Numerical simulation of yield stress fluid flows

Master's thesis

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Promotor: Jean-François Remacle

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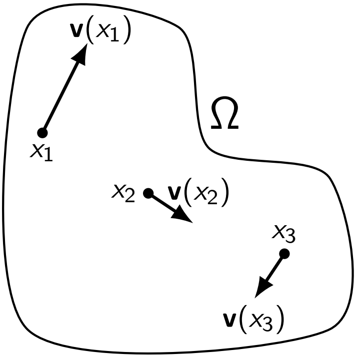
- Domain Ω
- Position vector $\mathbf{x} \in \Omega$
- Velocity field $\mathbf{v}(\mathbf{x})$
- Fluid undergoes stress $\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau}$
- Need to relate $\boldsymbol{\tau}$ to $\mathbf{v}$



Velocity modes

$$\nabla \mathbf{v} = \mathbf{D}_s + \mathbf{D}_d + \mathbf{W}$$

(a) expansion (b) shear (c) rotation

Velocity modes

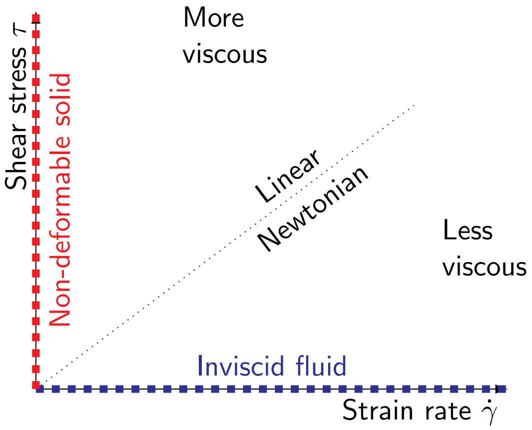
$$\nabla \mathbf{v} = \mathbf{D}_s + \mathbf{D}_d + \mathbf{W}$$
$$\boldsymbol{\tau} = \mu \, 2\mathbf{D}_d \qquad \text{(Newtonian fluids)}$$

(a) expansion

(b) shear

(c) rotation

Flow curve


More
viscous
Shear stress τ
Non-deformable solid
Linear
Newtonian
Less
viscous
Inviscid fluid
Strain rate $\dot{\gamma}$

Non-Newtonian fluids

- Generalized Newtonian model

$$\boldsymbol{\tau} = \mu(\dot{\gamma}, T)\,\dot{\boldsymbol{\gamma}} \qquad \text{where} \quad \begin{cases} \dot{\boldsymbol{\gamma}} = 2\mathbf{D} = \nabla\mathbf{v} + \nabla\mathbf{v}^\top \\ \dot{\gamma} = \|\dot{\boldsymbol{\gamma}}\|_F = \sqrt{\mathrm{Tr}(\dot{\boldsymbol{\gamma}} \cdot \dot{\boldsymbol{\gamma}})} \end{cases}$$

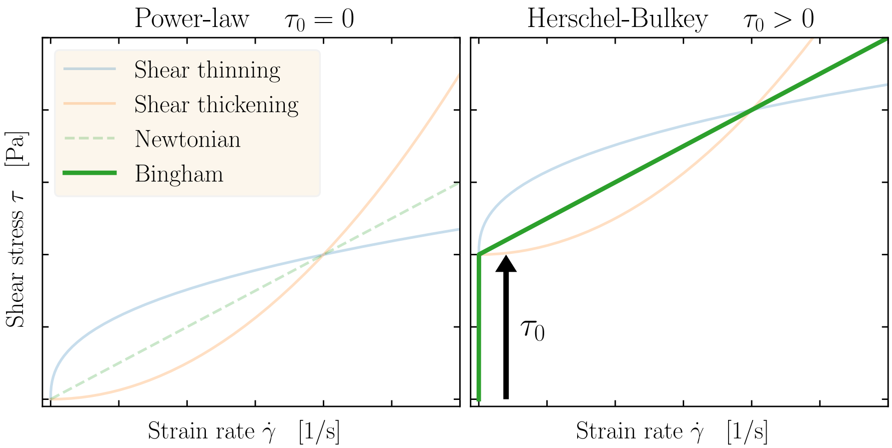
- Power-law model

$$\boldsymbol{\tau} = (K\dot{\gamma}^n)\,\dot{\boldsymbol{\gamma}}$$

- Herschel-Bulkley model (Bingham with $n = 1$)

$$\begin{aligned} &\dot{\boldsymbol{\gamma}} = 0 && \text{if} \quad \tau < \tau_0 \\ &\boldsymbol{\tau} = \left(K\dot{\gamma}^{n-1} + \frac{\tau_0}{\dot{\gamma}}\right)\dot{\boldsymbol{\gamma}} && \text{if} \quad \tau \geq \tau_0 \end{aligned}$$

Non-Newtonian fluids



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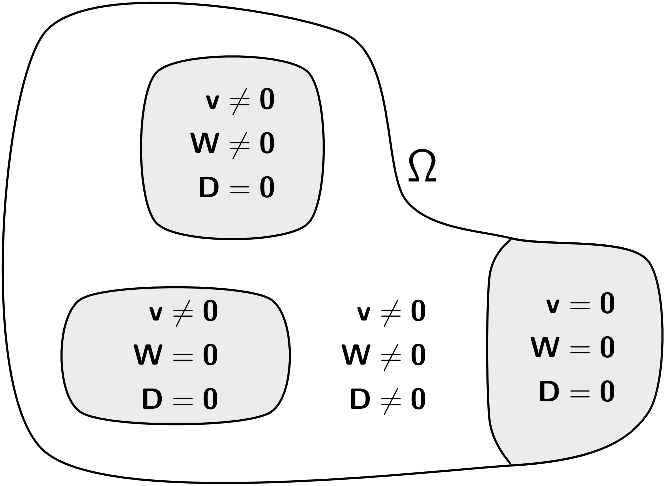
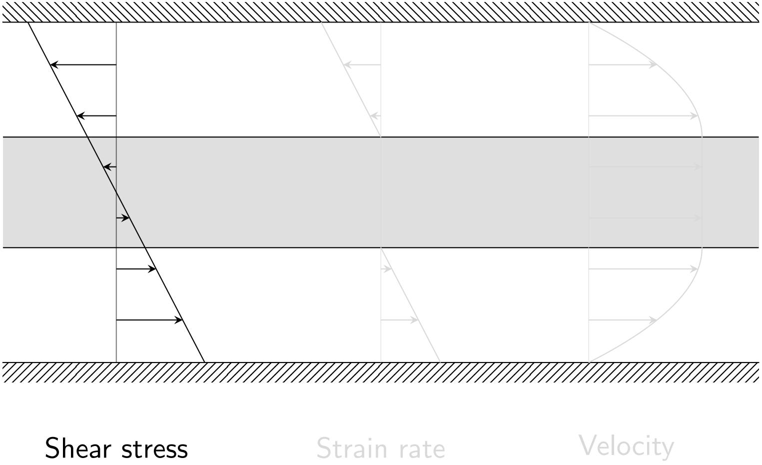
Solid-Liquid subdomains



Interface tracking

1. Simulate Flow
2. Locate interface(s)
3. Deform the mesh (X-MESH)
4. Repeat until convergence

Interface tracking benefits - Poiseuille flow



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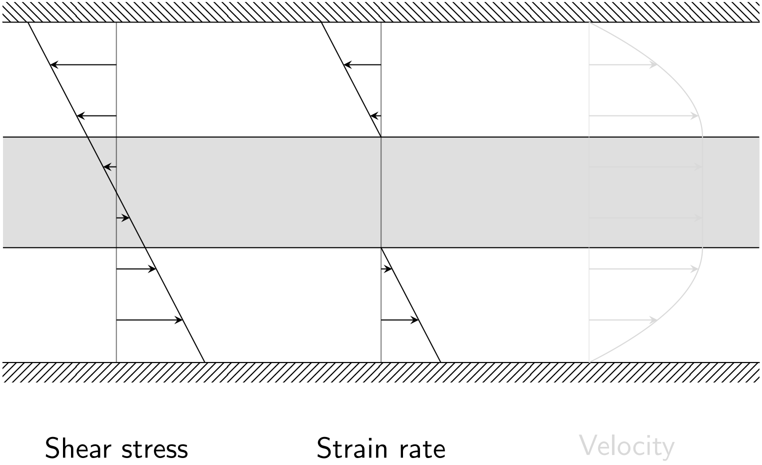

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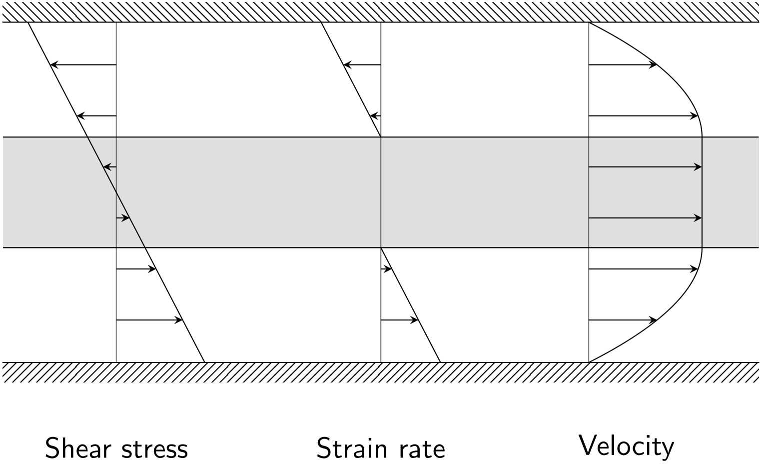

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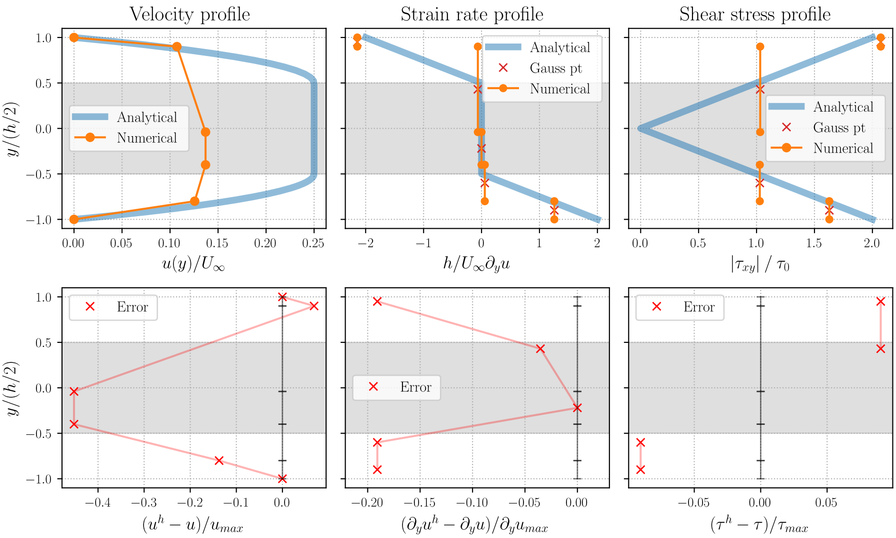
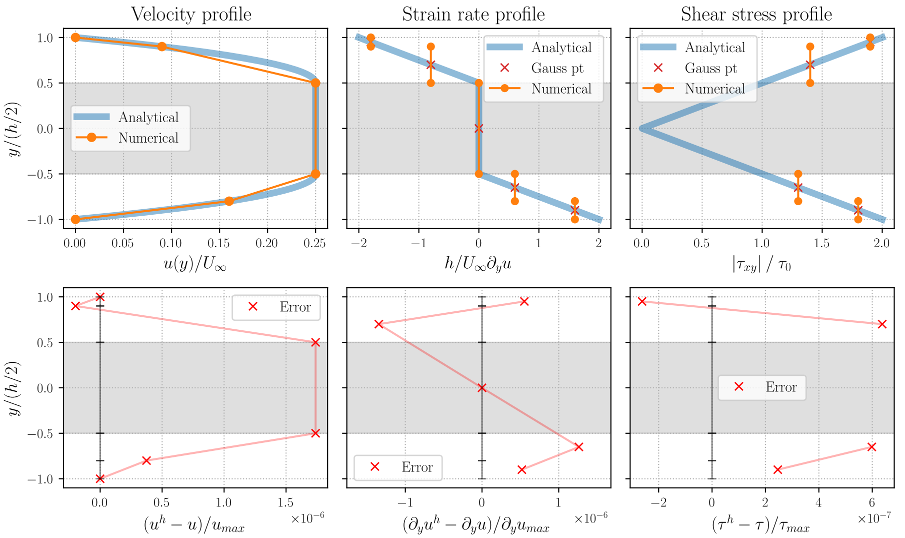


Interface tracking benefits - Poiseuille flow



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Equations

- Conservation laws for incompressible fluids:

$$\nabla \cdot \mathbf{v} = 0 \qquad \text{in } \Omega$$

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{f} \qquad \text{in } \Omega$$

- Constitutive law

$$\dot{\gamma} = 0 \qquad \text{if} \quad \tau < \tau_0$$

$$\boldsymbol{\tau} = (K + \tau_0 / \dot{\gamma})\, \dot{\boldsymbol{\gamma}} \qquad \text{if} \quad \tau \geq \tau_0$$

- Boundary conditions

$$\mathbf{v} = \mathbf{U} \qquad \text{on } \partial\Omega_D$$

$$\hat{\mathbf{n}} \cdot \boldsymbol{\sigma} = \mathbf{g} \qquad \text{on } \partial\Omega_N$$

Equations

- Conservation laws for incompressible fluids, with low Reynolds:

$$\begin{aligned} \nabla \cdot \mathbf{v} &= 0 && \text{in } \Omega \\ 0 &= -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{f} && \text{in } \Omega \end{aligned}$$

- Constitutive law

$$\begin{aligned} \dot{\boldsymbol{\gamma}} &= 0 && \text{if} \quad \tau < \tau_0 \\ \boldsymbol{\tau} &= (K + \tau_0/\dot{\gamma})\,\dot{\boldsymbol{\gamma}} && \text{if} \quad \tau \geq \tau_0 \end{aligned}$$

- Boundary conditions

$$\begin{aligned} \mathbf{v} &= \mathbf{U} && \text{on } \partial\Omega_D \\ \hat{\mathbf{n}} \cdot \boldsymbol{\sigma} &= \mathbf{g} && \text{on } \partial\Omega_N \end{aligned}$$

Equations

- Conservation laws for incompressible fluids:

$$\begin{aligned} \nabla \cdot \mathbf{v} &= 0 && \text{in } \Omega \\ 0 &= -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{f} && \text{in } \Omega \end{aligned}$$

- Constitutive law

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- Boundary conditions

$$\begin{aligned} \mathbf{v} &= \mathbf{U} && \text{on } \partial\Omega_D \\ \hat{\mathbf{n}} \cdot \boldsymbol{\sigma} &= \mathbf{g} && \text{on } \partial\Omega_N \end{aligned}$$

Energy functional

System of PDE's is equivalent to

$$\mathbf{v} = \arg\min_{\mathbf{u}\in\mathcal{V}} \mathcal{J}(\mathbf{u})$$

$$\mathcal{V} = \left\{ \mathbf{u} \in H^1(\Omega)^d \;\middle|\; \int_\Omega q \nabla \cdot \mathbf{u} = 0 \;\; \forall q \in L^2(\Omega),\; \mathbf{u} = \mathbf{U} \text{ on } \partial\Omega_D \right\}$$

$$\mathcal{J}(\mathbf{u}) = \overbrace{\frac{K}{2} \int_\Omega \|\dot{\gamma}(\mathbf{u})\|^2 \,\mathrm{d}x}^{\text{Viscous}} + \overbrace{\tau_0 \int_\Omega \|\dot{\gamma}(\mathbf{u})\| \,\mathrm{d}x}^{\text{Yield}} - \underbrace{\int_\Omega \mathbf{f} \cdot \mathbf{u} \,\mathrm{d}x}_{\text{Body forces}} - \underbrace{\int_{\partial\Omega_N} \mathbf{g} \cdot \mathbf{u} \,\mathrm{d}s}_{\text{Boundary forces}}$$

Choice of element

Discretize velocity-pressure fields, over a mesh of triangles, with either:

- Mini element: $(\mathcal{P}_1^C \oplus \mathcal{B}_3) - \mathcal{P}_1^C$
- Taylor-Hood element: $\mathcal{P}_2^C - \mathcal{P}_1^C$

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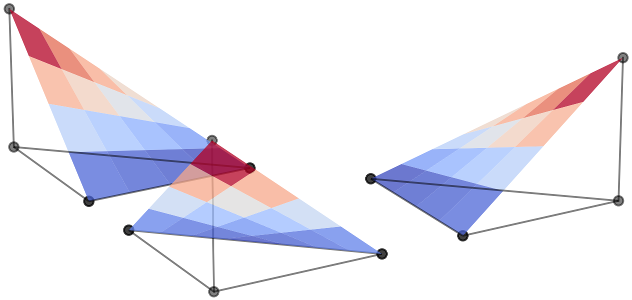

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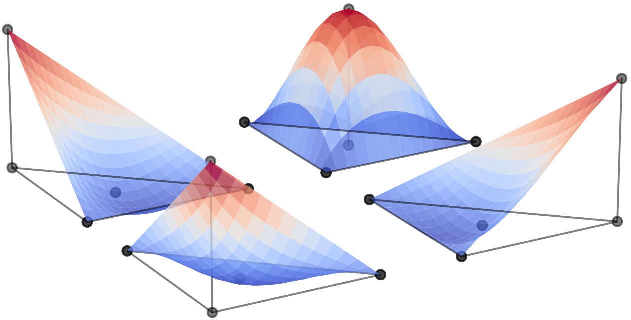

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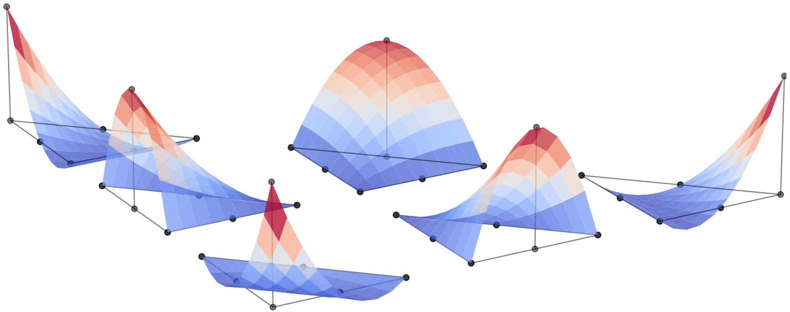


Finite element approximation

- Finite element approximation:

$$\mathbf{v}^h(\mathbf{x}) = \sum_{\text{nodes } j} \mathbf{V}_j \phi_j(\mathbf{x})$$

- Discrete functional:

$$\mathcal{J}(\mathbf{v}^h) = \sum_i \sum_g \omega_g \left[\frac{K}{2} \overbrace{\|\dot{\boldsymbol{\gamma}}(\mathbf{v}^h)\|^2}^{\leq S_{i,g}} + \tau_0 \overbrace{\|\dot{\boldsymbol{\gamma}}(\mathbf{v}^h)\|}^{\leq T_{i,g}} - \mathbf{f} \cdot \mathbf{v}^h \right] \det \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\boldsymbol{\xi}}_{i,g}$$
$$- \sum_e \sum_g \tilde{\omega}_g \, \mathbf{g} \cdot \mathbf{v}^h \, \det \frac{\mathrm{d}\tilde{\mathbf{x}}}{\mathrm{d}\tilde{\xi}}_{e,g}$$

Finite element approximation

- Finite element approximation:

$$\mathbf{v}^h(\mathbf{x}) = \sum_{\text{nodes } j} \mathbf{V}_j \phi_j(\mathbf{x})$$

- Discrete functional, with additional variables $S_{i,g}$ and $T_{i,g}$:

$$\mathcal{J}(\mathbf{v}^h) = \sum_i \sum_g \omega_g \left[\frac{K}{2} \overbrace{\|\dot{\gamma}(\mathbf{v}^h)\|^2}^{\leq S_{i,g}} + \tau_0 \overbrace{\|\dot{\gamma}(\mathbf{v}^h)\|}^{\leq T_{i,g}} - \mathbf{f} \cdot \mathbf{v}^h \right] \det \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\boldsymbol{\xi}}_{i,g}$$
$$- \sum_e \sum_g \tilde{\omega}_g \, \mathbf{g} \cdot \mathbf{v}^h \, \det \frac{\mathrm{d}\tilde{\mathbf{x}}}{\mathrm{d}\tilde{\xi}}_{e,g}$$

Objective and constraints

$$\underset{\mathbf{V}_j, S_{i,g}, T_{i,g}}{\text{minimize}} \quad \sum_{i,g} \omega_g \left[\frac{K}{2} S_{i,g} + \tau_0 T_{i,g} - \mathbf{f} \cdot \mathbf{v}^h \right] \det \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\boldsymbol{\xi}}_{i,g} - \sum_{e,g} \tilde{\omega}_g \, \mathbf{g} \cdot \mathbf{v}^h \det \frac{\mathrm{d}\tilde{\mathbf{x}}}{\mathrm{d}\tilde{\xi}}_{e,g}$$

$$\text{such that} \quad S_{i,g} \geq (2\partial_x u^h)^2 + (2\partial_y v^h)^2 + (\partial_y u^h + \partial_x v^h)^2 \qquad \forall i, g$$

$$T_{i,g} \geq \sqrt{(2\partial_x u^h)^2 + (2\partial_y v^h)^2 + (\partial_y u^h + \partial_x v^h)^2} \qquad \forall i, g$$

$$0 = \sum_{i,g} \omega_g \psi_I|_{\mathbf{x}_g} \left(\partial_x u^h + \partial_y v^h \right) \det \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\boldsymbol{\xi}}_{i,g} \qquad \forall \ I$$

$$\mathbf{V}_j = \mathbf{U} \qquad \forall \ j \in \partial\Omega_D$$

Reformulation for conic optimization

$$
\begin{aligned}
\underset{\mathbf{V}_j, S_{i,g}, T_{i,g}}{\text{minimize}} \quad & \sum_{i,g} \omega_g \left[\frac{K}{2} S_{i,g} + \tau_0 T_{i,g} - \mathbf{f} \cdot \mathbf{v}^h \right] \det \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\boldsymbol{\xi}}_{i,g} - \sum_{e,g} \tilde{\omega}_g \, \mathbf{g} \cdot \mathbf{v}^h \det \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\boldsymbol{\xi}}_{e,g} \\
\text{such that} \quad & 0 \preceq_{L_R^5} \left(S_{i,g}, \frac{1}{2}, \sqrt{2}\partial_x u^h, \sqrt{2}\partial_y v^h, \partial_y u^h + \partial_x v^h \right) && \forall i, g \\
& 0 \preceq_{L^4} \left(T_{i,g}, \sqrt{2}\partial_x u^h, \sqrt{2}\partial_y v^h, \partial_y u^h + \partial_x v^h \right) && \forall i, g \\
& 0 = \sum_i \sum_g \omega_g \psi_l |_{\mathbf{x}_g} \left(\partial_x u^h + \partial_y v^h \right) \det \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\boldsymbol{\xi}}_{i,g} && \forall \, l \\
& \mathbf{V}_j = \mathbf{U} && \forall \, j \in \partial\Omega_D
\end{aligned}
$$

Conic solver

Conic optimization problem:

- Objective is linear in variables U_j, V_j, $S_{i,g}$, $T_{i,g}$
- Equality constraints are linear
- Inequality constraints are cones

Can find the optimum with an interior-point method:

- Encode each constraint with barrier g_n
- Minimize a modified functional $\mathcal{J} + \mu \sum g_n$
- Alternatively:
  - perform Newton iterations (stay optimal)
  - and decrease $\mu \to 0$ (minimize $\mathcal{J}$ only)
- Cones provide special barriers (self-concordant)
- Solution obtained with Newton–Raphson method, within accuracy ϵ, after $\mathcal{O}(\sqrt{\nu} \log \frac{1}{\epsilon})$ iterations, where $\nu \propto$ number of variables

Interior-point solver example

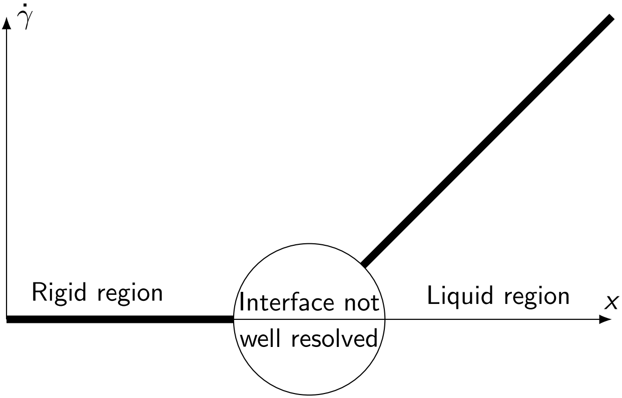
Minimize x with linear inequalities over x and y

Interface tracking

Once we have the velocity field, minimum of $\mathcal{J}$:

1. Estimate the interface position based on the strain rate field $\dot{\boldsymbol{\gamma}}(\mathbf{v}^h)$
   - Not trivial, as it is not a level set of $\dot{\gamma}$
2. Move the nodes of the mesh towards the interface estimation
   - X-MESH algorithm allowing extreme deformations of the mesh

Locating the interface



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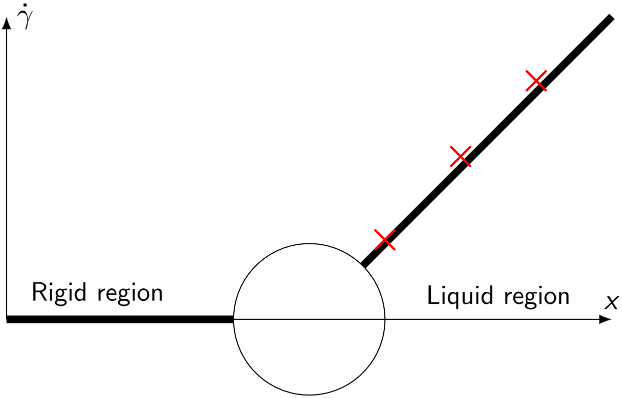

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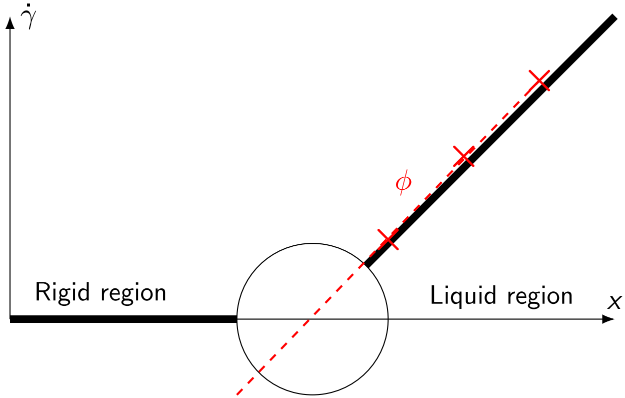
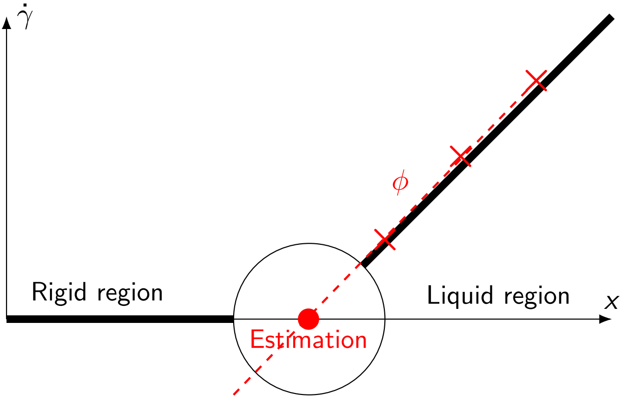
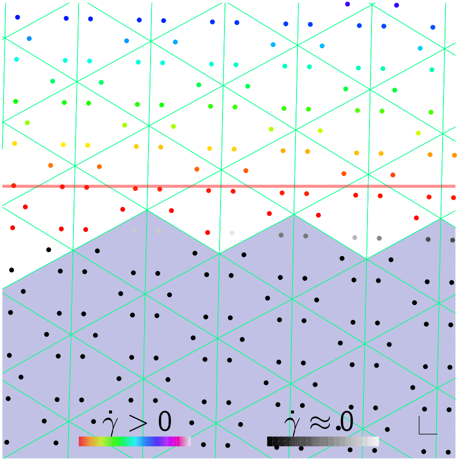


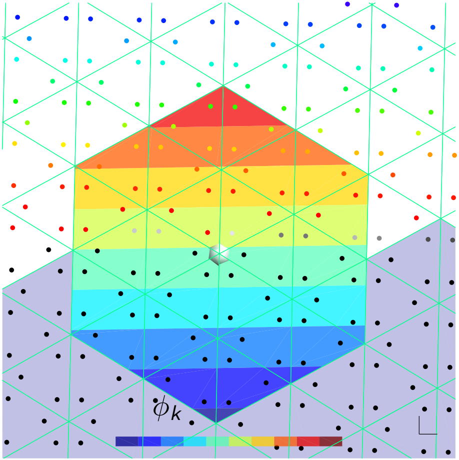
Locating the interface



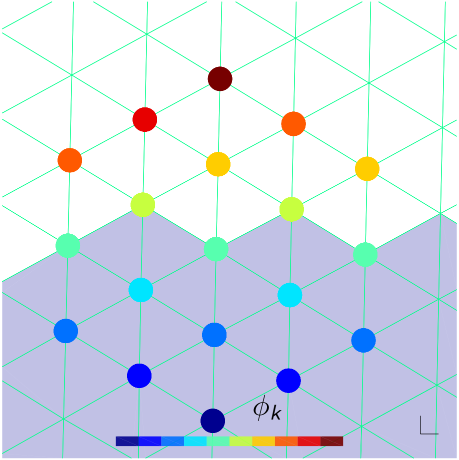
Locating the interface - Predictor



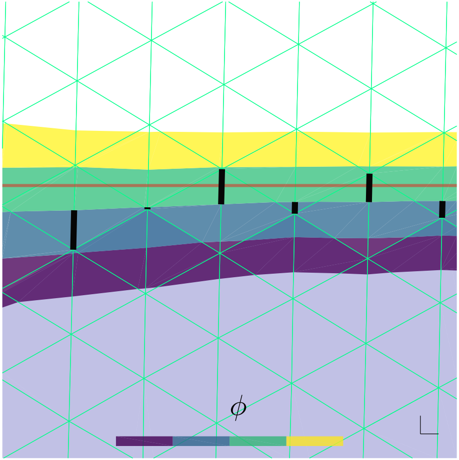
Locating the interface - Compute linear approximation



Locating the interface - Evaluate linear approximation



Locating the interface - Average linear approximations



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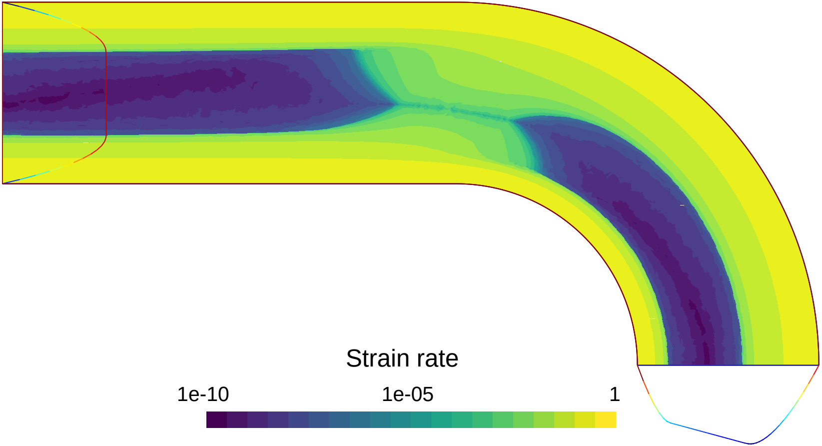
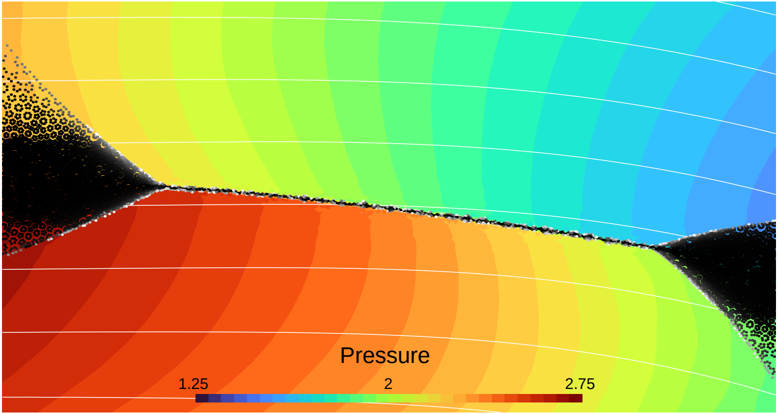
Curved channel



Curved channel - Pressure discontinuity

Jump condition

$$[\![\boldsymbol{\sigma}\cdot\hat{\mathbf{n}}]\!] = 0 \implies [\![p\hat{\mathbf{n}}]\!] = [\![\boldsymbol{\tau}\cdot\hat{\mathbf{n}}]\!] = [\![K\dot{\boldsymbol{\gamma}}\cdot\hat{\mathbf{n}}]\!] + \tau_0[\![\dot{\boldsymbol{\gamma}}/\dot{\gamma}\cdot\hat{\mathbf{n}}]\!]$$



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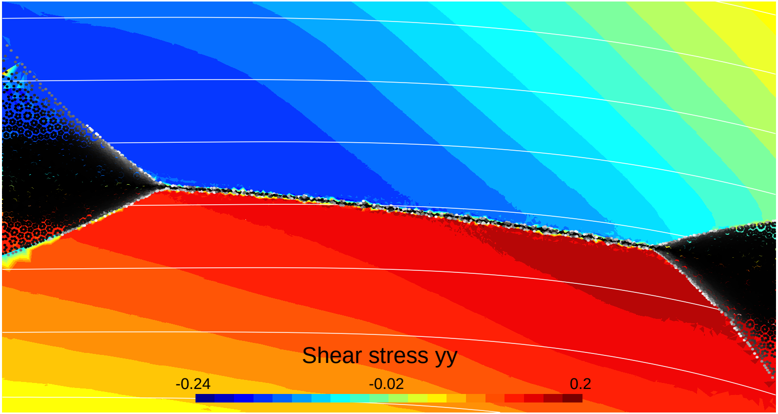
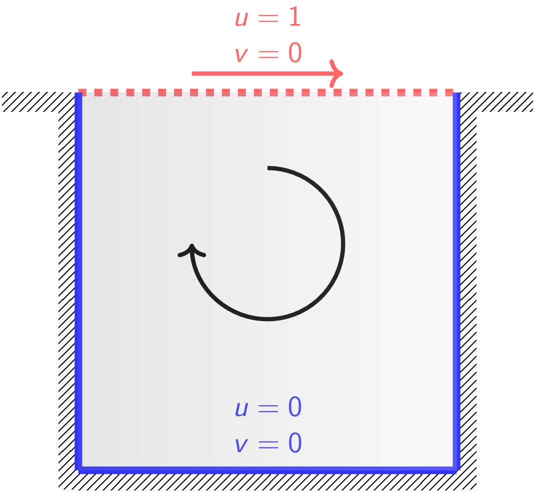
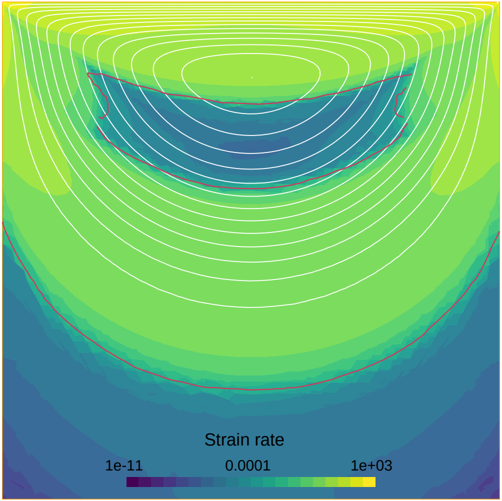


Curved channel - Increasing Bingham

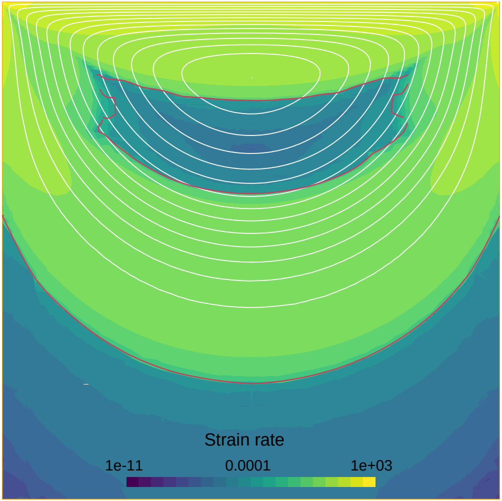
Lid-driven cavity



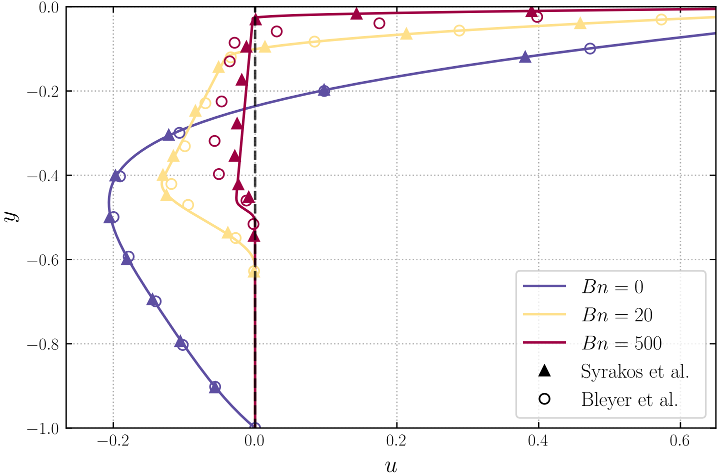
Lid-driven cavity - before/after interface tracking



Lid-driven cavity - before/after interface tracking



Lid-driven cavity - comparison with the literature



Lid-driven cavity - Rigid body motion

Flow around an obstacle

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