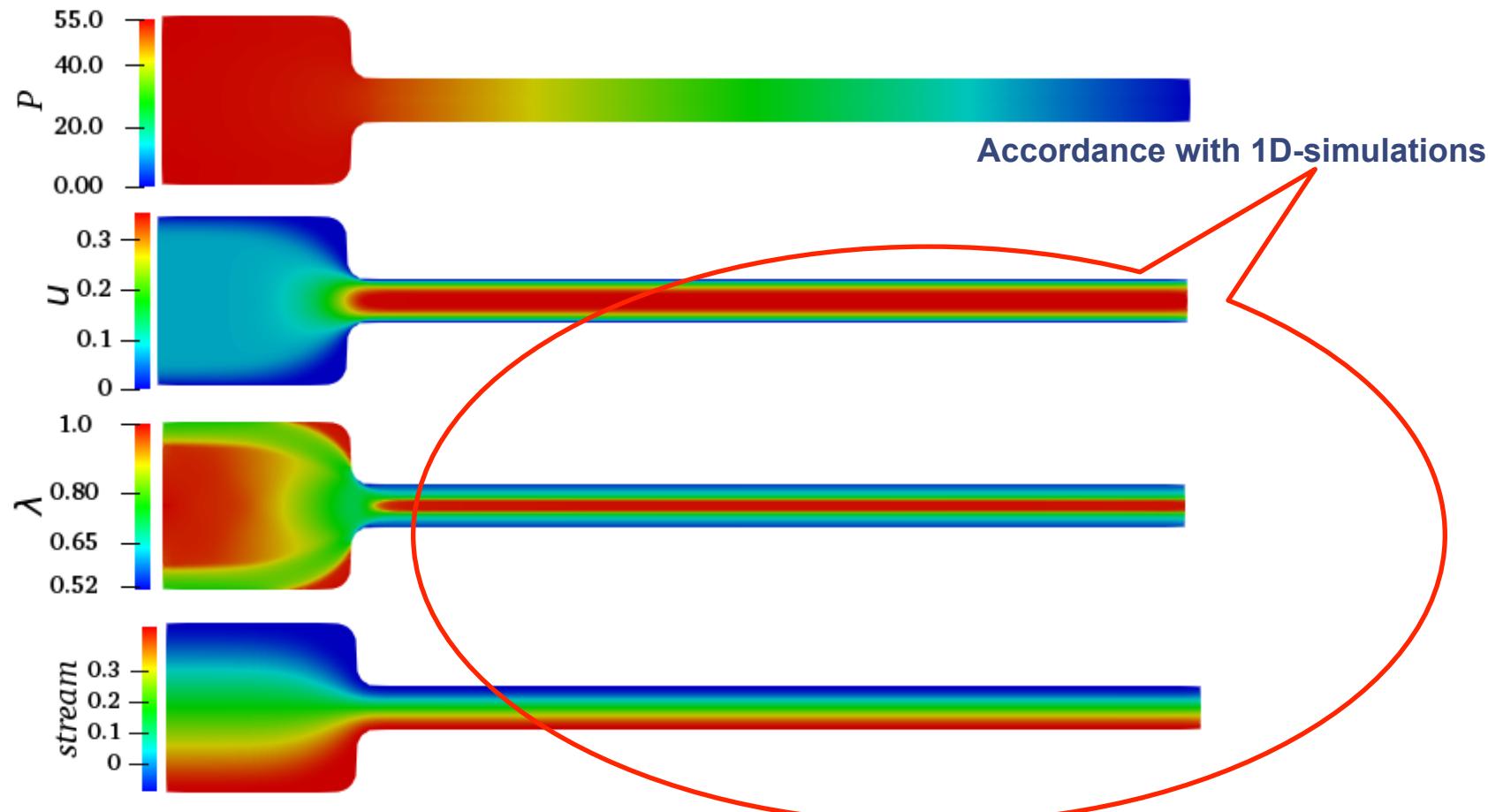
- 2D-FEM simulation results for thixotropic flow- validation of 1D tool
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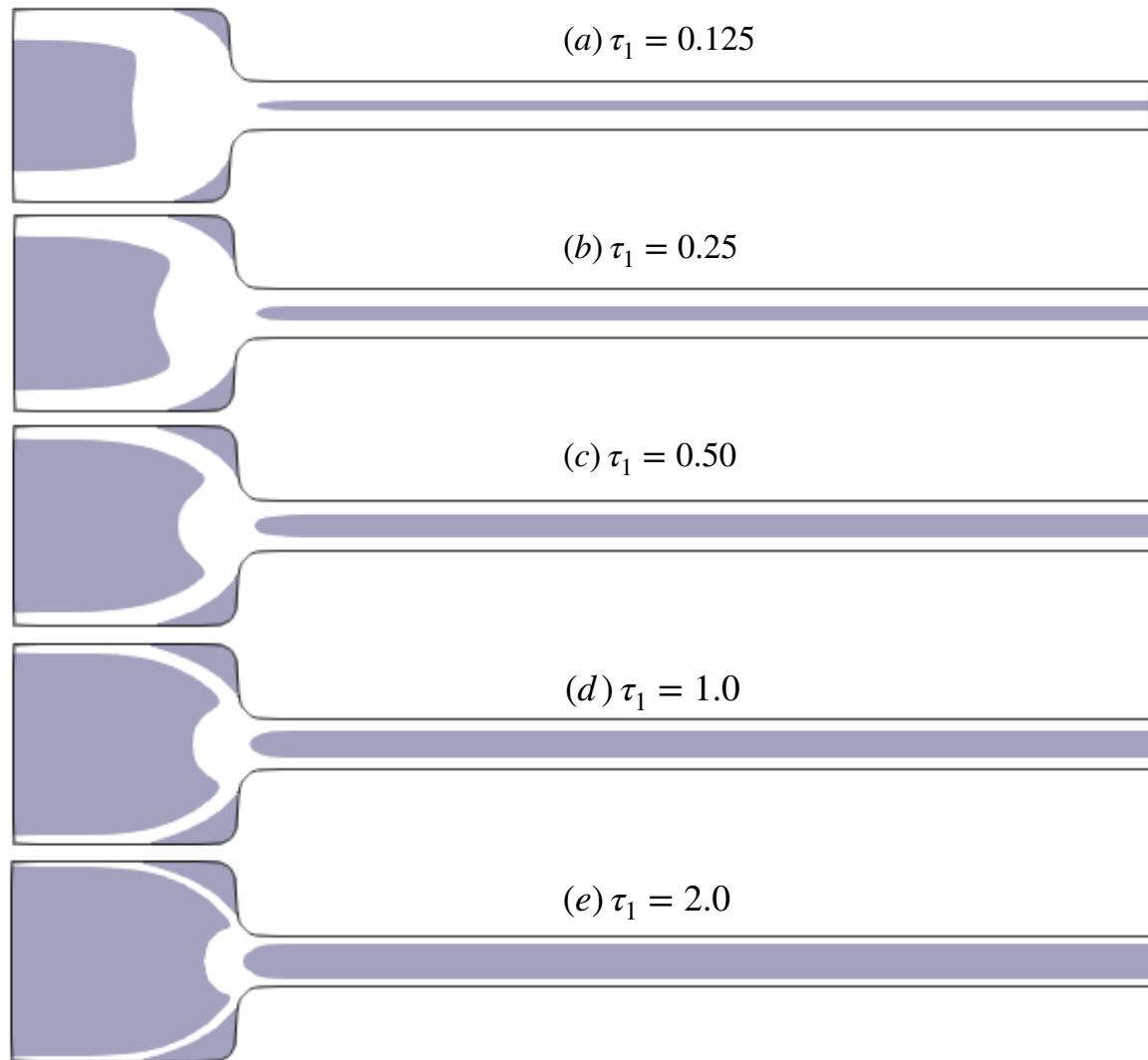


## Contraction flow (smoothed)

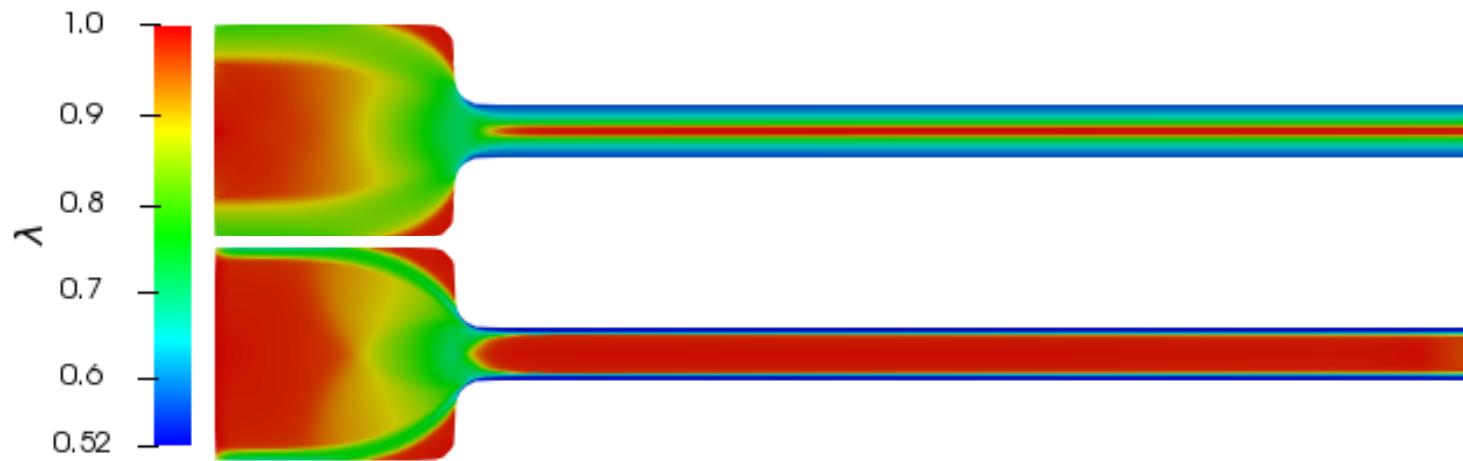


- ✓ As predicted  $(u, \lambda, p)$  solutions
- ✓ Structuring level is predicting shape and extent of rigid zones

- **progressive growth of unyielded zones (shaded)**



- Material structural behaviour w.r.t. yield stress



**To Do:** “Further investigation” regarding material structuring and prediction of plug-zones in the reservoir with sharp/abrupt contraction.

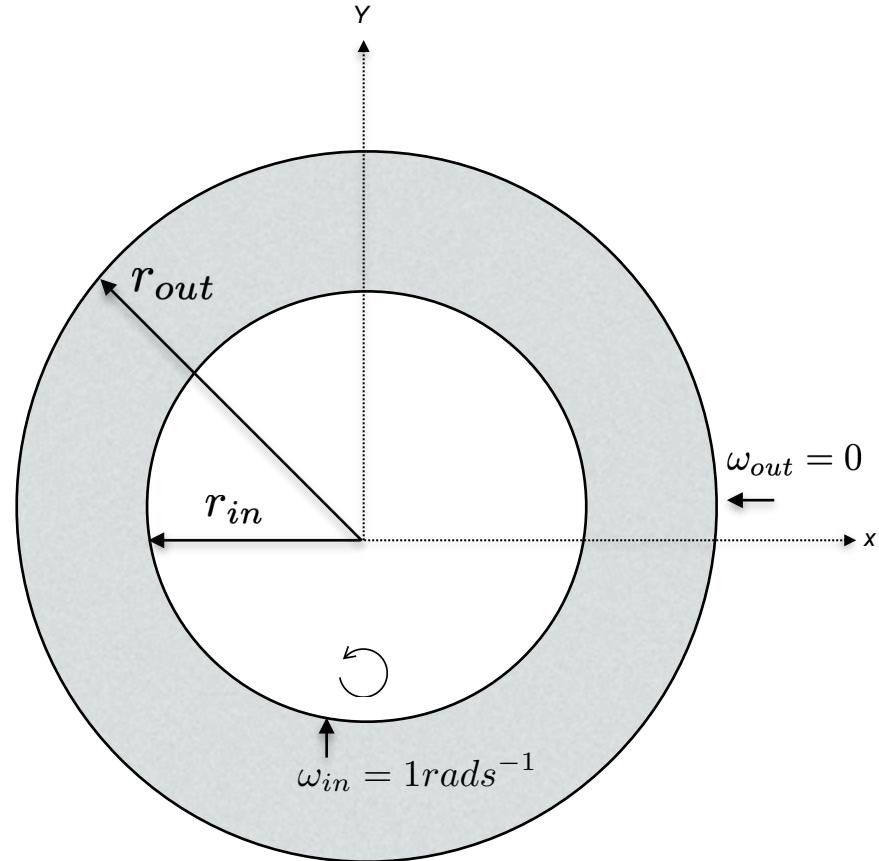
## Continuous axial-Flow Couette device:

The material is sheared in the annulus between the interior and exterior cylinder shells of radii  $r_{in}$  and  $r_{out}$  respectively.

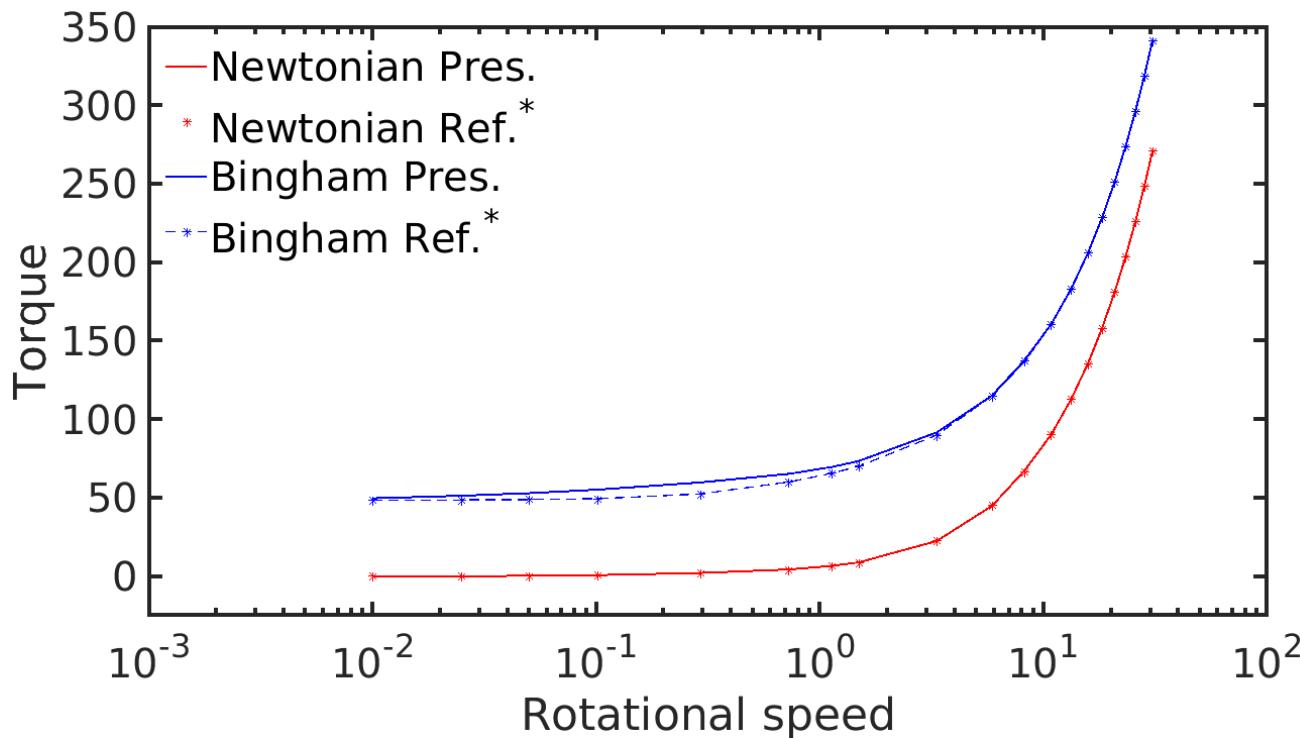
- ▶ Concentric cylinders
- ▶ Rotating inner cylinder with  $\omega_{in} = 1 \text{ rads}^{-1}$
- ▶ Stationary outer cylinder
- ▶ Vertical flow super-imposed in radial direction
- ▶ Torque is computed via:

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

where  $S$  is the surface of inner cylinder, and  $X_0$  the center of concentric couette device.



- “Validation”: Results for classical Newtonian and Bingham model are recovered



Material 1. Newtonian

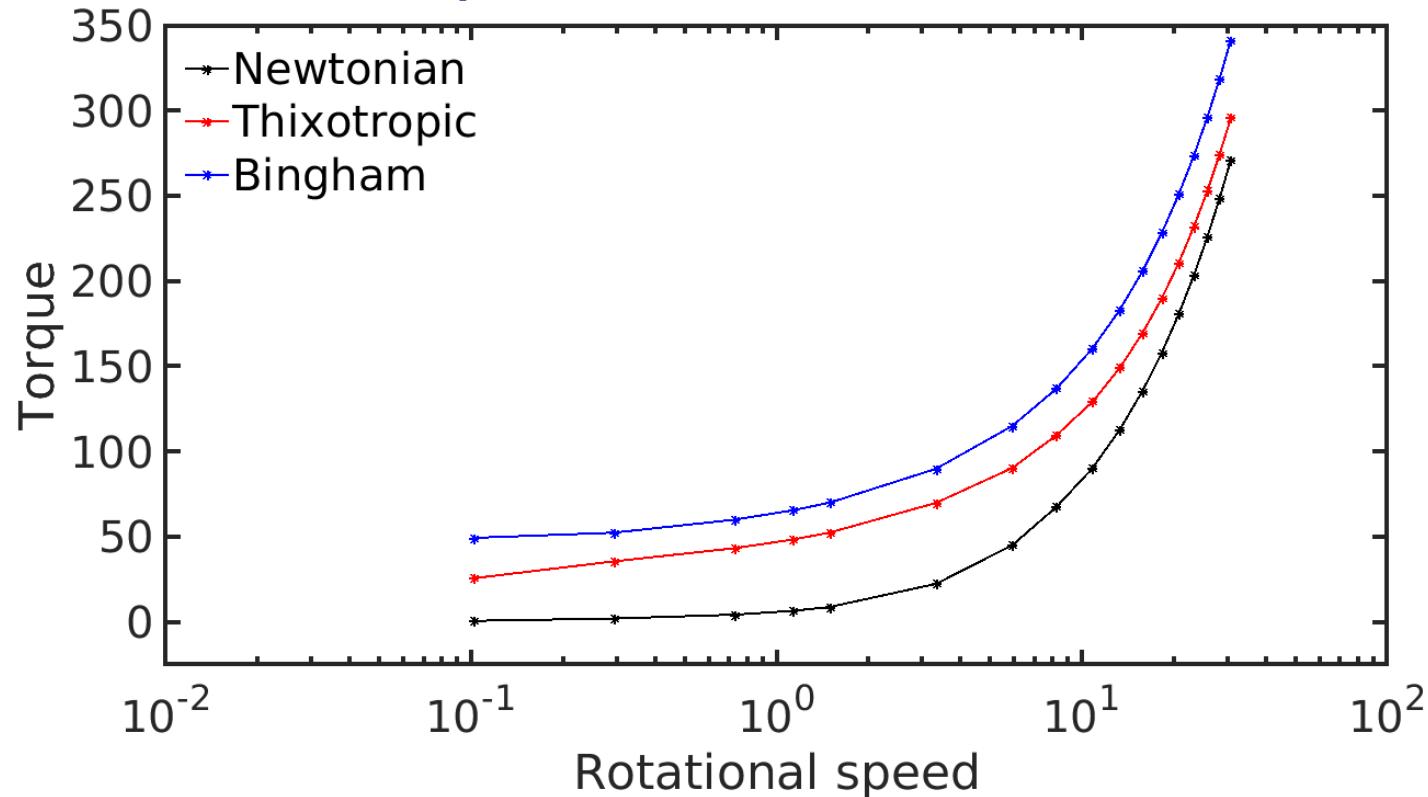
Material 2. Viscoplastic described by Bingham-Papanastasiou's model

Material 3. Thixotropic described by Houska's Model

Material	$\eta_0$	$\eta_1$	$\tau_0$	$\tau_1$
Newtonian	1.0	0.0	0.0	0.0
Viscoplastic	1.0	0.0	0.48	0.0
Thixotropic	1.0	0.0	0.0	0.48

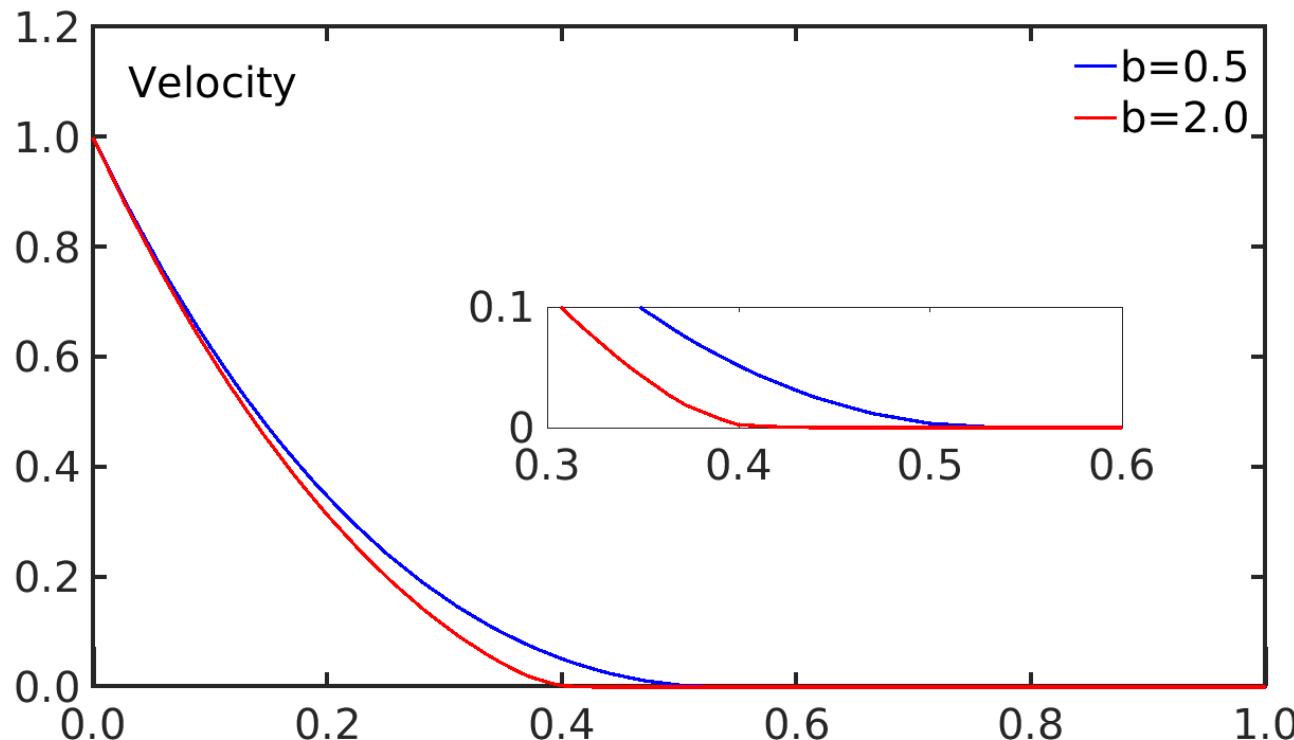
\*M. Kheiripour Langroudi, S. Turek, A. Ouazzi, G.I. Tardos, An investigation of frictional and collisional powder flows using a unified constitutive equation, Powder Technology, 197, 2010, 91-101.

- **Torque results for thixotropic material**



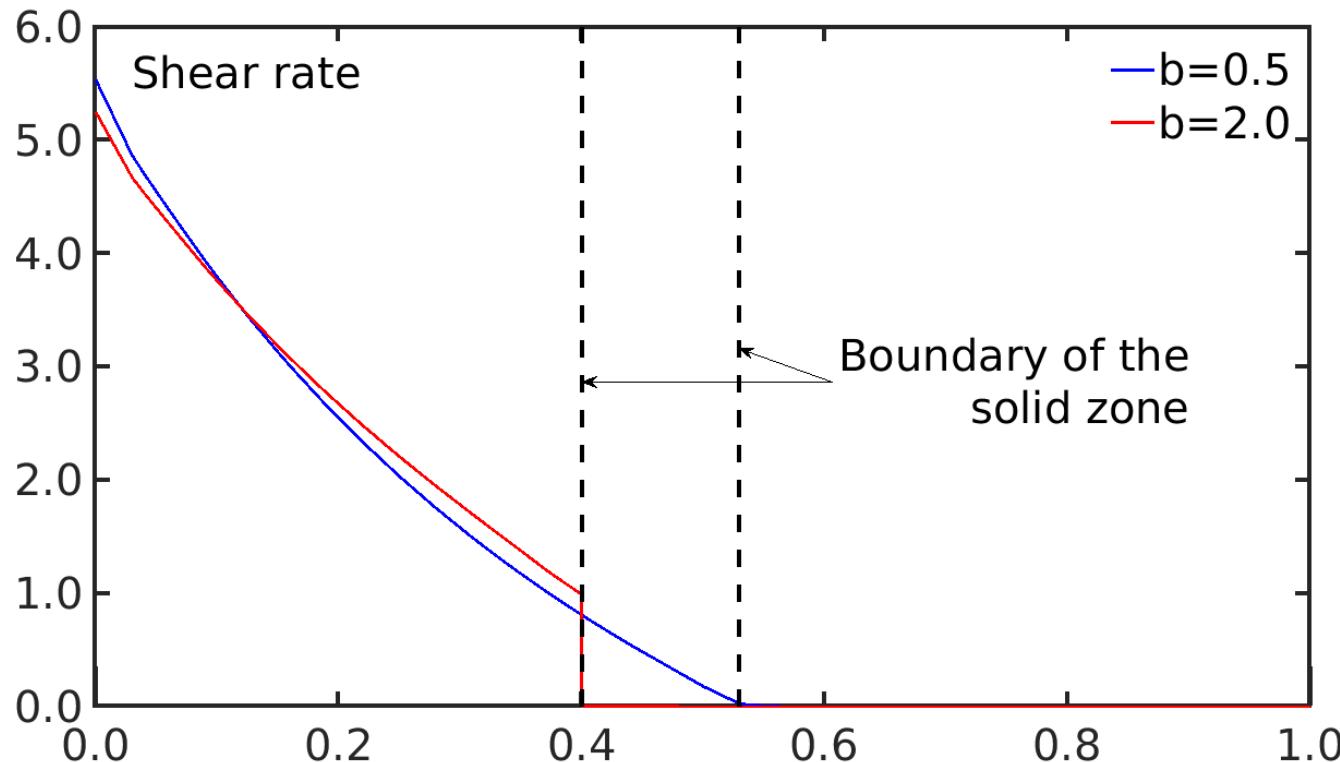
- Thixotropic material also yields a constant torque at small shear rates but then behaves like a Newtonian/Bingham and, data becomes indistinguishable where rotational speed is  $\geq 10 rads^{-1}$
- “Observation”: inherent thixotropy of Houska’s model controls the transitions between solid/liquid and liquid/solid.

- Velocity profile at cut-line positions  $c; c \in [0, 2\pi]$  in a Couette device w.r.t breakdown parameter



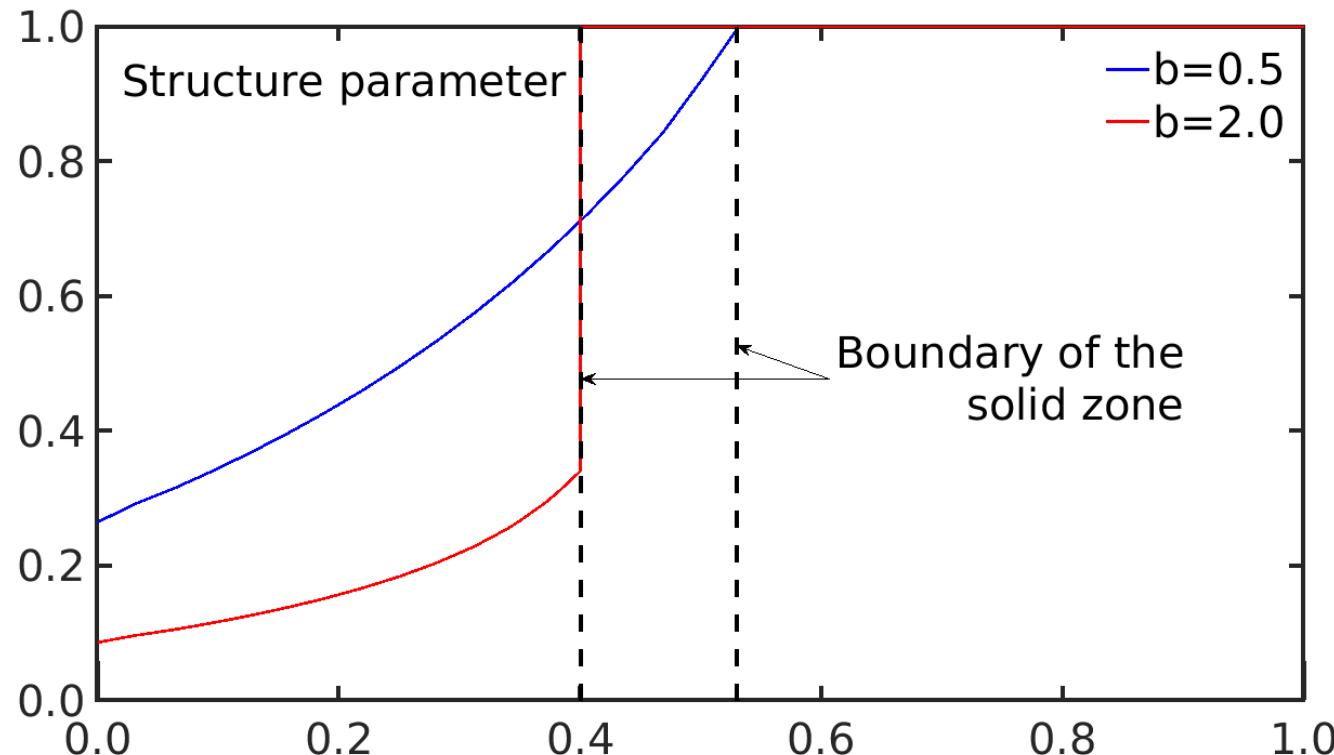
- ✓ Localization
- ✓ Shear banding

- Shear rate at cut-line positions  $c; c \in [0, 2\pi]$  in a Couette device w.r.t breakdown parameter



- ✓ Smooth and sharp transition are possible
- ✓ Transition point matches with the velocity

- Structure parameter at cut-line positions  $c; c \in [0, 2\pi]$  in a couette w.r.t. breakdown parameter



- ✓ Transition point matches with the velocity
- ✓ Structuring level is predicting shape and extent of rigid zones

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A quasi-Newtonian model for simulating thixotropic materials via time and shear rate dependent extended viscosity is analysed and validated for different prototypical flow simulations

- ✓ exact solution in simple channel
- ✓ complex flow geometry with curved contraction and in Couette devices

using robust numerical algorithms

- ✓ Monolithic Finite element method
- ✓ Generalized Newton's method w.r.t. singularities with global convergent property
- ✓ Fast Multigrid solver with local MPSC smoother

