Flow-type dependent rheologies and multiscale simulations

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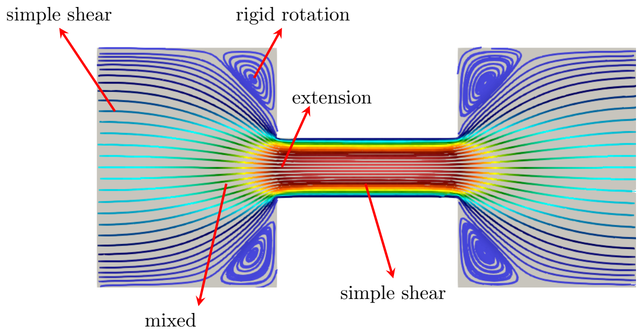
Generic flows feature multiple local flow types



Problems:

1. We can find flow-type dependence in the non-Newtonian response
2. We wish to avoid redundant computation in multiscale schemes

Stress projections

A general orthogonal basis for the stress tensor (planar 3D case)

We use the eigenvectors $\boldsymbol{d}_1$, $\boldsymbol{d}_2$, and $\boldsymbol{d}_3$ of $\mathsf{D} = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$ and set

$$\hat{\mathsf{D}} \equiv \boldsymbol{d}_1 \boldsymbol{d}_1 - \boldsymbol{d}_2 \boldsymbol{d}_2, \quad \text{with } \mathsf{D} = \dot{\varepsilon}\hat{\mathsf{D}} \text{ and } \boldsymbol{d}_3 \text{ the vorticity direction,}$$

$$\hat{\mathsf{E}} \equiv -\frac{1}{2}\boldsymbol{d}_1 \boldsymbol{d}_1 - \frac{1}{2}\boldsymbol{d}_2 \boldsymbol{d}_2 + \boldsymbol{d}_3 \boldsymbol{d}_3 \quad \text{and} \quad \hat{\mathsf{G}}_3 \equiv \boldsymbol{d}_1 \boldsymbol{d}_2 + \boldsymbol{d}_2 \boldsymbol{d}_1$$

With these, $(\mathsf{I}, \hat{\mathsf{D}}, \hat{\mathsf{E}}, \hat{\mathsf{G}}_3)$ are symmetric tensors, orthogonal to each other, and we recover well-known quantities in simple shear:

$$\sigma = \frac{1}{2}\boldsymbol{\sigma} : \hat{\mathsf{D}}, \qquad N_1 = -\boldsymbol{\sigma} : \hat{\mathsf{G}}_3, \qquad N_0 = N_2 + \frac{1}{2}N_1 = -\boldsymbol{\sigma} : \hat{\mathsf{E}}$$

Our definitions work for simple shear, extensional flow, and any mixed flow

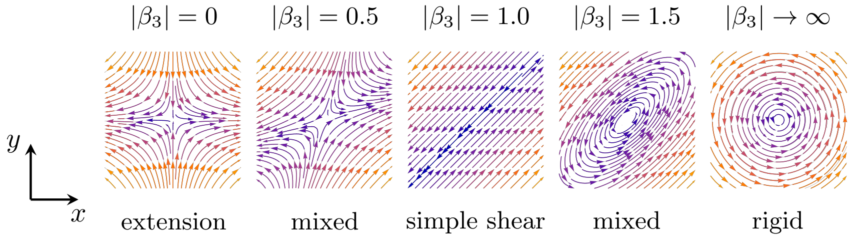
Details in: Giusteri & Seto, *J. Rheol.* 62(3), 713–723, 2018

Local flow calassification

$$\nabla \boldsymbol{u} = \mathsf{D} + \mathsf{W}$$

$$\mathsf{D} = \dot{\varepsilon}\left(\hat{\boldsymbol{d}}_1 \hat{\boldsymbol{d}}_1 - \hat{\boldsymbol{d}}_2 \hat{\boldsymbol{d}}_2\right) \qquad \mathsf{W} = \dot{\varepsilon}\beta_3\left(\hat{\boldsymbol{d}}_2 \hat{\boldsymbol{d}}_1 - \hat{\boldsymbol{d}}_1 \hat{\boldsymbol{d}}_2\right)$$

Deformation rate: $|\dot{\varepsilon}| = \sqrt{\frac{\mathrm{tr}\,\mathsf{D}^2}{2}}$ and flow type: $\beta_3 = \frac{\nabla \times \boldsymbol{u}}{2\dot{\varepsilon}} \cdot \hat{\boldsymbol{d}}_3$



Stress reconstruction and multiscale coupling

Once we have sampled the material coefficients

$$\eta\left(\dot{\varepsilon},\beta_3\right) := \frac{1}{2\dot{\varepsilon}}\frac{\boldsymbol{\sigma} : \hat{\mathsf{D}}}{||\hat{\mathsf{D}}||^2} \qquad \text{and} \qquad \lambda_3\left(\dot{\varepsilon},\beta_3\right) := \frac{1}{2\dot{\varepsilon}}\frac{\boldsymbol{\sigma} : \hat{\mathsf{G}}_3}{||\hat{\mathsf{G}}_3||^2},$$

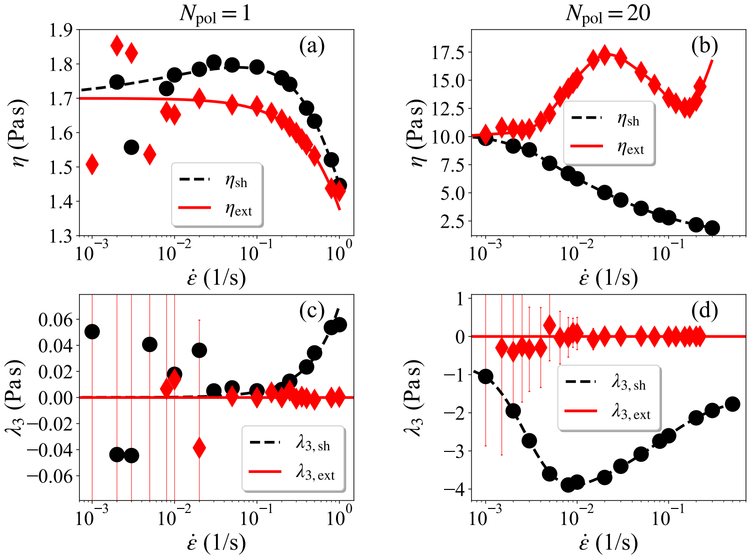
we can interpolate and extrapolate ($\sim$) the data and reconstruct the *macroscopic* stress (for a 2D flow) as

$$\boldsymbol{\sigma}(\dot{\varepsilon},\beta_3) = -p\mathsf{I} + 2\tilde{\eta}(\dot{\varepsilon},\beta_3)\mathsf{D} + 2\tilde{\lambda}_3(\dot{\varepsilon},\beta_3)\mathsf{G}_3,$$

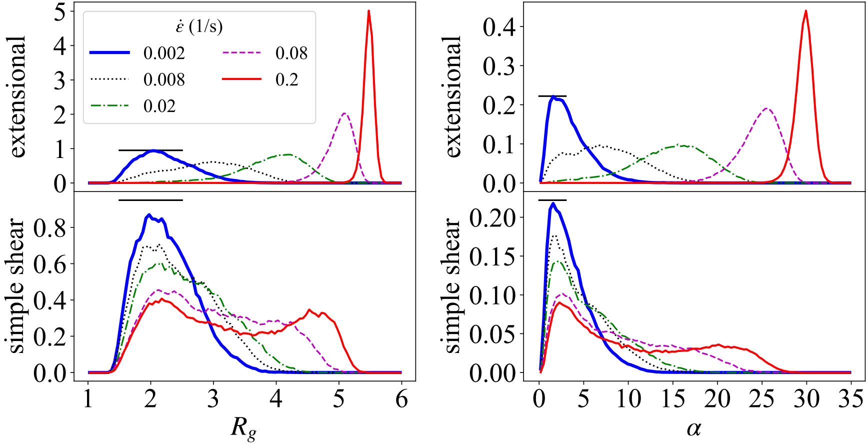
where $\mathsf{G}_3 = \frac{1}{2}\left(\mathsf{AD} - \mathsf{DA}\right)$ with $\mathsf{A} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$.

Details in: Tedeschi *et al.*, *Math. Eng.* 4(6), 1–22, 2021

Microscopic data



Origin of the flow-type dependence



Radius of gyration R_g and asphericity α describe the different behavior of polymer chains in the $N_{\mathrm{pol}} = 20$ case

Extrapolation of the material functions

$\tilde{\eta}(\dot{\varepsilon}, \beta_3)$ is an even function of β_3

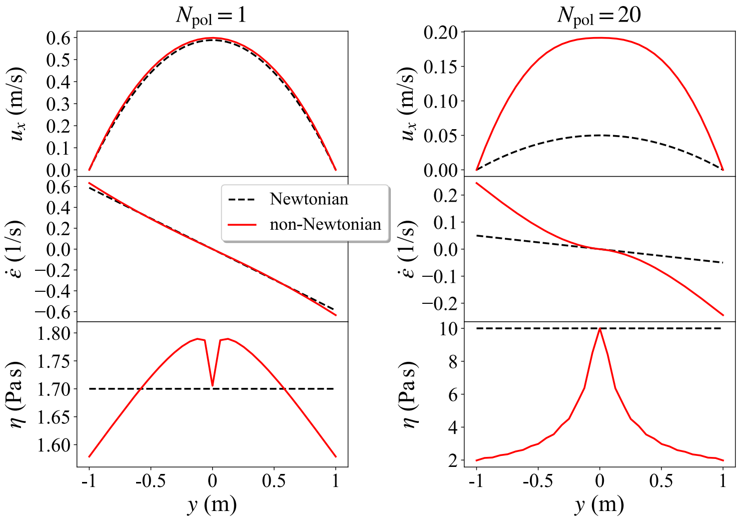
We set $$\tilde{\eta}(\dot{\varepsilon}, \beta_3) = \begin{cases} (1 - |\beta_3|)\eta_{\rm ext}(\dot{\varepsilon}) + |\beta_3|\eta_{\rm sh}(\dot{\varepsilon}) & \beta_3 \in [-1, 1] \\ \eta_{\rm sh}(\dot{\varepsilon}) & |\beta_3| > 1 \end{cases}$$

$\tilde{\lambda}_3(\dot{\varepsilon}, \beta_3)$ is an odd function of β_3

We set $$\tilde{\lambda}_3(\dot{\varepsilon}, \beta_3) = \begin{cases} \beta_3 \lambda_{3,\rm sh}(\dot{\varepsilon}) & \beta_3 \in [-1, 1] \\ \pm\, \lambda_{3,\rm sh}(\dot{\varepsilon}) & \beta_3 \gtrless \pm 1 \end{cases}$$

(*These choices should be improved, see below . . .*)

Channel flow



$L = 5$ m

$W = 2$ m

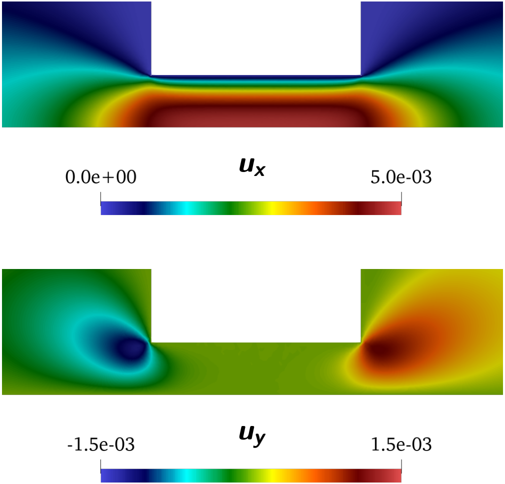
$\rho = 1$ kg/m^3

$C = 1$ Pa/m

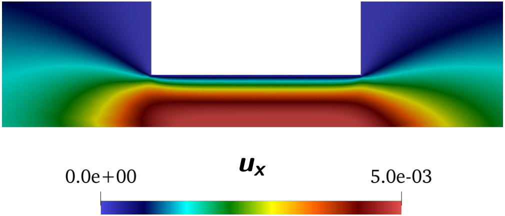
$\Delta t = 10^{-3}$ s

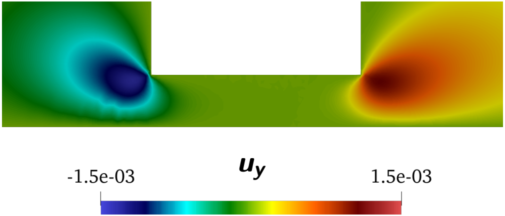
$T = 2$ s

Flow through a contraction

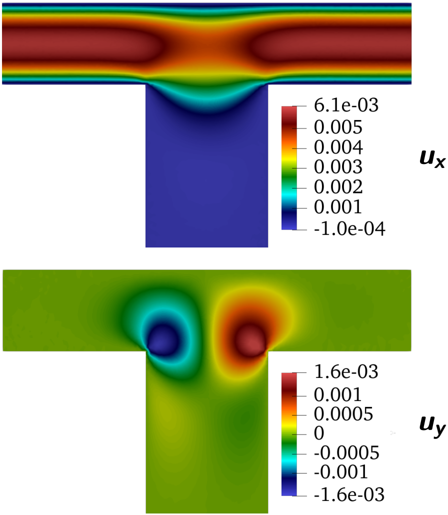


Flow through a contraction*





Flow past a deep hole



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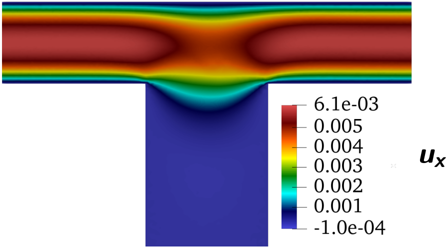
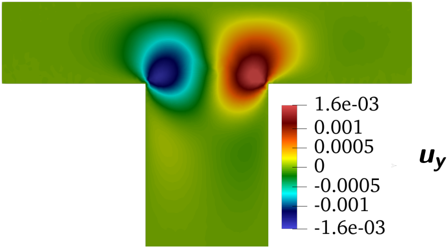
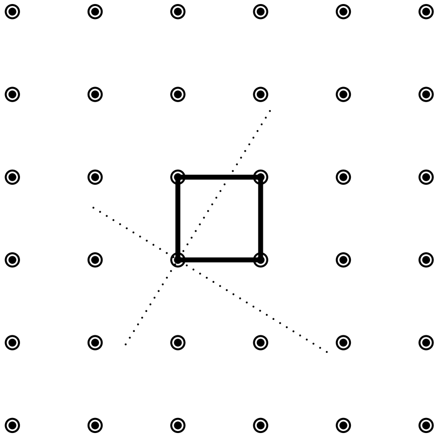


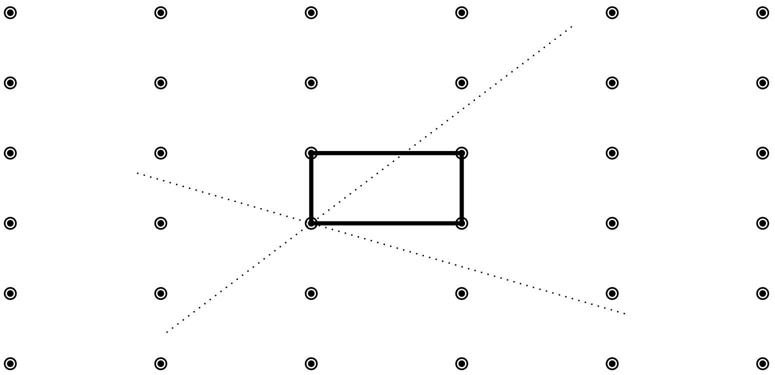


Kraynik–Reinelt method for extensional flow



Strain period $\tau_p = \log\left(\frac{3+\sqrt{5}}{2}\right)$ and tilt angle $\vartheta = \frac{1}{2}\left(\frac{\pi}{2} - \arcsin\left(\frac{1}{\sqrt{5}}\right)\right)$

Extension to the case of mixed flows

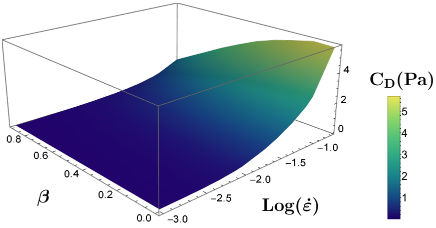


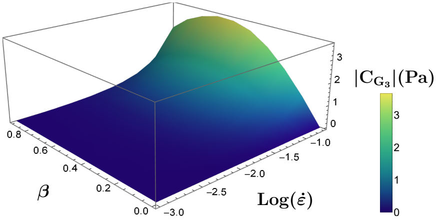
$$\beta = 0.6, \quad a = 2.143563, \quad \vartheta = 0.28070777, \quad \tau_p = 1.20302956$$

PMF: a LAMMPS package for Planar Mixed Flows.

`https://github.com/francescat93/user-pmf.git`

Rheological surfaces for stress components





We obtained data for the component of the stress related to η (left) and λ_3 (right) and found that the assumed linear interpolation is quite wrong (*Ready for further work!*)

We still need to investigate the chain conformation in mixed flows

Take-home messages

1. We have an economic approach for the identification of stress components to be used in multiscale schemes
2. It is essential to take the flow-type dependence into account (rheological surfaces)
3. Computational rheology that investigates mixed flows gives important information for the development of models (needed for extrapolation)

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Thank you! *. . . and open for questions!*