Newton-multigrid FEM solver for the simulation of thixo-viscoplastic flow problems

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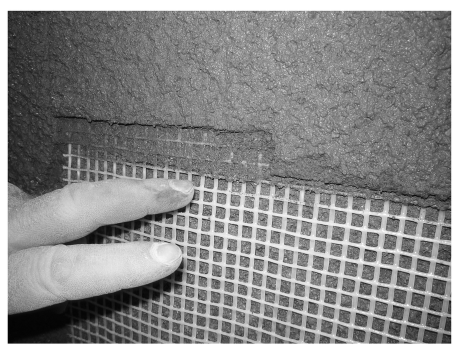
Motivation

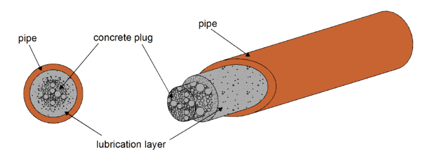
Thixotropic materials:

- 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

Thixo-viscoplastic (TVP) Models

➢ Thixo-viscoplastic constitutive stress based on Bingham Model

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

➢ Structure parameter equation

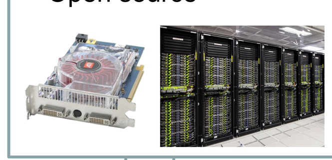
$$\left(\frac{\partial}{\partial t} + u\cdot\nabla\right)\lambda = \mathcal{F} - \mathcal{G}$$

➢ Examples of thixotropic models

	η	τ	$\mathcal{F}$	$\mathcal{G}$
Worrall & Tulliani	$\lambda\eta_0$	τ_0	$a(1-\lambda)\|\mathbf{D}\|$	$b\lambda\|\mathbf{D}\|$
Coussot et al.	$\lambda^g\eta_0$		a	$b\lambda\|\mathbf{D}\|$
Houška	$(\eta_0+\eta_1\lambda)\|\mathbf{D}\|^{n-1}$	$(\tau_0+\tau_1\lambda)$	$a(1-\lambda)$	$b\lambda^m\|\mathbf{D}\|$
Burgos et al.	η_0	$\lambda\eta_0$	$a(1-\lambda)$	$b\lambda\|\mathbf{D}\|e^{g\|\mathbf{D}\|}$
Mujumbar et al.	$-\eta_0\lambda\|\mathbf{D}\|^{n-1}$	$\lambda^{g+1}G_0\Lambda_c$	$a(1-\lambda)$	$b\lambda\|\mathbf{D}\|$
Dullaert & Mewis	$\lambda\eta_0$	$\lambda G_0(\lambda\|\mathbf{D}\|)\Lambda_c$	$(a_1+a_2\|\mathbf{D}\|)(1-\lambda)t^p$	$b\lambda\|\mathbf{D}\|t^{-p}$

Realization in FeatFlow

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):
- – interface capturing (Level Set)
- – interface tracking (FBM)
- – combination of both

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

Newton-multigrid FEM solver

Quasi-Newtonian approach

➢ Viscosity model for TVP flow i.e. extended viscosity defined on all domains

$$\mu(D_{\mathrm{II}},\lambda) = \eta(D_{\mathrm{II}},\lambda) + \tau(D_{\mathrm{II}},\lambda)\frac{\sqrt{2}}{2}\frac{1}{\sqrt{D_{\mathrm{II}}}}\left(1-e^{-k\sqrt{D_{\mathrm{II}}}}\right)$$

➢ Full set of equations

$$\begin{cases} \left(\dfrac{\partial}{\partial t} + u\cdot\nabla\right)u - \nabla\cdot\left(2\mu(D_{\mathrm{II}},\lambda)\mathbf{D}(u)\right) + \nabla p = 0 \\ \nabla\cdot u = 0 \\ \left(\dfrac{\partial}{\partial t} + u\cdot\nabla\right)\lambda - \mathcal{F}(D_{\mathrm{II}},\lambda) + \mathcal{G}(D_{\mathrm{II}},\lambda) = 0 \end{cases}$$

Adaptive Newton's Method

➢ The Newton's method assuming invertible Jacobian

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

➢ Continuous adaptive Newton via operator-adaptive splitting

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

➢ Discrete adaptive Newton via adaptive step-length control parameter

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

Continuous thixo-viscoplastic problem

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

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

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

➢ Compatibily constraints

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

Discrete thixo-viscoplastic problem

➢ Conforming Approximations

$$\mathbb{T}_h \subset \mathbb{T}, \quad \mathbb{V}_h \subset \mathbb{V}, \quad \mathbb{Q}_h \subset \mathbb{Q}$$
$$\mathcal{A}_{\tilde{\boldsymbol{u}}_h} = \mathcal{A}_{\tilde{\boldsymbol{u}}},\ \mathcal{B}_h = \mathcal{B}$$

➢ Discrete inf-sup condition

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

Robust conforming FEM

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

$$J_{\tilde{u}}(\tilde{u}_h,\tilde{v}_h) = \sum_{e\in\mathcal{E}_h}\gamma_{\tilde{u}}h^2\int_e [\nabla\tilde{u}_h]:[\nabla\tilde{v}_h]\,ds$$

➢ Inf-sup conditions is satisfied
➢ Discontinuous pressure
  ➢ Good for the solver
  ➢ Straightforward element-wise mass conservation
➢ Discrete problem is well-posed
➢ Highly consistent and symmetric stabilization
➢ Robust & efficient solver w.r.t. the monolitic approach

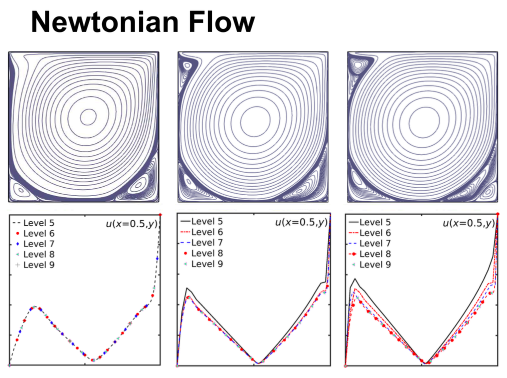
Monolithic-multigrid linear solver

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

➢ Standard Geometric multigrid solver
➢ Local Multilevel Pressure Schur Complement via Vanka-like smoother

Thixo-viscoplastic flow in Lid-driven cavity

Newtonian Flow

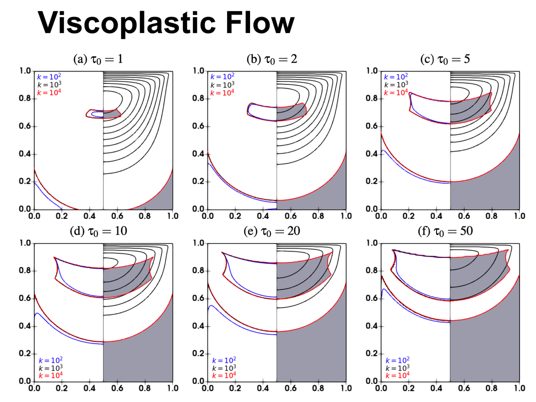


Re		1000		5000		10000	
Level	cells	Energy$\times 10^2$	N/M	Energy$\times 10^2$	N/M	Energy$\times 10^2$	N/M
5	1024	4.541506	5/1	6.082524	6/1	7.940472	7/1
6	4096	4.458877	5/1	4.955858	5/1	5.369527	6/1
7	16384	4.452357	3/1	4.768669	4/1	4.868399	5/1
8	65536	4.451904	3/1	4.744815	3/2	4.783917	4/2
9	262144	4.451846	3/1	4.742921	3/1	4.773500	3/2
10	1048576	4.451834	2/1	4.742815	3/1	4.772692	3/1
$Ref.values \approx$		4.45		4.74		4.77	

Re	1000		5000		10000	
Level	ψ_{max}	$\psi_{min}\times 10^3$	ψ_{max}	$\psi_{min}\times 10^3$	ψ_{max}	$\psi_{min}\times 10^3$
6	0.1190073	−1.72813	0.1249471	−3.145666	0.1586626	−5.7535749
7	0.1189360	−1.72649	0.1225439	−3.077555	0.1236127	−3.2070181
8	0.1189361	−1.72851	0.1222499	−3.072411	0.1225210	−3.1831353
9	0.1189362	−1.72963	0.1222269	−3.073524	0.1224097	−3.1910101
10	0.1189366	−1.72965	0.1222259	−3.073589	0.1223892	−3.1797390
$Ref.$	0.1189	−1.729	0.1221	−3.070		

✓ Point-wise mesh convergence for Newtonian
✓ Efficient non-linear solver and mesh refinement independent linear solver

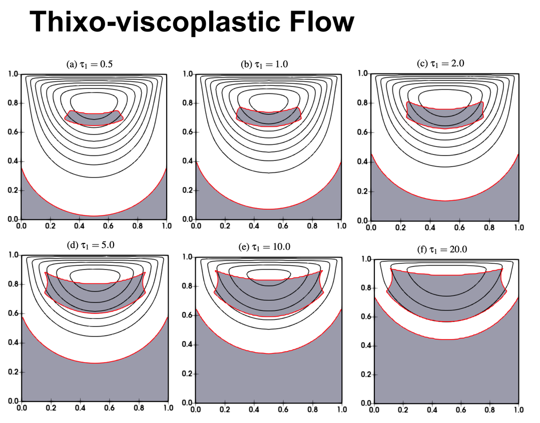
Viscoplastic Flow



$k\backslash L$	5	6	7	5	6	7	5	6	7
	$\tau_0=1$			$\tau_0=2$			$\tau_0=5$		
1×10^1	3/1	3/1	3/1	3/1	3/1	3/1	4/1	4/1	4/1
5×10^1	2/1	2/1	2/1	2/1	2/1	2/1	3/1	3/1	3/1
1×10^2	3/1	3/1	3/1	3/1	3/1	3/1	4/1	4/1	4/1
5×10^2	3/1	2/1	2/1	3/1	2/1	3/1	3/2	3/2	3/1
1×10^3	2/2	3/2	3/1	3/1	3/1	4/1	4/1	5/2	5/2
5×10^3	2/1	2/1	4/1	3/1	3/2	6/2	4/1	8/2	6/1
1×10^4	2/1	2/2	5/1	3/1	3/1	6/1	4/1	5/4	6/3
	$\tau_0=10$			$\tau_0=20$			$\tau_0=50$		
1×10^1	5/1	5/1	5/1	6/1	6/1	6/1	5/1	7/1	7/1
5×10^1	4/1	3/1	3/1	4/1	4/1	3/2	5/4	4/2	4/2
1×10^2	5/2	4/1	4/1	5/2	5/2	5/1	6/5	5/4	5/1
5×10^2	5/3	3/2	3/1	4/4	3/4	4/3	5/4	4/2	4/3
1×10^3	5/2	7/4	9/1	5/5	7/2	8/1	5/5	9/2	9/2
5×10^3	5/1	7/3	8/2	6/3	6/4	6/4	6/4	7/2	8/2
1×10^4	6/1	7/2	8/3	6/3	5/5	7/3	6/3	7/3	8/2

✓ Accurate track of interface is captured via larger k solutions and finer mesh refinement
✓ Existence of pair (k, L) beyond which no further improvement in solutions is expected
✓ Efficient non-linear solver and mesh independent linear solver for all values of yield-stress
✓ Solutions are obtained with continuation strategy w.r.t. k

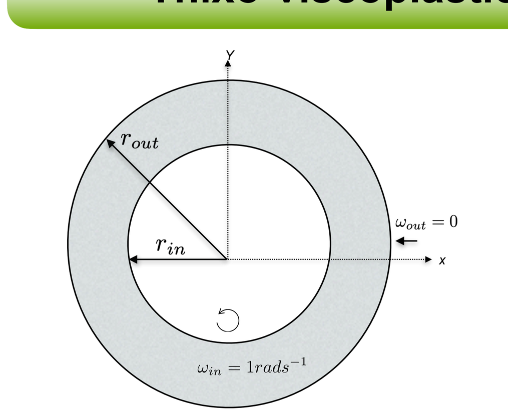
Thixo-viscoplastic Flow



$k\backslash L$	5	6	7	5	6	7	5	6	7
	$\tau_1=0.5$			$\tau_1=1$			$\tau_1=2$		
1×10^1	5/2	5/3	6/2	5/2	5/2	9/1	5/2	5/2	9/1
5×10^1	4/2	4/2	4/2	3/2	3/3	7/1	3/2	3/3	8/1
1×10^2	4/1	4/2	5/1	4/1	4/2	7/1	4/2	4/2	8/1
5×10^2	4/1	4/1	5/1	3/1	4/1	6/1	4/2	4/2	8/1
1×10^3	4/1	4/1	4/1	4/2	4/2	8/1	4/4	6/1	7/1
5×10^3	4/1	4/1	3/2	7/1	9/1	5/1	6/1	9/1	8/1
1×10^4	4/1	4/2	4/2	5/1	7/1	4/1	7/1	10/1	8/2
	$\tau_1=5.0$			$\tau_1=10.0$			$\tau_1=20.0$		
1×10^1	6/2	6/2	10/1	11/1	8/2	11/1	10/1	9/2	11/1
5×10^1	4/2	3/2	11/1	11/1	4/2	7/1	12/1	5/3	9/1
1×10^2	4/2	5/2	11/1	10/1	5/3	8/1	12/1	6/3	10/1
5×10^2	5/2	4/2	10/1	9/1	5/3	5/1	8/1	5/5	11/1
1×10^3	5/2	9/1	10/1	10/1	9/1	7/1	8/2	9/1	9/2
5×10^3	5/1	5/1	5/1	8/1	8/2	6/1	8/1	7/1	11/1
1×10^4	5/1	5/2	5/1	8/3	7/1	5/1	8/2	7/1	9/1

✓ Main rheological characteristics of TVP materials is captured for increasing thixotropic yield-stress
✓ Efficient non-linear solver and mesh independent linear solver for all values of yield-stress
✓ Solutions are obtained with continuation strategy w.r.t. k

Thixo-viscoplastic flow in Couette devices



Flow configuration

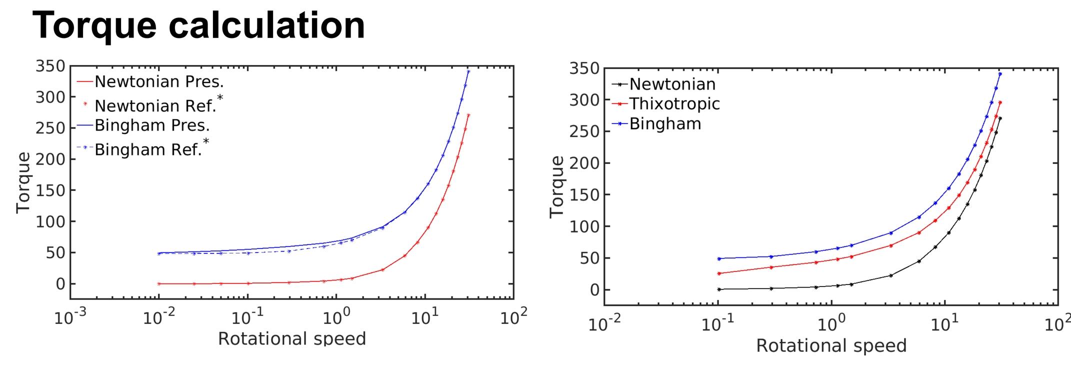
The material is sheared in two Concentric cylinders
- Rotating inner cylinder with $\omega_{in} = 1rads^{-1}$
- Stationary outer cylinder

Investigations of thixo-viscoplastic phenomena
- Torque at the surface of inner cylinder

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

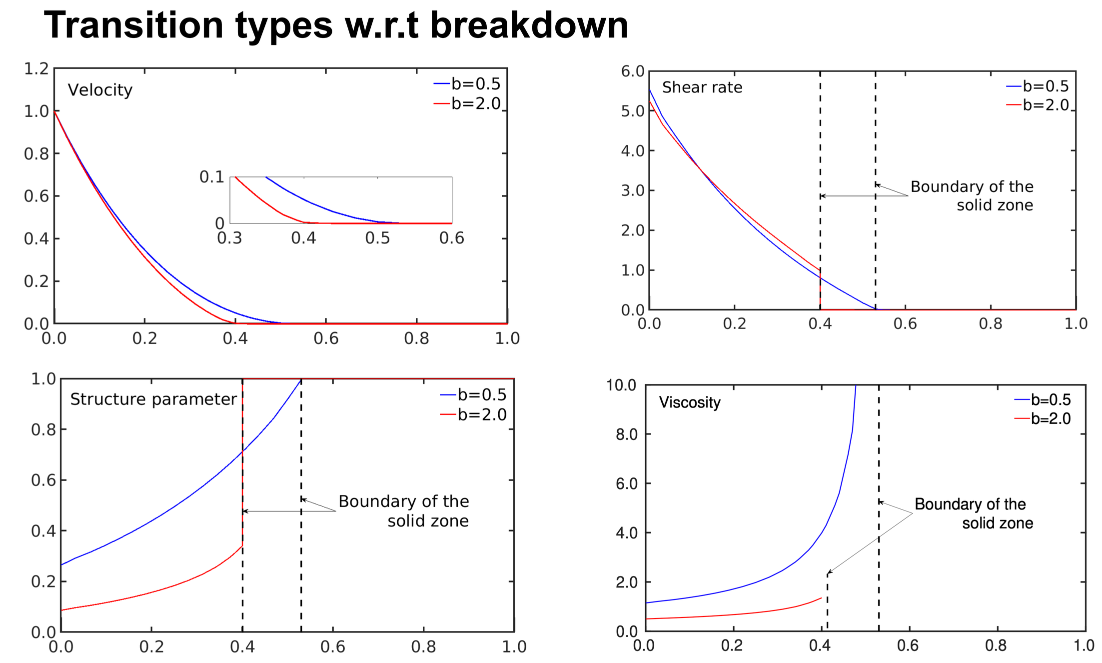
- Shear localization
- Shear banding

Torque calculation



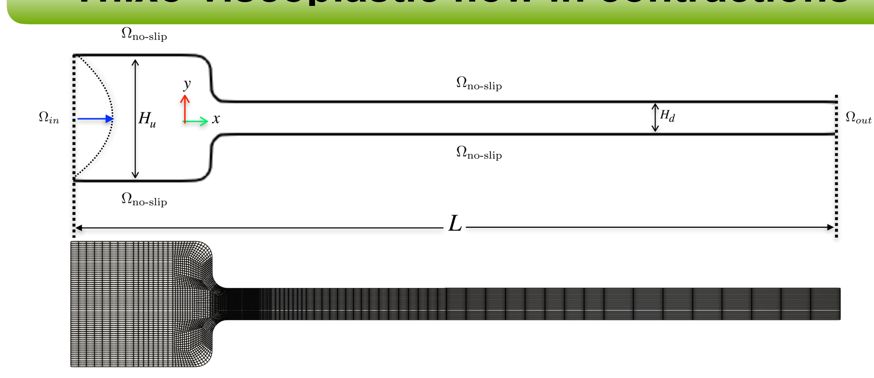
✓ Agreement with Ref. [5] for Torque for Non-thixotropic flow
✓ Thixotropic flow is encompassed between the two extremities, Newtonian liquid and Bingham plastic, as predicted by Houska's model

Transition types w.r.t breakdown

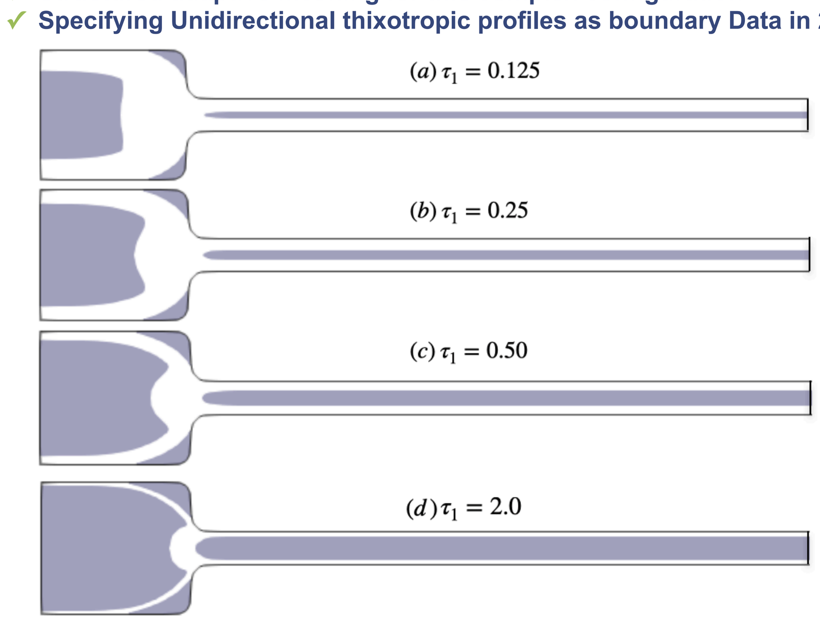


✓ Shear Localization & shear banding transition types w.r.t breakdown parameter
✓ Transition point for shear-rate and structure parameter match with velocity
✓ Structure parameter predicts the shape and extent of rigid zones

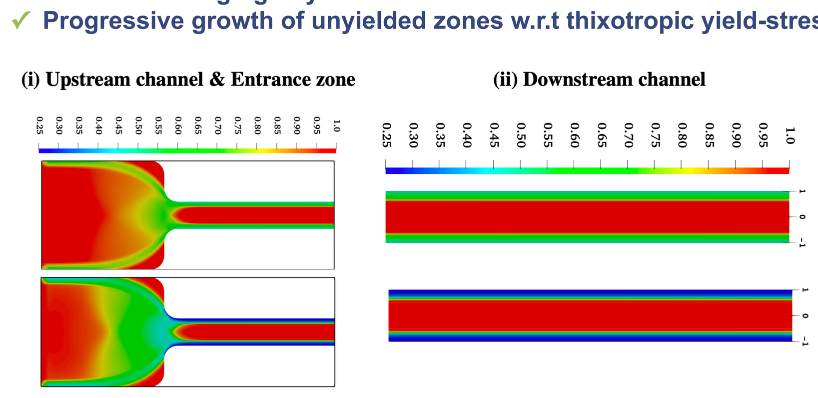
Thixo-viscoplastic flow in contractions



✓ Structured adaptive meshing for this complex configuration
✓ Specifying Unidirectional thixotropic profiles as boundary Data in 2D



✓ Three non-merging unyielded-zones
✓ Progressive growth of unyielded zones w.r.t thixotropic yield-stress



✓ Appearance of more breakdown layers w.r.t pronounced breakdown parameter
  ➡ Restart pressure in pipelines should not be over-estimated

✓ Three non-merging unyielded-zones
  ➡ Further investigation regarding material structuring in thixo-elasovisocplastic

Summary

Accurate, robust, and efficient numerical solver for TVP flows is developed using
- ✓ Higher order finite element method
- ✓ Monolitic Newton-multigrid
  - Adaptive discrete Newton's method with global convergent property
  - Geometric multigrid with local MPSC

To analyze the quasi-Newtonian model for TVP materials for different flow simulations
- ✓ Newtonian, VP, and TVP flow in Lid-driven cavity
- ✓ TVP flow in Couette devices
- ✓ TVP flow in curved contractions

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