FEM simulations of thixo-viscoplastic flow problems

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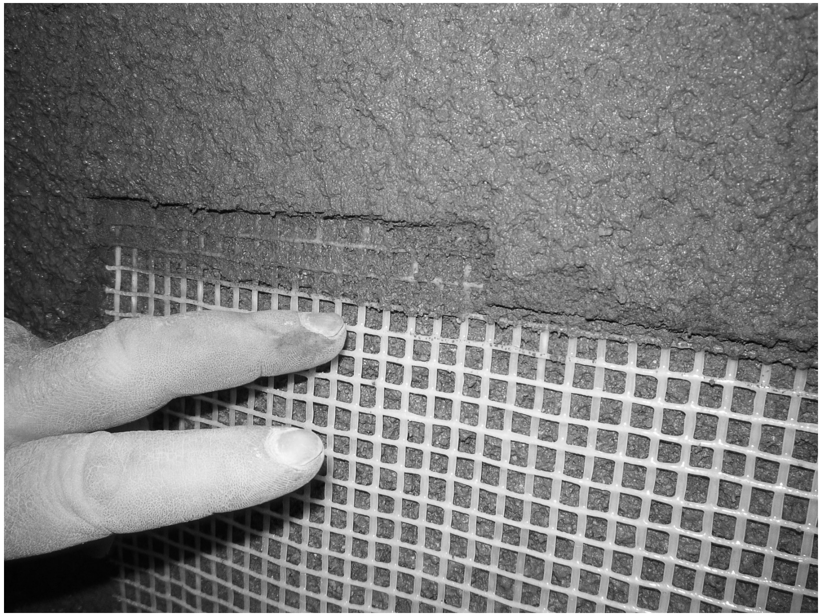
Why "Thixotropic materials?

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

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

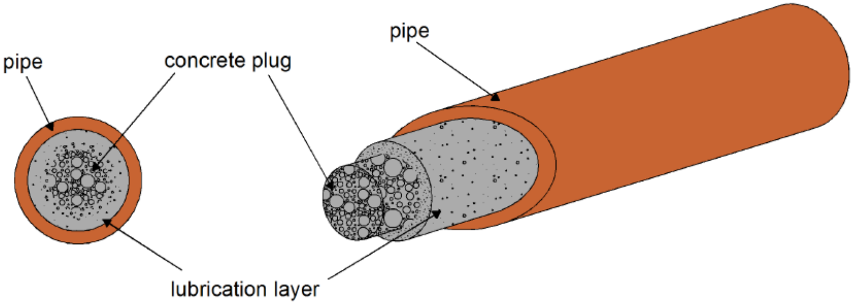
- **Physically fascinating due to improved mechanical properties**



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

Introduction

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- 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 / Buildup
  - ➢ At rest or under slow flow: fluid ages
    Increases of the viscosity in time

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):
•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

Governing equations

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

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

$$\nabla\cdot\boldsymbol{u}=0,$$

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

$$\boldsymbol{\sigma}=2\eta_s\boldsymbol{D}(\boldsymbol{u})$$ **: η_s is constant viscosity**

- **non-linear material behaviour- structurally viscous / viscoplastic**

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

- **Power-law, Carreau, Bingham, Herschel-Bulkley, Houska, …**

- **structure paremeter λ**

Rheological Models

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- **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	$\lambda\eta_0$	τ_0
Coussot *et al.*	$\lambda^a\eta_0$	–
Houska	$(\eta_0+\eta_1\lambda)\,D_{\mathrm{II}}^{\frac{(n-1)}{2}}$	$(\tau_0+\tau_1\lambda)$
Mujumbar *et al.*	$(\eta_0+\eta_1\lambda)\,D_{\mathrm{II}}^{\frac{(n-1)}{2}}$	$\lambda^{a+1}\mathrm{G}_0\Lambda_c{}^*$
Burgos *et al.*	η_0	$\lambda\tau_0$
Dullaert and Mewis	$\lambda\eta_0$	$\lambda\mathrm{G}_0\left(\lambda D_{\mathrm{II}}^{\frac{1}{2}}\right)\Lambda_c^*$

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

Rheological Models

- **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	$c_1(1-\lambda)D_{\mathrm{II}}^{\frac{1}{2}}$	$c_2\lambda D_{\mathrm{II}}^{\frac{1}{2}}$
Coussot *et al.*	c_1	$c_2\lambda D_{\mathrm{II}}^{\frac{1}{2}}$
Houska	$c_1(1-\lambda)$	$c_2\lambda^m D_{\mathrm{II}}^{\frac{1}{2}}$
Mujumbar *et al.*	$c_1(1-\lambda)$	$c_2\lambda D_{\mathrm{II}}^{\frac{1}{2}}$
Burgos *et al.*	$c_1(1-\lambda)$	$c_2\lambda D_{\mathrm{II}}^{\frac{1}{2}} \exp(aD_{\mathrm{II}}^{\frac{1}{2}})$
Dullaert and Mewis	$(c_1 + c_3 D_{\mathrm{II}}^{\frac{1}{2}})(1-\lambda)t^{-b}$	$c_2\lambda D_{\mathrm{II}}^{\frac{1}{2}} t^{-b}$

Thixo-viscoplastic model

- **Viscoplastic (VP) flow**

$$\begin{cases} \boldsymbol{\sigma} = 2\,\eta_0 \boldsymbol{D}(\boldsymbol{u}) + \sqrt{2}\,\tau_0 \dfrac{\boldsymbol{D}(\boldsymbol{u})}{\sqrt{D_{\mathrm{II}}}} & \text{if } D_{\mathrm{II}} \neq 0 \\ \sigma_{\mathrm{II}} \leq \tau_0 & \text{if } D_{\mathrm{II}} = 0 \end{cases}$$

- **Thixo-viscoplastic (TVP) flow**

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

- **Micro-structure equation**

$$\left(\frac{\partial}{\partial t} + u \cdot \nabla\right)\lambda + \mathcal{M}(D_{\mathrm{II}}, \lambda) = f_\lambda$$

$$\mathcal{M} := \mathcal{G} - \mathcal{F}$$

Quasi-Newtonian TVP model

➢ 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

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

Sobolev spaces and notations

- $H^0(\Omega) := L^2(\Omega) = \left\{ v \,|\, \int_\Omega |v|^2 d\Omega < \infty \right\}$

  $L^2_0(\Omega) = \left\{ v \in L^2(\Omega) \,|\, \int_\Omega v d\Omega = 0 \right\}, \quad \|v\|_{0,\Omega} = \left(\int_\Omega |v|^2 d\Omega \right)^{\frac{1}{2}}$

- $H^1(\Omega) = \{ v \in L^2(\Omega) \,|\, \nabla v \in L^2(\Omega) \}, \quad \|v\|_{1,\Omega} = \left(\|v\|^2_{0,\Omega} + \|\nabla v\|^2_{0,\Omega} \right)^{\frac{1}{2}}$

  $H^1_\Gamma(\Omega) = \{ v \in H^1(\Omega) \,|\, v_{|\Gamma} = 0, \Gamma \subset \partial\Omega \}$

  $H^1_0(\Omega) = \{ v \in H^1(\Omega) \,|\, v_{|\partial\Omega} = 0 \}$

- $H(\boldsymbol{u}, \Omega) = \{ v \in L^2(\Omega), \boldsymbol{u} \cdot \nabla v \in L^2(\Omega) \}, \quad \|v\|_{1,\boldsymbol{u}} = \left(\|v\|^2_{0,\Omega} + \|\boldsymbol{u} \cdot \nabla v\|^2_{0,\Omega} \right)^{\frac{1}{2}}$

  $\Gamma^- = \{ x \in \Gamma \subset \partial\Omega \,|\, \boldsymbol{u} \cdot \boldsymbol{n} < 0 \}, \quad \Gamma^+ = \{ x \in \Gamma \subset \partial\Omega \,|\, \boldsymbol{u} \cdot \boldsymbol{n} > 0 \}$

  $< v, w >_\pm = \int_{\Gamma^\pm} |\boldsymbol{u} \cdot \boldsymbol{n}| v w ds, \quad < v >_\pm = < v, v >^{\frac{1}{2}}_\pm$

Continuous thixo-viscoplastic problem

- **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.**

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

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

  - ➢ **Compatibily constraints**

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

➢ **Weak Formulation**

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

➢ **Operators**

$$\Big\langle \mathcal{K}(\lambda, \boldsymbol{u}, p), (\xi, \boldsymbol{v}, q) \Big\rangle = a_\lambda(\tilde{\boldsymbol{u}})(\lambda, \xi) + a_{\boldsymbol{u}}(\tilde{\boldsymbol{u}})(\boldsymbol{u}, \boldsymbol{v}) + b(\boldsymbol{v}, p) - b(\boldsymbol{u}, q)$$

$$\mathcal{A}_{\tilde{\boldsymbol{u}}}(\tilde{\boldsymbol{u}})\tilde{\boldsymbol{u}} = \mathcal{A}_\lambda(\tilde{\boldsymbol{u}})\lambda + \mathcal{A}_{\boldsymbol{u}}(\tilde{\boldsymbol{u}})\boldsymbol{u}$$

$$\Big\langle \mathcal{A}_\lambda(\tilde{\boldsymbol{u}})\lambda, \xi \Big\rangle = a_\lambda(\tilde{\boldsymbol{u}})(\lambda, \xi) = \Big(\mathcal{M}(D_{\mathrm{II}}, \lambda), \xi\Big) + \Big(\boldsymbol{u} \cdot \nabla\lambda, \xi\Big)$$

$$\Big\langle \mathcal{A}_{\boldsymbol{u}}(\tilde{\boldsymbol{u}})\boldsymbol{u}, \boldsymbol{v} \Big\rangle = a_{\boldsymbol{u}}(\tilde{\boldsymbol{u}})(\boldsymbol{u}, \boldsymbol{v}) = \Big(2\mu(D_{\mathrm{II},r}, \lambda)\boldsymbol{D}(\boldsymbol{u}), \boldsymbol{D}(\boldsymbol{v})\Big) + \Big(\boldsymbol{u} \cdot \nabla\boldsymbol{u}, \boldsymbol{v}\Big)$$

$$\Big\langle \mathcal{B}\boldsymbol{v}, \mathrm{q} \Big\rangle = b(\boldsymbol{v}, q) = -\Big(\nabla \cdot \boldsymbol{v}, q\Big)$$

$$\Big\langle \mathcal{L}, (\xi, \boldsymbol{u}, q) \Big\rangle = \Big(f_\lambda, \xi\Big) + \Big(\boldsymbol{f}_{\boldsymbol{u}}, \boldsymbol{v}\Big)$$

Wellposedness of thixo-viscoplastic problem !

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.*

Remark

- *Coercivity*

$$a_{\tilde{\boldsymbol{u}}}(\tilde{\boldsymbol{v}})(\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{v}}) \geq \mathcal{M}_a \|\xi\|_{0,\Omega}^2 + \frac{1}{2} \langle\xi\rangle^2 + \eta_0 \mathcal{C}_K \|\boldsymbol{v}\|_{1,\Omega}^2 \qquad \forall\, \tilde{\boldsymbol{v}} \in \mathbb{W}_0$$

- *Pressure*

$$\|p\|_0 = \mathcal{O}(k \|\boldsymbol{f_u}\|_0)$$

Coercivity in weaker norm for the microstructure !
Pressure is underdertmined in regid zone !

Theorem [Nonsingular solution]

Let $\boldsymbol{f_u} \in (L^2(\Omega))^2$ *and* $f_\lambda \in L^2(\Omega)$. *Assume in addition*

$$\max\left(\frac{3}{2}\frac{\mathcal{M}_b\|\boldsymbol{f_u}\|_0}{\eta_0\mathcal{C}_K\mathcal{M}_a}, \frac{\|\boldsymbol{f_u}\|_0}{\eta_\infty(\eta_0\mathcal{C}_K)^2\mathcal{M}_a}\right) \leq \ 1$$

Then, the thixo-viscoplastic problem has a unique nonsingular solution $(\tilde{\boldsymbol{u}}, p) = (\lambda, \boldsymbol{u}, p) \in \mathbb{W} \times \mathbb{Q}$.

Proof:

- $$\left\langle \frac{\partial A_{\tilde{\boldsymbol{u}}}\tilde{\boldsymbol{u}}}{\partial \tilde{\boldsymbol{u}}}\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{v}} \right\rangle \geq 2\left(\mathcal{M}_a - \frac{3}{2}\frac{\mathcal{M}_b}{\eta_0\mathcal{C}_K}\|\boldsymbol{f_u}\|_0\right)\|\xi\|^2_{0,\Omega} + \langle\xi\rangle^2 + \left(\eta_0\eta_\infty\mathcal{C}_K - \frac{1}{\eta_0\mathcal{C}_K}\|\boldsymbol{f_u}\|_0\right)\|\boldsymbol{v}\|^2_{1,\Omega} \qquad \forall\, \tilde{\boldsymbol{v}} \in \mathbb{W}_0$$

Approximated TVP problem

- **Conforming approximations**

$$\mathbb{T}_h \subset \mathbb{T},\ \mathbb{V}_h \subset \mathbb{V},\ \mathbb{Q}_h \subset \mathbb{Q},\ \mathbb{W}_h := \mathbb{T}_h \times \mathbb{V}_h$$

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

- **Discrete inf-sup condition**

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

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

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

Order of convergence !

➢ Coercivity in a weaker norm for microstructure

➢
$$\|\xi_h - \lambda_h\|_0^2 \;\leq\; \mathcal{C}_{\lambda,\lambda}\|\lambda - \xi_h\|_0^2 + \mathcal{C}_{\lambda,\boldsymbol{u}}|\boldsymbol{u} - \boldsymbol{v}_h|_{1,\infty}^2 + \mathcal{C}_{\lambda,\boldsymbol{u}}|\boldsymbol{u}_h - \boldsymbol{v}_h|_{1,\infty}^2$$

$$|\boldsymbol{v}_h - \boldsymbol{u}_h|_{1,\infty}^2 \leq \mathcal{C}_{\boldsymbol{u},\boldsymbol{u}}|\boldsymbol{u} - \boldsymbol{v}_h|_1^2 + \mathcal{C}_{\boldsymbol{u},\lambda}\|\lambda - \xi_h\|_1^2 + \mathcal{C}_{\boldsymbol{u},\lambda}\|\lambda_h - \xi_h\|_0^2 + \mathcal{C}_{\boldsymbol{u},p}\|p - p_h\|_0^2$$

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

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

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

➢ Regularization

$$\tilde{\mathcal{C}}_{\boldsymbol{u},\boldsymbol{u}}(\mathcal{M}_a, \mathcal{M}_b, \|\lambda\|_0, \eta_0, \eta_\infty, \tau_\infty k, \mathcal{C}_K, |\boldsymbol{u}|_1) = \mathcal{O}(\mathcal{C}_{\boldsymbol{u},\boldsymbol{u}}) = \mathcal{O}(k^2)$$

$$\mathcal{C}_{\boldsymbol{u},\boldsymbol{u}}(\eta_0, \eta_\infty, \tau_\infty k, \mathcal{C}_K, |\boldsymbol{u}|_1) = 4\left(\frac{2\eta_\infty + 2\tau_\infty k + |\boldsymbol{v}_h|_1 + |\boldsymbol{u}|_1}{\eta_0 \mathcal{C}_K - |\boldsymbol{v}_h|_1}\right)^2$$

Coercivity in a stronger norm for the microstructure eq. !
FEM choices to counterbalance the regularisation/sub-optimality !

Numerical challenges

- **Discretization of TVP model have to address the following challenges**
  - ➢ **Stable FEM spaces**
  - ➢ **Coercivity in a weaker norm**
  - ➢ **Regularization**

- **TVP Newton-multigrid Solver have to deal with**
  - ➢ **Different source of nonlinearities**
  - ➢ **Strong coupling of equations**
  - ➢ **Robustness and efficiency**

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**

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

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

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

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- **Coercivity in a Stronger norm for microstructure**

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

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

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

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

- **Regularisation for TVP model**

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

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

Stabilization recover the optimal order of convergence
Higher order FEM counterbalance regularization

Let $\{\varphi_i, i=1,2,\dots,\mathtt{dim}\mathbb{W}_h\}$ **and** $\{\psi_i,\ i=1,\dots,\mathtt{dim}\mathbb{Q}_h\}$ **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 $\mathcal{R}(\mathcal{U})\in\mathbb{R}^{\mathtt{dim}\mathbb{W}_h+\mathtt{dim}\mathbb{Q}_h}$

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

- **Update of the nonlinear iteration with the correction** $\delta\mathcal{U}$

$$\mathcal{U}^{l+1}=\mathcal{U}^l+\delta\mathcal{U}$$

- **The linearization of the residual provides**

$$\mathcal{R}(\mathcal{U}^{l+1})=\mathcal{R}(\mathcal{U}^l+\delta\mathcal{U})\simeq\mathcal{R}(\mathcal{U}^l)+\left(\frac{\partial\mathcal{R}(\mathcal{U}^l)}{\partial\mathcal{U}}\right)\delta\mathcal{U}$$

- **The Newton's method assuming invertible Jacobian**

$$\mathcal{U}^{l+1}=\mathcal{U}^l-\omega_l\left(\frac{\partial\mathcal{R}(\mathcal{U}^l)}{\partial\mathcal{U}}\right)^{-1}\mathcal{R}(\mathcal{U}^l)$$

Adaptive discrete Newton's method

The Jacobian matrix in discrete Newton is calculated using the finite difference

$$\left[\frac{\partial \mathcal{R}(\mathcal{U}^l)}{\partial \mathcal{U}}\right]_{ij} \approx \frac{\mathcal{R}_i(\mathcal{U}^l + \varepsilon_l \boldsymbol{e}_j) - \mathcal{R}_i(\mathcal{U}^l - \varepsilon_l \boldsymbol{e}_j)}{2\varepsilon_l}$$

- **Damping of the updated solution,** $\omega_l \in (0,1)$ **, s.t.**

$$\|\mathcal{R}(\mathcal{U}^{l+1})\| \leq \|\mathcal{R}(\mathcal{U}^l)\|$$

! Not sufficient for TVP problem

- **Operator-adaptive splitting**

$$\left(\frac{\partial \mathcal{R}(\mathcal{U}^l)}{\partial\, \mathcal{U}}\right) = \left(\frac{\partial \tilde{\mathcal{R}}(\mathcal{U})}{\partial \mathcal{U}}\right) + \delta_l \left(\frac{\partial \hat{\mathcal{R}}(\mathcal{U})}{\partial \mathcal{U}}\right)$$

$$\delta_{l+1} = f(r_l)\delta_l,\ \ r_l := \|\mathcal{R}(\mathcal{U}^l)\| / \|\mathcal{R}(\mathcal{U}^{l-1})\|,\ \ f(r_l) = 0.2 + 4/(0.7 + e^{1.5 r_l})$$

! Requires a priori analysis of the Jacobian

- **Adaptive step-length control**

$$\varepsilon_{l+1} = g(r_l)\varepsilon_l,\ \ g(r_l) = 1/f(r_l)$$

! Robust

Convergence analysis of the <u>method</u> !

Monolithic Multigrid solver

The discretization and linearization of TVP leads to systems of following linearized discrete TVP saddle point problem

$$\left(\frac{\partial \mathcal{R}(\mathcal{U})}{\partial \mathcal{U}}\right)\delta\mathcal{U} = \begin{pmatrix} \frac{\partial \mathcal{R}_{\tilde{\boldsymbol{u}}}(\tilde{\boldsymbol{u}})}{\partial \tilde{\boldsymbol{u}}} & \frac{\partial \mathcal{R}_{\tilde{\boldsymbol{u}}}(\tilde{\boldsymbol{u}})}{\partial p} \\ \frac{\partial \mathcal{R}_{p}(\tilde{\boldsymbol{u}})}{\partial \tilde{\boldsymbol{u}}} & 0 \end{pmatrix} \begin{pmatrix} \delta\tilde{\boldsymbol{u}} \\ \delta p \end{pmatrix} = -\begin{pmatrix} \mathcal{R}_{\tilde{\boldsymbol{u}}} \\ \mathcal{R}_{p} \end{pmatrix}.$$

- **Coupled geometric multigrid methods CGMG**
  - **Hierarchy of multilevel triangulations**
  - **Relaxation/smoothing**
  - **Coarse-grid correction**
  - **Grid transfer operator**
  - **Local Multilevel Pressure Schur Complement**

- **Setting local subproblem,**
  - **Prolongation/Restriction:** $\mathcal{P}_K = (\mathcal{P}_K^{\tilde{\boldsymbol{u}}}, \mathcal{P}_K^p),\ \mathcal{P}_K^{\mathrm{T}} = (\mathcal{P}_K^{\tilde{\boldsymbol{u}}\,\mathrm{T}}, \mathcal{P}_K^{p\,\mathrm{T}})$

$$\mathcal{P}_K^{\tilde{\boldsymbol{u}}} : \mathbb{W}_h(K) \longrightarrow \mathbb{W}_h,\ \mathcal{P}_K^p : \mathbb{Q}_h(K) \longrightarrow \mathbb{Q}_h, \quad \forall\, K \in \mathcal{T}_h,$$

$$\mathcal{P}_K^{\tilde{\boldsymbol{u}}\,\mathrm{T}} : \mathbb{W}_h \longrightarrow \mathbb{W}_h(K),\ \mathcal{P}_K^{p\,\mathrm{T}} : \mathbb{Q}_h \longrightarrow \mathbb{Q}_h(K), \quad \forall\, K \in \mathcal{T}_h,$$

- **Algebraically counterpart**
  - **Prolongation/Restriction:** $\boldsymbol{\mathcal{P}}_K = (\boldsymbol{\mathcal{P}}_K^{\tilde{\boldsymbol{u}}}, \boldsymbol{\mathcal{P}}_K^p),\ \boldsymbol{\mathcal{P}}_K^{\mathrm{T}} = (\boldsymbol{\mathcal{P}}_K^{\tilde{\boldsymbol{u}}\,\mathrm{T}}, \boldsymbol{\mathcal{P}}_K^{p\,\mathrm{T}})$

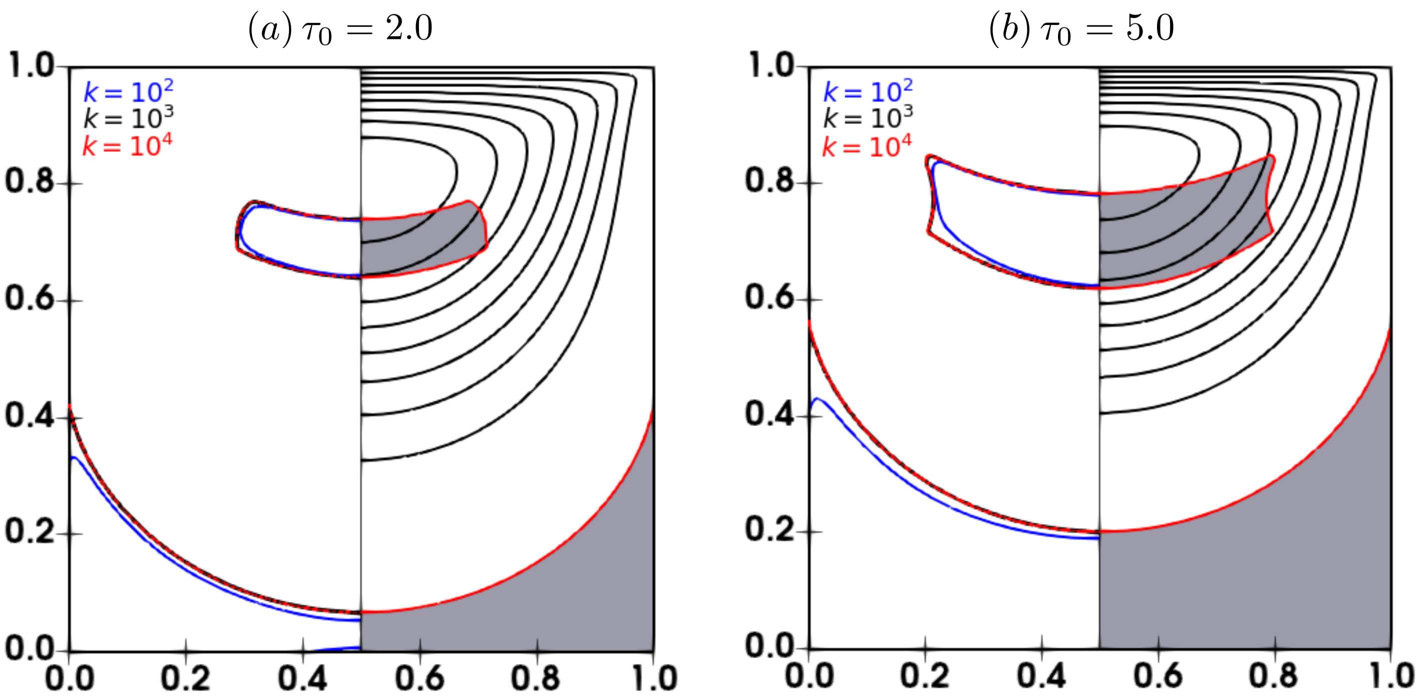
$$\begin{aligned} \mathcal{U}_K &= (\tilde{\boldsymbol{u}}_K, p_K) := \boldsymbol{\mathcal{P}}_K^{\mathrm{T}} \mathcal{U} = (\boldsymbol{\mathcal{P}}_K^{\tilde{\boldsymbol{u}}\,\mathrm{T}} \tilde{\boldsymbol{u}}, \boldsymbol{\mathcal{P}}_K^{p\,\mathrm{T}} p) \\ \mathcal{U} &= (\tilde{\boldsymbol{u}}, p) := \sum_{K \in \mathcal{T}_h} \boldsymbol{\mathcal{P}}_K \mathcal{U}_K = \sum_{K \in \mathcal{T}_h} (\boldsymbol{\mathcal{P}}_K^{\tilde{\boldsymbol{u}}} \tilde{\boldsymbol{u}}, \boldsymbol{\mathcal{P}}_K^p p) \end{aligned}$$

- **Block Gauss-Seidel iteration reads**

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

Coupled Monolithic Multigrid Solver !

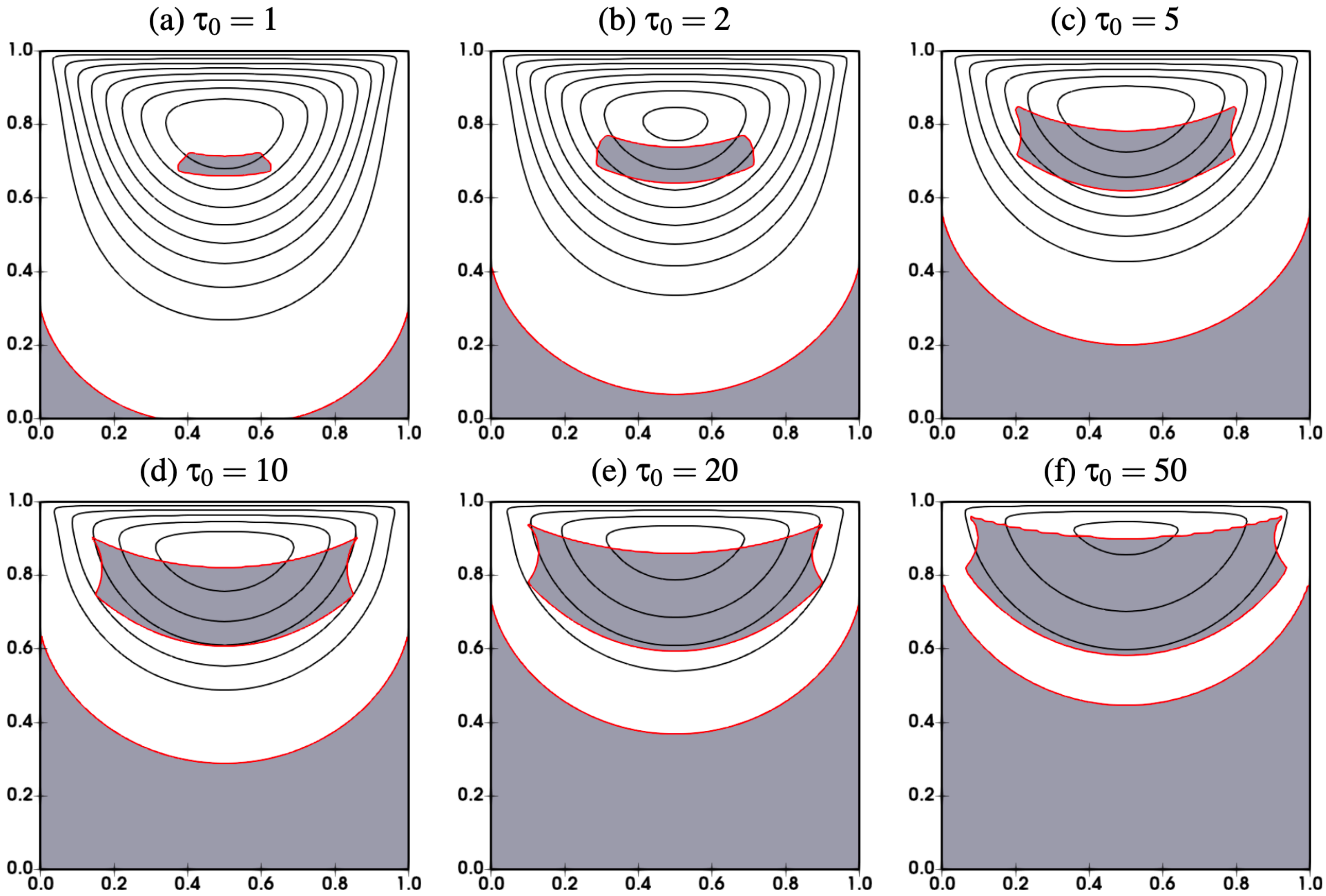
- **Boundary limit for rigid-zone w.r.t regularization k**



- **Accurate track of interface requires**
  - ✓ **larger k solutions**
  - ✓ **finer mesh refinement**
- **Existence of pair (k, L) beyond which no further improvement in solutions is expected**

Viscoplastic flow in Lid-driven cavity

- **progressive growth of unyielded zones for non-thixotropic (Bingham Plastic) flow**



✓ **Unyielded zones's shape and extent is in agreement with Ref. Results**

- **Solver behaviour w.r.t Regulariztaion and mesh refinement**

$k\backslash L$	5	6	7	5	6	7	5	6	7
	$\tau_0 = 1.0$			$\tau_0 = 2.0$			$\tau_0 = 5.0$		
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
	$\tau_0 = 10.0$			$\tau_0 = 20.0$			$\tau_0 = 50.0$		
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

✓ **Efficient non-linear solver**

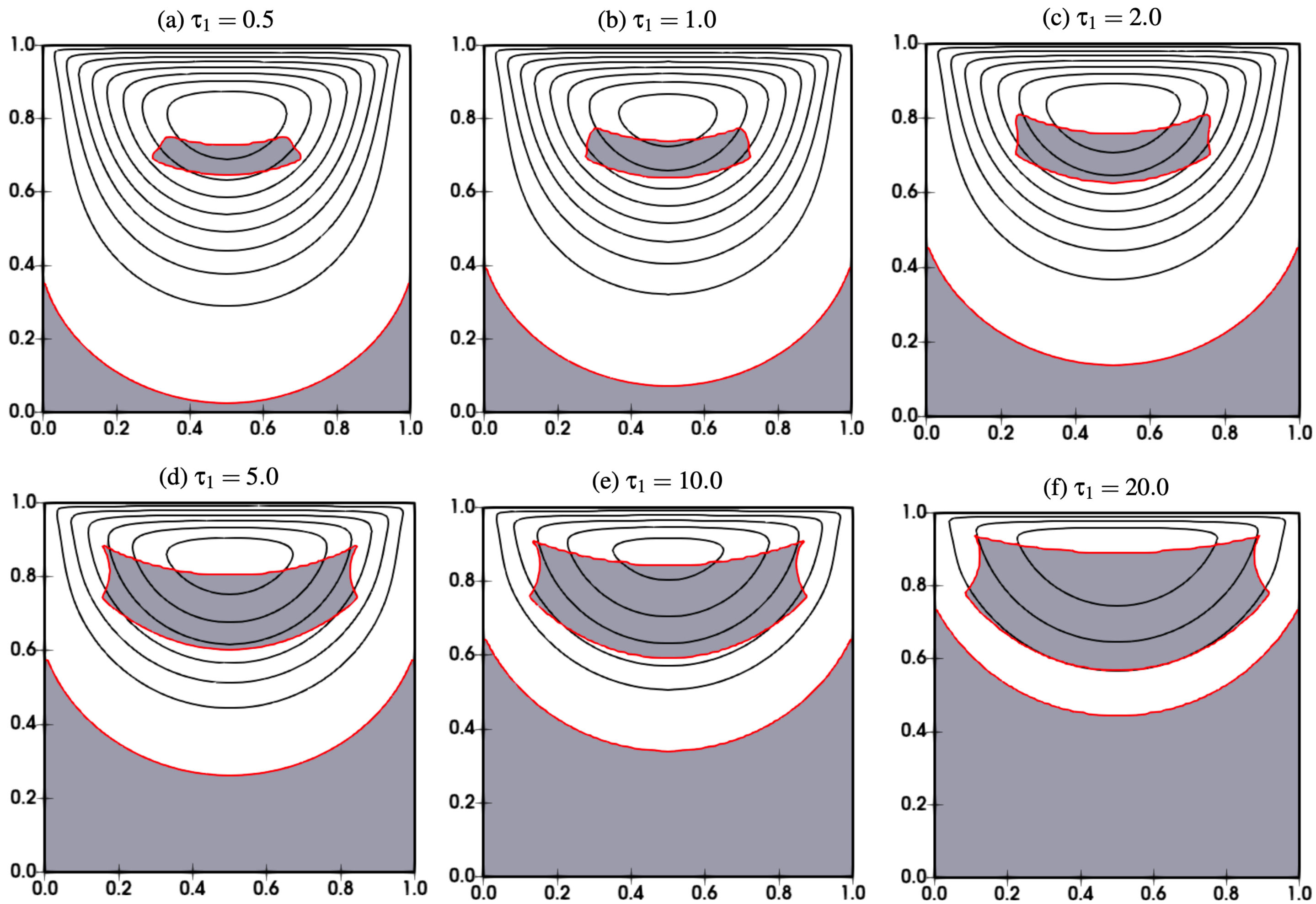
✓ **Mesh independent linear solver**

✓ **Solutions are obtained with continuation strategy w.r.t. k**

➡ **Integration of continuation strategy w.r.t. k in the solver**

Thixo-viscoplastic flow in Lid-driven cavity

- **Impact of thixotropic yield stress on morphology of unyielded zones in TVP flow**



✓ **Main rheological characteristics of materials with yield stress is preserved** technische universität dortmund

- **Solver behaviour w.r.t Regulariztaion and mesh refinement**

$k\backslash L$	5	6	7	5	6	7	5	6	7
	$\tau_1 = 0.5$			$\tau_1 = 1.0$			$\tau_1 = 2.0$		
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

✓ **Robust non-linear solver**

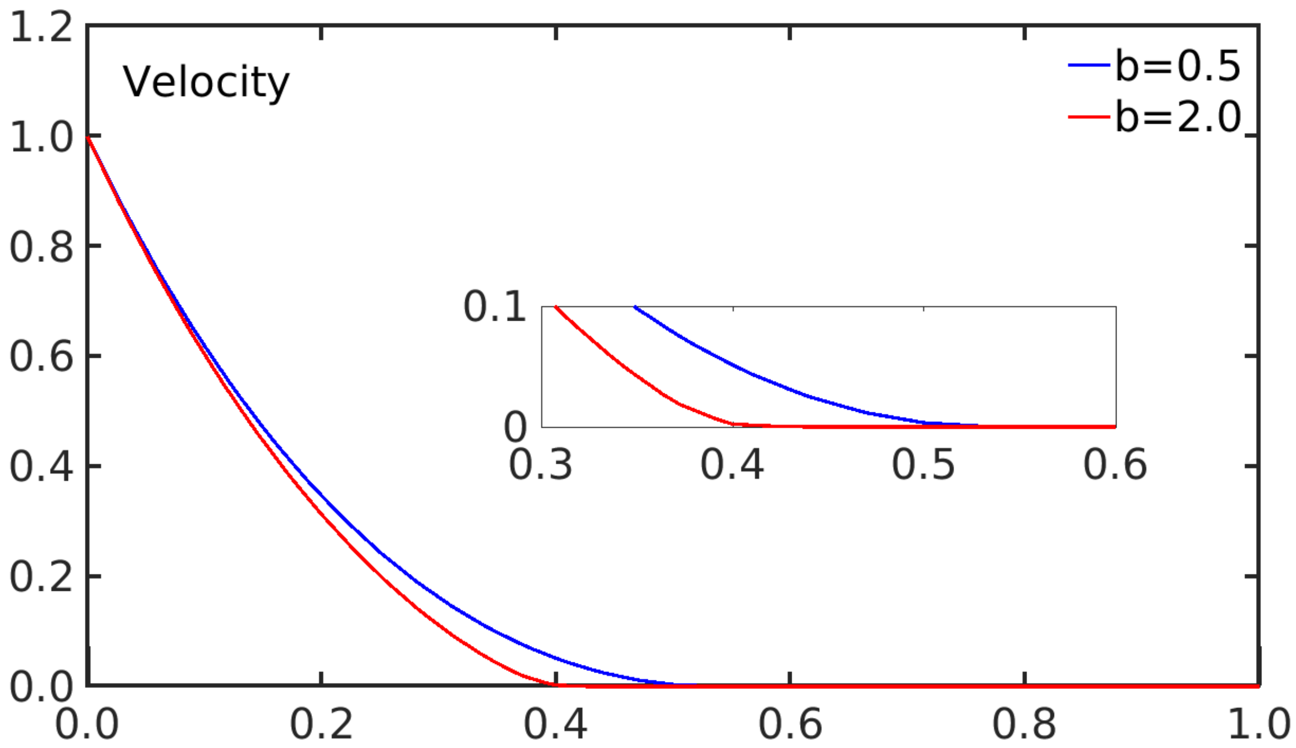
✓ **Mesh independent linear solver**

✓ **Solutions are obtained via continuation strategy w.r.t.** k

➡ **Integration of continuation strategy w.r.t.** k **in the solver**

Thixo-viscoplastic flow in Couette

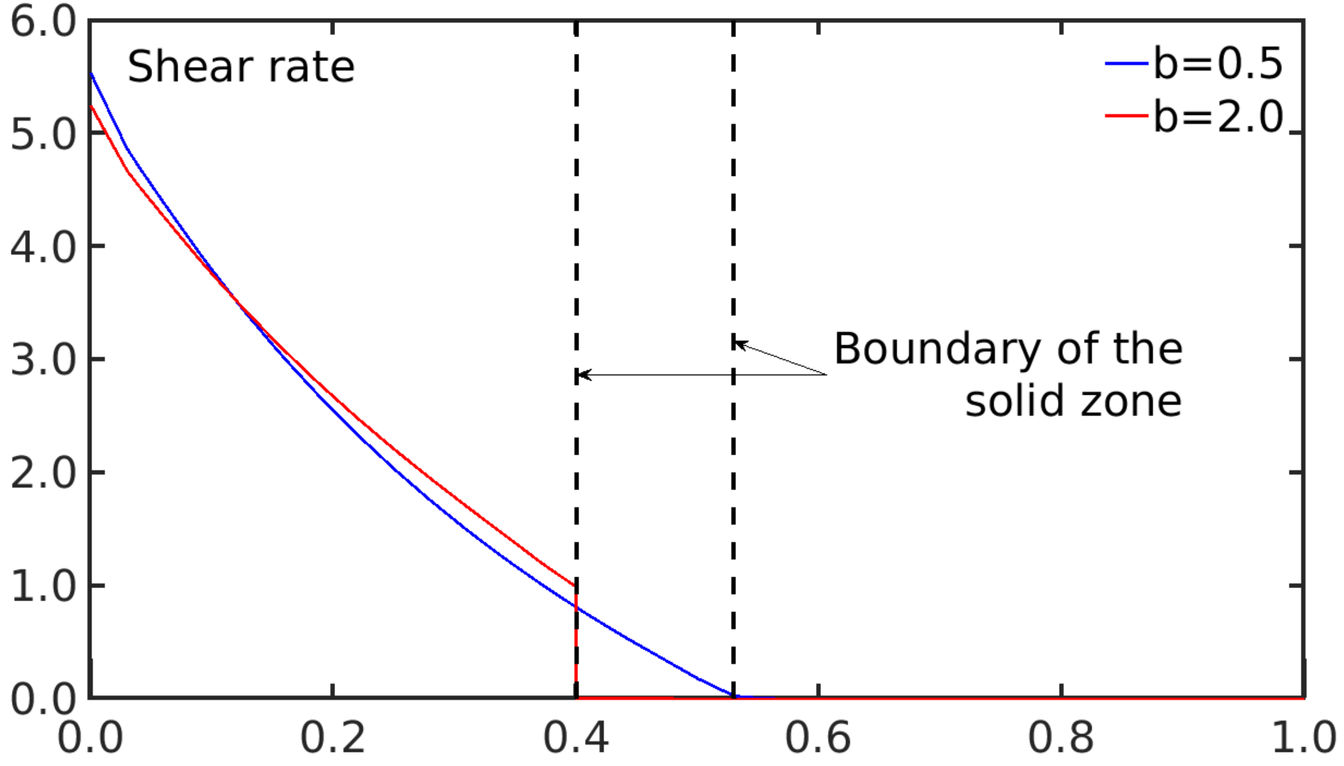
- **Velocity profile at cut-line positions $c; c \in [0, 2\pi]$ in a Couette device w.r.t breakdown parameter**



✓ **Localization**
✓ **Shear banding**

Thixo-viscoplastic flow in Couette

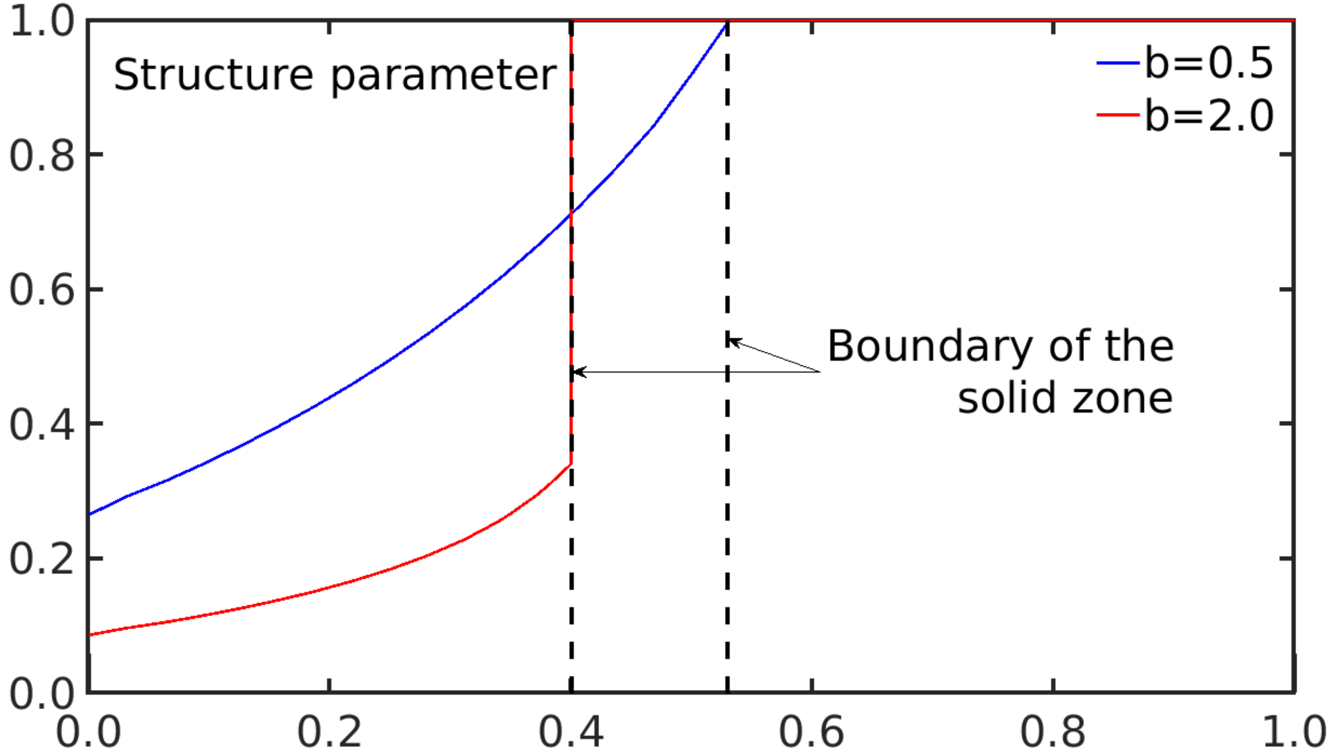
- **Shear rate at cut-line positions $c; c \in [0, 2\pi]$ in a Couette device w.r.t breakdown parameter**



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

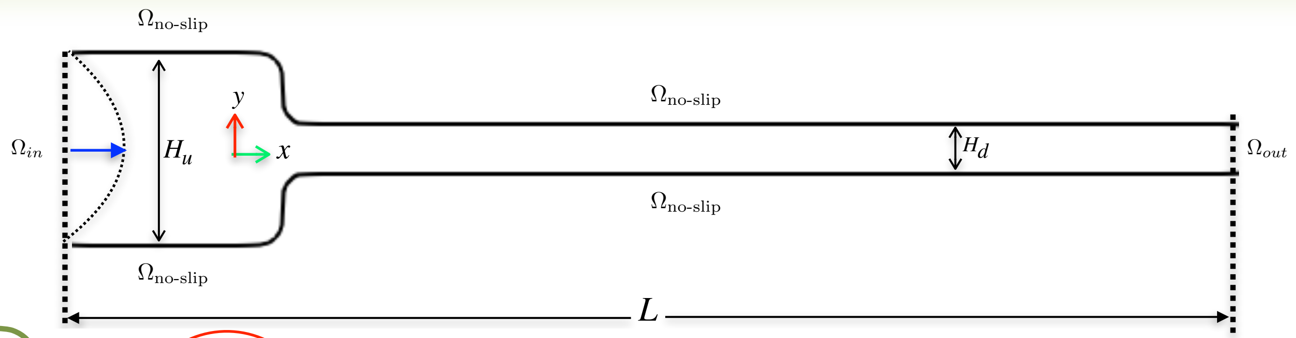
Thixo-viscoplastic flow in Couette

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

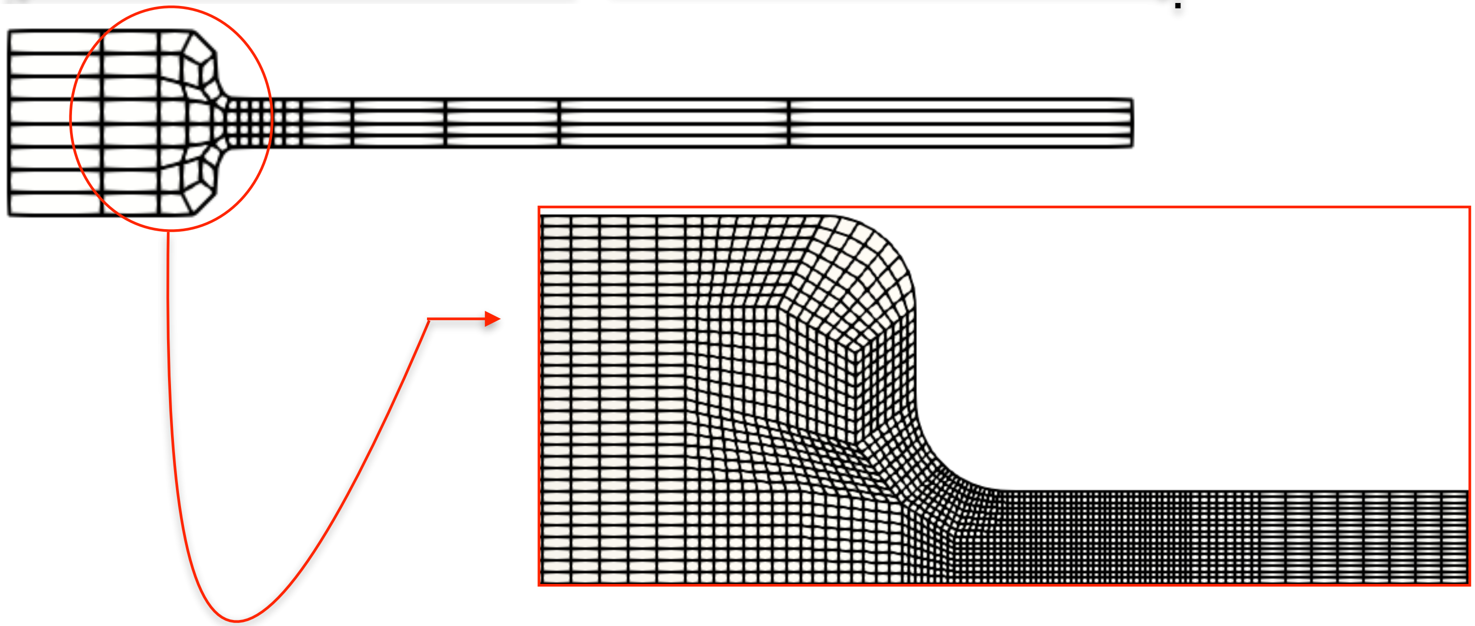


✓ **Transition point matches with the velocity**
✓ **Structuring level is predicting shape and extent of rigid zones**

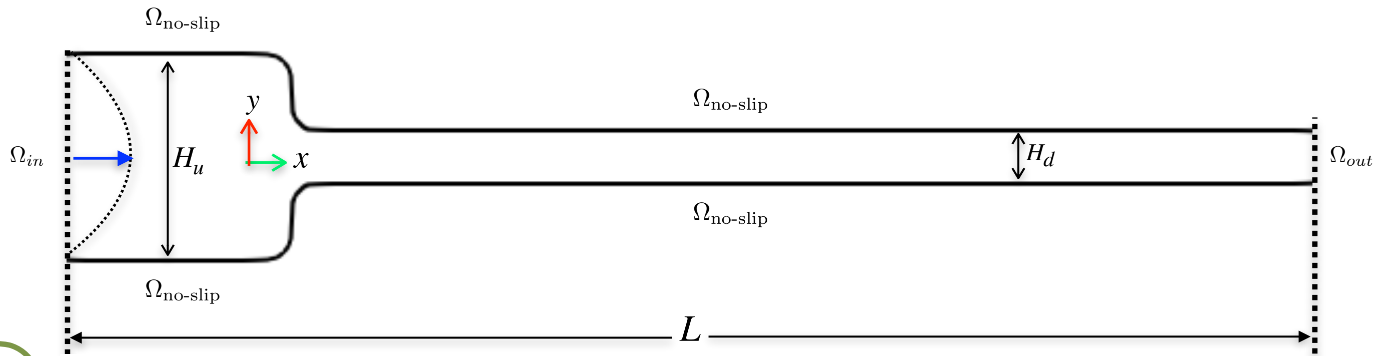
- **2D-FEM simulation results for thixo-viscoplastic flow- validation of 1D tool**
- **Specifying the "unidirectional profiles as boundary Data" in 2D for contraction**



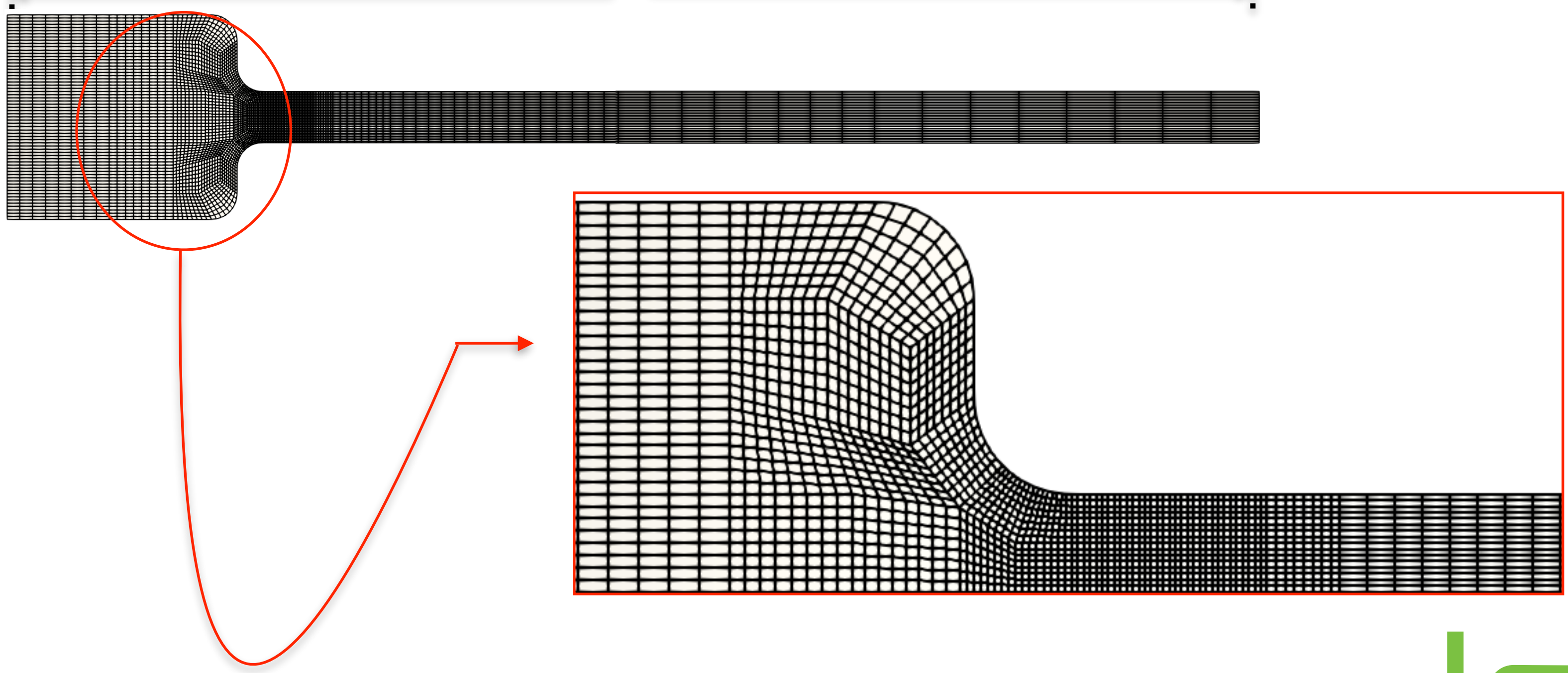
Coarse Mesh



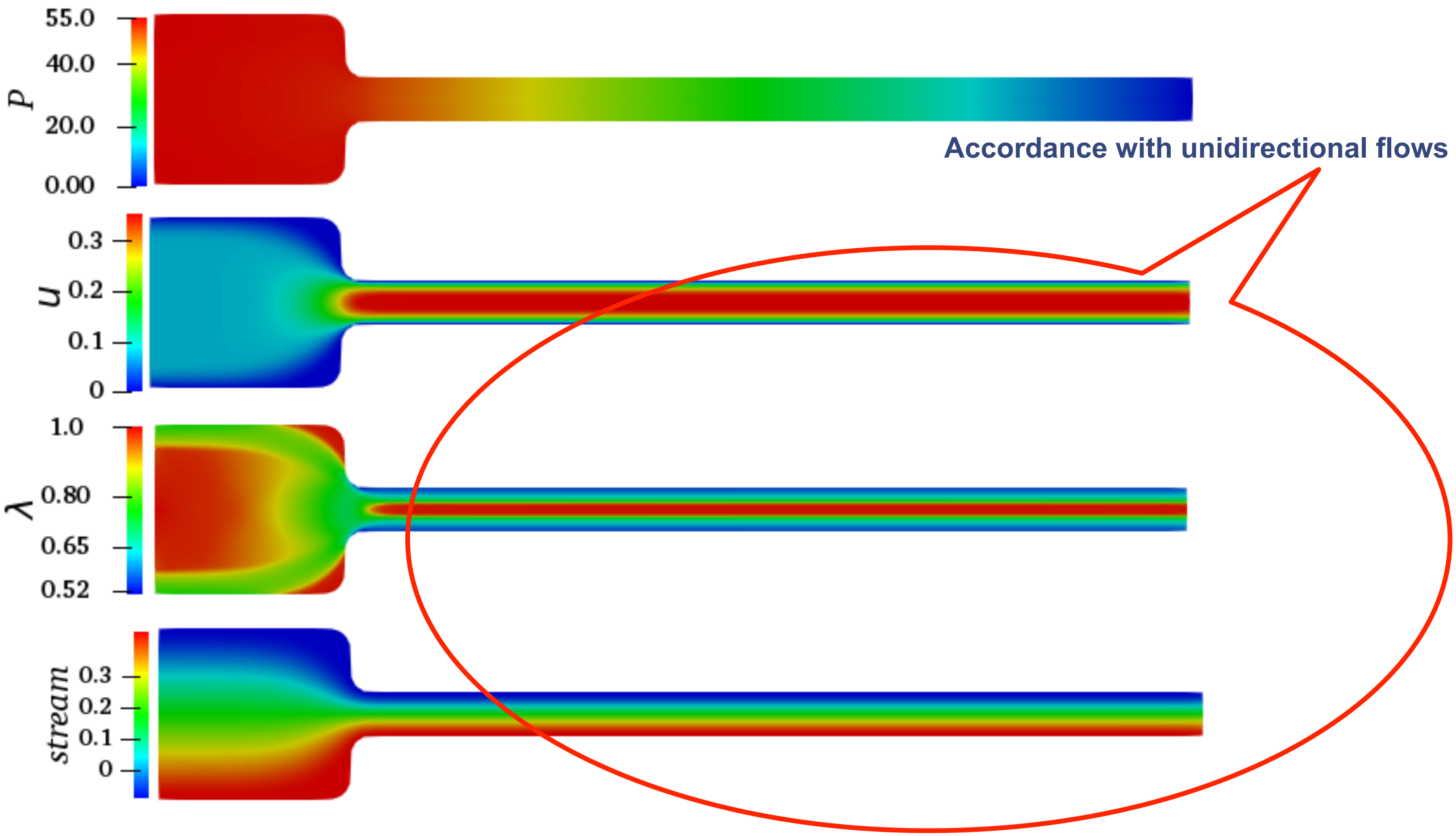
- **2D-FEM simulation results for thixotrpic flow- validation of 1D tool**
- **Specifying the “1D-profiles as boundary Data” in 2D simulations for contraction domain**



Computational Mesh



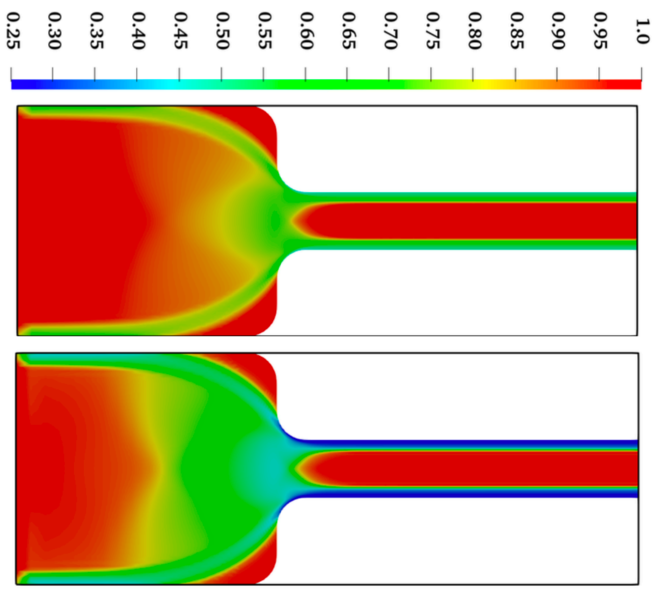
Contraction flow (smoothed)



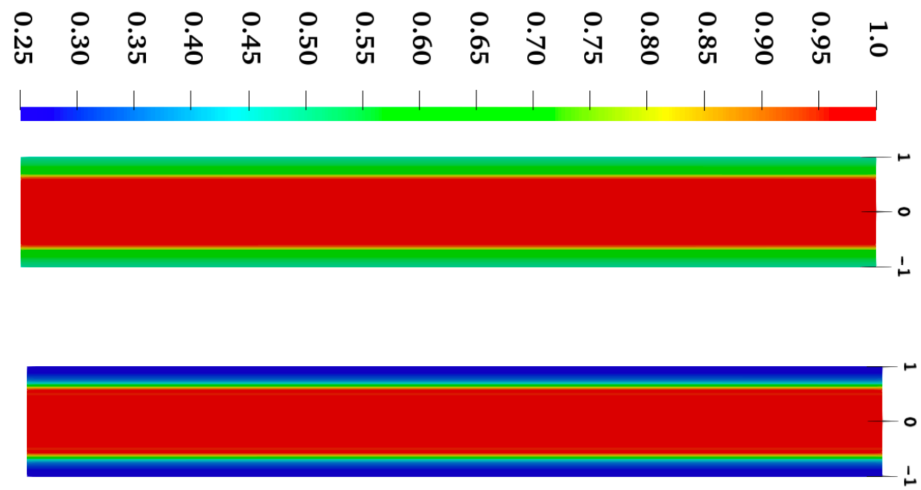
- ✓ As predicted (u, λ, p) solutions
- ✓ Structuring level is predicting shape and extent of rigid zones

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

(i) Upstream channel & Entrance zone



(ii) Downstream channel



- **Inherent thixotropy speed-up the breakdown**
  - ✓ **Appearance of more breakdown layers**
  - ✓ **Applications: restart pressure in pipelines should not be over-estimated**

Summary

We analysed FEM for regularized TVP problem

- ✓ **Wellposedness**
- ✓ **Convergence analysis**

Analyzed the accuracy, robustness, and efficiency of the TVP solver using

- ✓ **Higher order finite element method**
- ✓ **Monolithic Newton-multigrid**
  - **Adaptive discrete Newton's method with global convergent property**
  - **Geometric multigrid with local MPSC**

Simulations for TVP materials for Benchmarks in Lid-driven cavity, Couette devices and 4:1 contraction configuration

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