

The „Tensor Diffusion“-approach for simulating viscoelastic fluids with special emphasis on the „no solvent“-case

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Introduction

Simulation of viscoelastic fluids without solvent

Application in mind

- processing of (pure) **rubber melts** („Kautschuk“), industrial partner: ARLANXEO
- simulating viscoelastic fluids ...
 - ... consisting of wide relaxation time spectrum (over several decades)
 - „multi mode“-approach for adequate modelling
 - High Weissenberg Number Problem (HWNP)
 - ... **without „solvent contribution“**
- **plus:** solver often intended for **direct steady-state** solutions (relevant for applications)
- governing equations

$$- 2 \eta_s \nabla \cdot \mathbf{D}(\mathbf{u}) - \nabla \cdot \boldsymbol{\sigma} + \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0$$

plus constitutive equation for stress tensor $\boldsymbol{\sigma}$

Modelling approaches

1. **differential** material model (for multiple „modes“ $\Lambda_k, k = 1, \dots, K$)

$$\boldsymbol{\sigma} = \sum_{k=1}^K \boldsymbol{\sigma}_k, \quad (\mathbf{u} \cdot \nabla) \boldsymbol{\sigma}_k - \nabla \mathbf{u}^T \cdot \boldsymbol{\sigma}_k - \boldsymbol{\sigma}_k \cdot \nabla \mathbf{u} + \mathbf{f}(\Lambda_k, \eta_{p,k}, \boldsymbol{\sigma}_k) = 2 \frac{\eta_{p,k}}{\Lambda_k} \mathbf{D}(\mathbf{u})$$

- model function: $\mathbf{f}(\Lambda_k, \eta_{p,k}, \boldsymbol{\sigma}_k) = \frac{1}{\Lambda_k} \left(\boldsymbol{\sigma}_k + \alpha_k \frac{\Lambda_k}{\eta_{p,k}} \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_k \right)$ for $\alpha_k \in [0,1]$

2. **integral** material model („Deformation Fields Method“, c.f. Hulsen et al.)

$$\boldsymbol{\sigma} = \int_0^\infty M(s) \mathbf{g}(\mathbf{B}(s)) ds$$

for $s \in [0, \infty[$, $\mathbf{B}(0) = \mathbf{I}$: $\frac{\partial}{\partial s} \mathbf{B}(s) + (\mathbf{u} \cdot \nabla) \mathbf{B}(s) - \nabla \mathbf{u}^T \cdot \mathbf{B}(s) - \mathbf{B}(s) \cdot \nabla \mathbf{u} = 0$

- (multi-mode) memory function: $M(s) = \sum_{k=1}^K M_k(s) = \sum_{k=1}^K \frac{\eta_{p,k}}{\Lambda_k^2} \exp\left(-\frac{s}{\Lambda_k}\right)$
- in both cases for $\eta_s = 0$ („no solvent“):

Operator-Splitting not applicable vs. monolithic approach difficult

Monolithic approach

- „no solvent“ in Stokes equations (plus constitutive)

$$\cancel{-2\eta_s \nabla \cdot \mathbf{D}(\mathbf{u})} - \nabla \cdot \boldsymbol{\sigma} + \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0$$

- **differential** models for **single-mode**

$$\begin{pmatrix} 0 & B & -C \\ B^T & 0 & 0 \\ D & 0 & K(\mathbf{u}) \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \\ \boldsymbol{\sigma} \end{pmatrix} = \begin{pmatrix} \mathbf{r}_u \\ \mathbf{r}_p \\ \mathbf{r}_\sigma \end{pmatrix}$$

- standard Krylov-space methods: no diagonal preconditioning
 - multigrid
 - no diagonal smoothers applicable
 - Vanka-like smoothers behave unstable
 - stability problems w.r.t. additional LBB for $\mathbf{u}, \boldsymbol{\sigma}$
- not applicable for **integral** models

Operator-Splitting

1. for given $\boldsymbol{\sigma}^n$, solve **Stokes-problem** for $\mathbf{u}^{n+1}, p^{n+1}$ with non-zero RHS

$$-2\eta_s \nabla \cdot \mathbf{D}(\mathbf{u}^{n+1}) + \nabla p^{n+1} = \nabla \cdot \boldsymbol{\sigma}^n, \quad \nabla \cdot \mathbf{u}^{n+1} = 0$$

2. calculate $\boldsymbol{\sigma}^{n+1}$ from **differential** ($\boldsymbol{\sigma}_k^{n+1}$ for „multi-mode“ $\boldsymbol{\sigma} = \sum_{k=1}^K \nabla \cdot \boldsymbol{\sigma}_k$)
 $(\mathbf{u}^{n+1} \cdot \nabla) \boldsymbol{\sigma}^{n+1} - \nabla \mathbf{u}^{n+1 T} \cdot \boldsymbol{\sigma}^{n+1} - \boldsymbol{\sigma}^{n+1} \cdot \nabla \mathbf{u}^{n+1} + \mathbf{f}(\Lambda, \eta_p, \boldsymbol{\sigma}^{n+1}) = 2 \frac{\eta_p}{\Lambda} \mathbf{D}(\mathbf{u}^{n+1})$

or **integral** constitutive equation / DFM

$$\boldsymbol{\sigma}^{n+1} = \int_0^\infty M(s) \mathbf{g}(\mathbf{B}(s)) ds$$

$$\frac{\partial}{\partial s} \mathbf{B}(s) + (\mathbf{u}^{n+1} \cdot \nabla) \mathbf{B}(s) - \nabla \mathbf{u}^{n+1 T} \cdot \mathbf{B}(s) - \mathbf{B}(s) \cdot \nabla \mathbf{u}^{n+1} = 0$$

- Stokes problem without diffusive part
- not applicable for „no solvent“ - independently of actual model!

The „Tensor Diffusion“-approach

Assumption: „Tensor Diffusion“ μ via $\sigma = \mu \cdot D(\mathbf{u})$

- direct computation of (\mathbf{u}, p) -solution via „Tensor Stokes“-problem

$$-\nabla \cdot (\mu \cdot D(\mathbf{u})) + \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0$$

- σ computed in postprocessing
 - solve **linear „Stokes“-problem** instead of highly nonlinear system
- **monolithic** solution approach for „no-solvent“ (differential models only, single-mode)

$$\begin{pmatrix} -T(\mu) & B & 0 \\ B^T & 0 & 0 \\ D & 0 & K(\mathbf{u}) \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \\ \sigma \end{pmatrix} = \begin{pmatrix} \mathbf{r}_u \\ \mathbf{r}_p \\ \mathbf{r}_\sigma \end{pmatrix}$$

- no „zero-diagonal“ in Stokes-part
 - diagonal preconditioners / smoothers applicable
 - improved Vanka-behaviour
 - stabilizing character of „Tensor Diffusion“ w.r.t. LBB for \mathbf{u}, σ

Assumption: „Tensor Diffusion“ μ via $\sigma = \mu \cdot D(u)$

→ prototypical **Operator-Splitting** in iterative methods

1. for given μ^n (e.g. $\mu = I$ for $n = 0$) determine (u^{n+1}, p^{n+1}) from „Tensor Stokes“-problem

$$-\nabla \cdot (\mu^n \cdot D(u^{n+1})) + \nabla p^{n+1} = 0, \quad \nabla \cdot u^{n+1} = 0$$

2. for u^{n+1} , determine stress tensor σ^{n+1} from **integral or differential** model
3. determine (tensor) viscosity μ^{n+1} via $\sigma^{n+1} = \mu^{n+1} \cdot D(u^{n+1})$

- now, **non-vanishing velocity coupling** in momentum equation

→ Operator-Splitting applicable

Proof of concept

- **main idea:** postulate stress-decomposition $\boldsymbol{\sigma} = \boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})$ exists
 - incorporate into viscoelastic simulations (besides Stokes / constitutive equations)
- show feasibility of presented „Tensor Diffusion“-approach by
 1. solve full **differential model** in $(\mathbf{u}, \boldsymbol{\sigma}, p)$ (already **realized inside FEATFLOW**)
 2. calculating „Tensor Diffusion“ $\boldsymbol{\mu}$
 - a) analytically
 - b) based on differential $(\mathbf{u}, \boldsymbol{\sigma}, p)$ -solution
 3. solve pure „**Tensor Stokes**“-problem for (\mathbf{u}, p) with above $\boldsymbol{\mu}$
- „Tensor Stokes“-solution should give same as full 3-field $(\mathbf{u}, \boldsymbol{\sigma}, p)$ -formulation!

1D-flow configurations



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

- analytical solutions for \mathbf{B} inserted into **stress integral** (single-mode UCM)

$$\boldsymbol{\sigma} = \int_0^\infty \frac{\eta_p}{\Lambda^2} \exp\left(-\frac{s}{\Lambda}\right) (\mathbf{B}(s) - \mathbf{I}) ds = \left\{ 2 \int_0^\infty \frac{\eta_p}{\Lambda^2} \exp\left(-\frac{s}{\Lambda}\right) \begin{pmatrix} s & s^2 \frac{\partial u}{\partial y} \\ 0 & s \end{pmatrix} ds \right\} \mathbf{D}(\mathbf{u})$$

- (unsymmetric) tensor-valued quantity relating $\boldsymbol{\sigma}$ to $\mathbf{D}(\mathbf{u})$: $\boldsymbol{\mu}(\mathbf{u}) = 2\eta_p \begin{pmatrix} 1 & 2\Lambda \frac{\partial u}{\partial y} \\ 0 & 1 \end{pmatrix}$

- for **differential** (single-mode) UCM: $\boldsymbol{\sigma} = \begin{pmatrix} 2\Lambda\eta_p \left(\frac{\partial u}{\partial y}\right)^2 & \eta_p \frac{\partial u}{\partial y} \\ \eta_p \frac{\partial u}{\partial y} & 0 \end{pmatrix} = \boldsymbol{\mu}(\mathbf{u}) \cdot \mathbf{D}(\mathbf{u})$

- methodology can be analogously applied to **Giesekus / PSM** → $\boldsymbol{\mu}_{21} \neq \mathbf{0}$

Shear flow

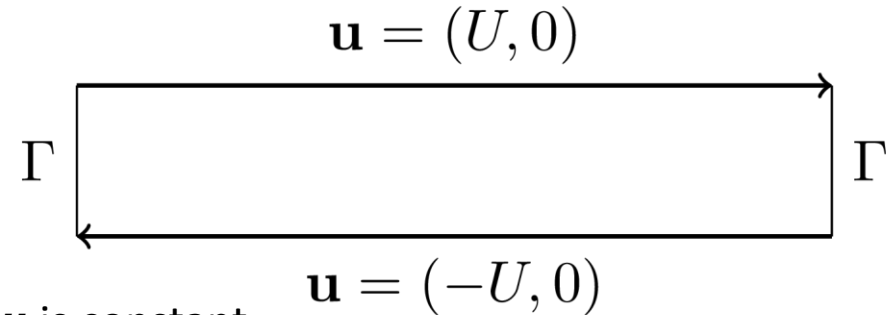
- velocity field $\mathbf{u} = \begin{pmatrix} u(y) \\ v \end{pmatrix} = \begin{pmatrix} Uy \\ 0 \end{pmatrix}$
- $\mathbf{D}(\mathbf{u})$ and $\boldsymbol{\sigma}$ are constant → viscosity tensor $\boldsymbol{\mu}$ is constant
- solve „Tensor Stokes“-problem with $\boldsymbol{\mu}$ prescribed globally

$$-\nabla \cdot (\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})) + \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0$$

- test configuration: set perturbed velocity profile on Γ

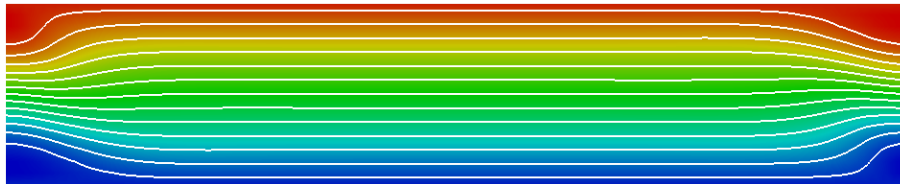
$$\tilde{\mathbf{u}} = \begin{pmatrix} w(y) \\ 0 \end{pmatrix}, \quad w(y) = Uy + \kappa y(1 - y^2)$$

- analytical flow profiles should be recovered inside of the channel

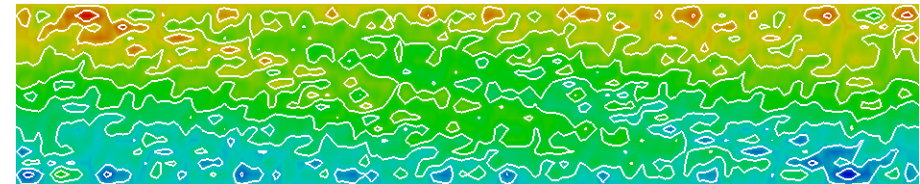


Shear flow

- for „low“ relaxation times Λ , analytical x -velocity is recovered
- for higher Λ , flow shows defects (due to unsymmetric $\boldsymbol{\mu}$!)



$u(y), \Lambda = 10.0$



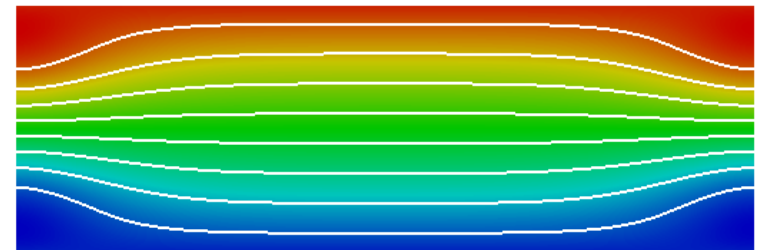
$u(y), \Lambda = 50.0$

- consider **symmetrized** „Tensor Stokes“-problem

$$-\frac{1}{2} \nabla \cdot (\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u}) + \mathbf{D}(\mathbf{u}) \cdot \boldsymbol{\mu}^T) + \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0$$

- x -velocity looks reasonable even for very large Λ !

$u(y), \Lambda = 1000.0$

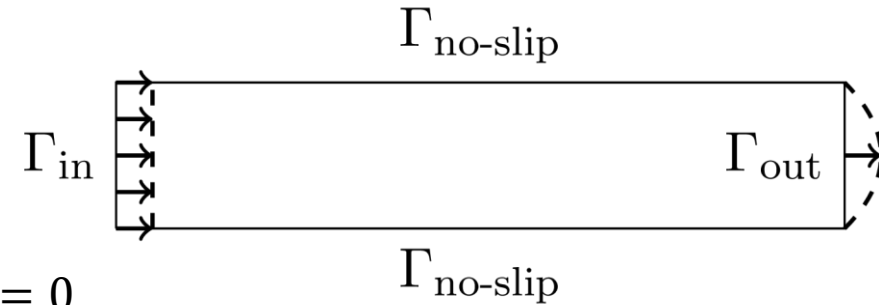


Poiseuille flow

- solve symmetrized „Tensor Stokes“-problem

$$-\frac{1}{2} \nabla \cdot (\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u}) + \mathbf{D}(\mathbf{u}) \cdot \boldsymbol{\mu}^T) + \nabla p = 0, \nabla \cdot \mathbf{u} = 0$$

- „fully developed“ Tensor Diffusion $\boldsymbol{\mu}$, „perturbed“ velocity profile on inflow edge

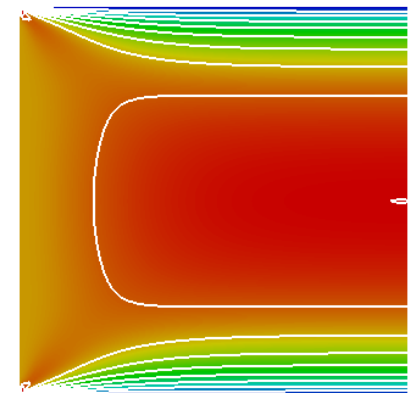
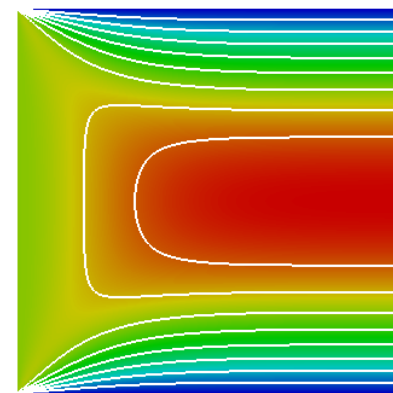
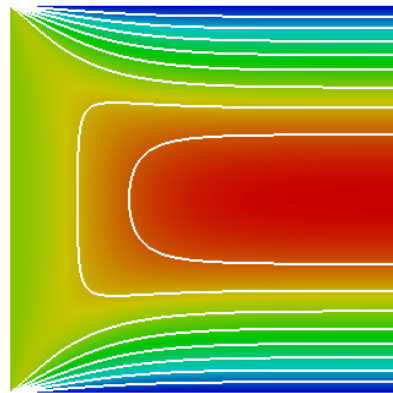
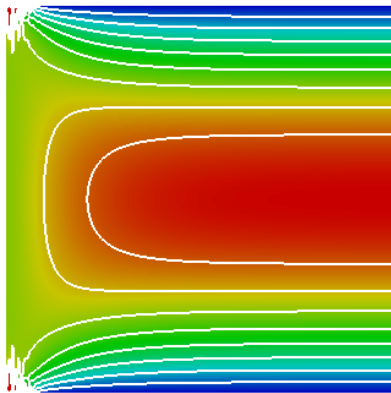


$\Lambda = 1.0$

$\Lambda = 50.0$

$\Lambda = 1.0, U_{\max} = 0.099$

$\Lambda = 50.0, U_{\max} = 0.083$



UCM

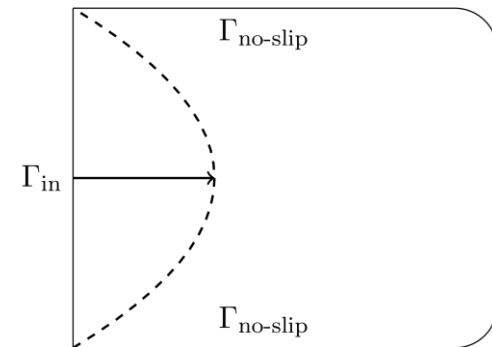
Giesekus, $\alpha = 0.1$

→ via solving purely **linear (Tensor-)Stokes** problem:

fully developed **viscoelastic(!) flow** recovered away from (perturbed) inflow!

Four-field formulation

- „Tensor Diffusion“ not known (semi-)analytically
- how to calculate $\boldsymbol{\mu}$ from differential $(\mathbf{u}, \boldsymbol{\sigma}, p)$ -solution?
- extend single-mode differential models for „no solvent“



$$-\nabla \cdot \boldsymbol{\sigma} + \nabla p = 0 \quad \text{or} \quad -\frac{1}{2} \nabla \cdot (\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u}) + \mathbf{D}(\mathbf{u}) \cdot \boldsymbol{\mu}^T) + \nabla p = 0,$$

$$(\mathbf{u} \cdot \nabla) \boldsymbol{\sigma} - \nabla \mathbf{u}^T \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \nabla \mathbf{u} + \mathbf{f}(\Lambda, \eta_p, \boldsymbol{\sigma}) = 2 \frac{\eta_p}{\Lambda} \mathbf{D}(\mathbf{u}),$$

$$\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u}) - \boldsymbol{\sigma} = 0, \quad \nabla \cdot \mathbf{u} = 0$$

- **1st alternative:** $(\mathbf{u}, \boldsymbol{\sigma}, p)$ -solution does not depend on $\boldsymbol{\mu}$ („postprocessing fashion“)
- **2nd alternative:** four-field formulation of „Tensor Stokes“-problem, $(\mathbf{u}, \boldsymbol{\sigma}, p)$ coupled with $\boldsymbol{\mu}$

Four-field formulation

- discrete operators and nonlinear systems via **FEM** with $Q_2/P_1^{\text{disc}}/Q_2/Q_0$
- plus „**Edge-Oriented FEM**“ stabilization (**EOFEM**) for $(\mathbf{u}, \boldsymbol{\sigma}, \boldsymbol{\mu})$
- solution via monolithic Newton-**multigrid**-scheme (even for higher Λ)
- for $\omega_n \in]0,1], \mathbf{x} = (\mathbf{u}, p, \boldsymbol{\sigma}, \boldsymbol{\mu})^T$:

$$\mathbf{x}^{n+1} = \mathbf{x}^n - \omega_n \mathbf{A}(\mathbf{u}^n, \boldsymbol{\sigma}^n, \boldsymbol{\mu}^n)^{-1} \mathbf{r}(\mathbf{u}^n, p^n, \boldsymbol{\sigma}^n, \boldsymbol{\mu}^n)$$
- residual \mathbf{r} and Jacobian matrix \mathbf{A} problem-dependent
- original approach

$$\mathbf{A}_C = \begin{pmatrix} J_u & B & -C & 0 \\ B^T & 0 & 0 & 0 \\ D + K_u(\boldsymbol{\tau}) & 0 & K_\sigma(\mathbf{w}) + J_\sigma & 0 \\ 0 & 0 & M & D(\mathbf{w}) + J_\mu \end{pmatrix}, \quad \mathbf{r}_C = \begin{pmatrix} Bq - C\boldsymbol{\tau} \\ B^T \mathbf{w} \\ D\mathbf{w} + K(\mathbf{w})\boldsymbol{\tau} \\ M\boldsymbol{\tau} + D(\mathbf{w})\mathbf{v} \end{pmatrix}$$

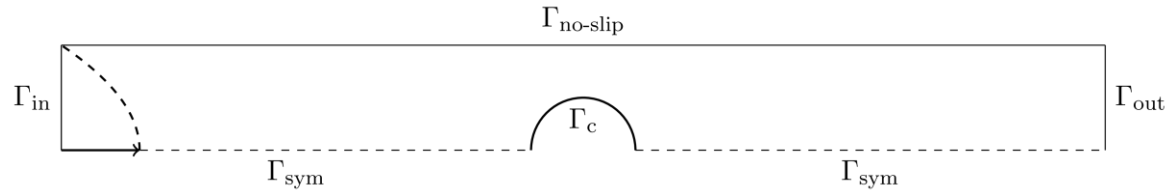
Four-field formulation

- discrete operators and nonlinear systems via **FEM** with $Q_2/P_1^{\text{disc}}/Q_2/Q_0$
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- residual \mathbf{r} and Jacobian matrix \mathbf{A} problem-dependent
- original approach, „Tensor Stokes“-problem

$$\mathbf{A}_T = \begin{pmatrix} -T_u(\mathbf{v}) + J_u & B & 0 & -T_\mu(\mathbf{w}) \\ B^T & 0 & 0 & 0 \\ D + K_u(\boldsymbol{\tau}) & 0 & K_\sigma(\mathbf{w}) + J_\sigma & 0 \\ 0 & 0 & M & D(\mathbf{w}) + J_\mu \end{pmatrix}, \quad \mathbf{r}_T = \begin{pmatrix} Bq - T(\mathbf{w})\mathbf{v} \\ B^T \mathbf{w} \\ D\mathbf{w} + K(\mathbf{w})\boldsymbol{\tau} \\ M\boldsymbol{\tau} + D(\mathbf{w})\mathbf{v} \end{pmatrix}$$

Flow around cylinder



- drag coefficient calculated via $C_D(\mathbf{T}) = \frac{2}{U_{\text{mean}R}^2} \int_{E_c} (T_{xx}n_1 + T_{xy}n_2) \frac{\partial \varphi}{\partial x} dx$

→ problem-dependent total stress tensor:

$$\mathbf{T}_C = -p\mathbf{I} + 2\eta_s\mathbf{D}(\mathbf{u}) + \boldsymbol{\sigma}, \quad \mathbf{T}_T = -p\mathbf{I} + 2\eta_s\mathbf{D}(\mathbf{u}) + \frac{1}{2}(\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u}) + \mathbf{D}(\mathbf{u}) \cdot \boldsymbol{\mu}^T)$$

Oldroyd-B ($\eta_s = 0.59$)

Λ	$C_D(\mathbf{T}_C)$	N_C	$C_D(\mathbf{T}_T)$	N_T	Ref.
0.1	130.342	2	130.348	3	130.36
0.6	117.695	3	117.970	3	117.78

Giesekus ($\alpha = 0.1, \eta_s = 0.59$)

Λ	$C_D(\mathbf{T}_C)$	N_C	$C_D(\mathbf{T}_T)$	N_T	Ref.
5.0	85.210	3	85.243	6	85.22
10.0	83.047	4	83.068	6	83.06

- very good agreement to reference and original approach
- appropriate solver behaviour

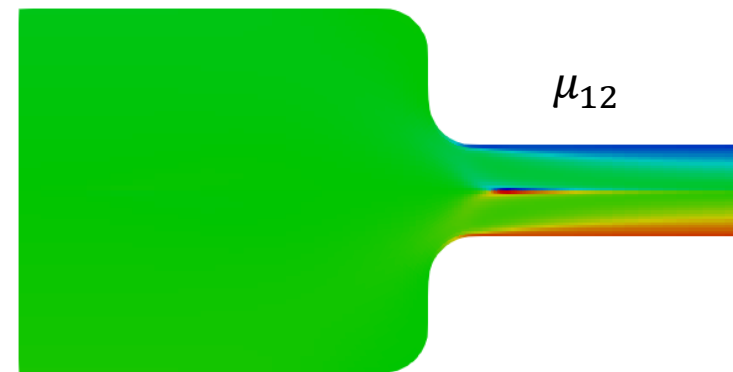
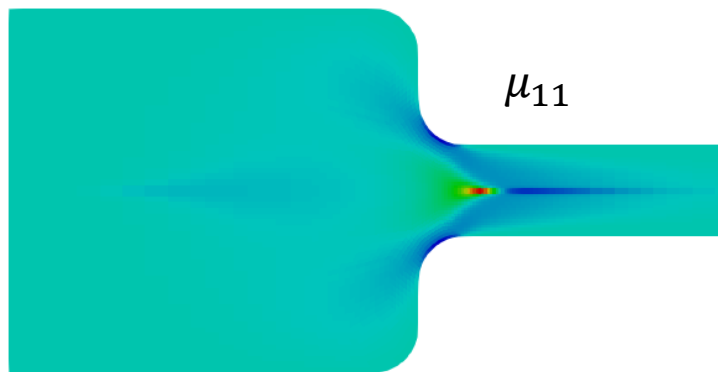
Summary and outlook

Summary

- new „**Tensor Diffusion**“-**approach** - particularly for „no solvent“-case
 - direct model for $\boldsymbol{\mu} = \boldsymbol{\mu}(\mathbf{u}, \mathbf{D}(\mathbf{u}))$ possible? (1D-flows: **YES!**)
 - solve **linear „Stokes“-problem** instead of highly nonlinear system
 - otherwise: numerical calculation from algebraic equation
 - validated for simple test cases, evaluated for more complex test cases
 - allows modified solvers w.r.t. Operator-Splitting and Newton-multigrid
 - more numerical tests
 - detailed numerical analysis/theoretical background for new „Tensor Stokes“?
- $$-\frac{1}{2} \nabla \cdot (\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u}) + \mathbf{D}(\mathbf{u}) \cdot \boldsymbol{\mu}^T) + \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0$$
- application to **integral models** possible?

Outlook

- (smoothed) contraction flow \rightarrow reasonable $(\mathbf{u}, \boldsymbol{\sigma}, p)$ -solution
- **but:** discontinuities/singularities(?) in $\boldsymbol{\mu}$ along symmetry line



- \rightarrow large amount of EOFEM (w.r.t. $\boldsymbol{\mu}$) to get smooth solution
- **alternative I:** Least-Squares $\frac{1}{2} (\|\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u}) - \boldsymbol{\sigma}\|^2 + \delta \|\nabla \boldsymbol{\mu}\|^2) \rightarrow \min$
- in four-field formulation: determine $\boldsymbol{\mu}$ from

$$\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u}) \cdot \mathbf{D}(\mathbf{u}) - \boldsymbol{\sigma} \cdot \mathbf{D}(\mathbf{u}) - \delta \Delta \boldsymbol{\mu} = 0$$

Outlook

- recall:

$$(\mathbf{u} \cdot \nabla) \boldsymbol{\sigma} - \nabla \mathbf{u}^T \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot \nabla \mathbf{u} + \mathbf{f}(\Lambda, \eta_p, \boldsymbol{\sigma}) = 2 \frac{\eta_p}{\Lambda} \mathbf{D}(\mathbf{u})$$

- inserting $\boldsymbol{\sigma} = \boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})$ into constitutive equation
- **but:** how to treat 2nd-order \mathbf{u} -derivatives in convective part?

$$(\mathbf{u} \cdot \nabla)[\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})] = (\mathbf{u} \cdot \nabla)[\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})] + (\nabla \cdot \mathbf{u}) \cdot (\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})) = \nabla \cdot [(\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})) \otimes \mathbf{u}]$$

→ alternative II: PDE for $\boldsymbol{\mu}$

- monolithic 3-field formulation in $(\mathbf{u}, \boldsymbol{\mu}, p)$

$$-\frac{1}{2} \nabla \cdot (\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u}) + \mathbf{D}(\mathbf{u}) \cdot \boldsymbol{\mu}^T) + \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0$$

$$\nabla \cdot [(\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})) \otimes \mathbf{u}] - \nabla \mathbf{u}^T \cdot [\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})] - [\boldsymbol{\mu} \cdot \mathbf{D}(\mathbf{u})] \cdot \nabla \mathbf{u} + \mathbf{f}(\Lambda, \eta_p, \boldsymbol{\mu}, \mathbf{u}) = 2 \frac{\eta_p}{\Lambda} \mathbf{D}(\mathbf{u})$$

→ improved calculation of $\boldsymbol{\mu}$, e.g. regarding „singularities“?