The „Tensor Diffusion approach“
for simulating viscoelastic fluids
with special emphasis on „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

- in CFD, consider „realistic“ 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“, i.e. *no* polymer solutions considered

- **plus**: solver often intended for **direct steady-state** solutions (relevant for applications)

- governing equations for „no solvent“-case
  
  \[- 2 \eta_s \nabla \cdot D(\mathbf{u}) - \nabla \cdot \mathbf{\sigma} + \nabla p = 0, \quad \nabla \cdot \mathbf{u} = 0\]

  plus constitutive equation for stress tensor \(\mathbf{\sigma}\)
Modelling approaches for constitutive equations

- **differential** material model (for multiple "modes"/relaxation times $\Lambda_k, k = 1, \ldots, K$)

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

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

- **integral** material model ("Deformation Fields Method", DFM, c.f. Hulsen et al.)

\[
\sigma = \int_0^\infty M(s) \mathbf{g}(\mathbf{B}(s)) \, ds, \quad \frac{\partial}{\partial s} \mathbf{B}(s) + (\mathbf{u} \cdot \nabla)\mathbf{B}(s) - \nabla \mathbf{u}^T \cdot \mathbf{B}(s) - \mathbf{B}(s) \cdot \nabla \mathbf{u} = 0
\]

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

- differential models for single-mode (matrix-vector-notation)
  \[
  \begin{pmatrix}
  0 & B & -C \\
  B^T & 0 & 0 \\
  D & 0 & K(u)
  \end{pmatrix}
  \begin{pmatrix}
  \mathbf{u} \\
  p \\
  \mathbf{\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 smoother applicable
    - only Vanka-like smoothers work - but not robust
  - stability problems w.r.t. additional LBB for \( \mathbf{u}, \mathbf{\sigma} \)

- how to apply for integral models?!
Operator-Splitting

• given \( u^n, \sigma^n, p^n \)

1. solve **Stokes-problem** for \( u^{n+1}, p^{n+1} \) with non-zero RHS

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

2. calculate \( \sigma^{n+1} \) from **differential** (\( \sigma_k^{n+1} \) for „multi-mode“ \( \sigma = \sum_{k=1}^{K} \sigma_k \))

\[
(u^{n+1} \cdot \nabla)\sigma^{n+1} - \nabla u^{n+1T} \cdot \sigma^{n+1} - \sigma^{n+1} \cdot \nabla u^{n+1} + f(\Lambda, \eta_p, \sigma^{n+1}) = 2 \frac{\eta_p}{\Lambda} D(u^{n+1})
\]

or **integral** constitutive equation / DFM

\[
\sigma^{n+1} = \int_0^\infty M(s) g(B(s)) \, ds
\]

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

• not applicable for „no solvent“ - independently of actual model!

→ **Stokes problem without diffusive part**
The „Tensor Diffusion“ approach
Assumption: „Tensor Diffusion“ $\mu$ via $\sigma = \mu \cdot D(u)$

- idea: in 2D („no solvent“) Stokes equations, replace $\sigma$ by $\mu \cdot D(u)$, $\mu \in \mathbb{R}^{2 \times 2}$ or $\mathbb{R}^{3 \times 3}$
  \[
  - \nabla \cdot \sigma + \nabla p = 0, \quad \nabla \cdot u = 0
  \]
- consider newly defined (symmetrized) „Tensor Stokes“-problem
  \[
  - \frac{1}{2} \nabla \cdot (\mu \cdot D(u) + D(u) \cdot \mu^T) + \nabla p = 0, \quad \nabla \cdot u = 0
  \]

- issues to tackle
  - how to determine „Tensor Diffusion“ $\mu$?
  - (potential) benefits?
  - reasonable assumption / approach?
„Tensor Diffusion“ $\mu$ given/known

- consider (symmetrized) „Tensor Stokes“-problem

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

- **approach I:** „Tensor Diffusion“ $\mu$ known from „somewhere“
  - original problem: Stokes equations coupled with nonlinear diff./int. model
  - fully coupled nonlinear system in $(u, \sigma, p)$
  - but by introducing „Tensor Diffusion“:

  **direct computation of „nonlinear“ solution via pure $(u, p)$-problem**

- $\sigma$ computed in postprocessing, only


„Tensor Diffusion“ $\mu$ from algebraic equation

- **approach II**: determine „Tensor Diffusion“ $\mu$ from algebraic equation
  - consider single-mode differential models for „no-solvent“
    
    $- \nabla \cdot \sigma + \nabla p = 0 \quad \text{or} \quad -\frac{1}{2} \nabla \cdot (\mu \cdot D(u) + D(u) \cdot \mu^T) + \nabla p = 0$, with:
    
    $(u \cdot \nabla)\sigma - \nabla u^T \cdot \sigma - \sigma \cdot \nabla u + f(\Lambda, \eta_p, \sigma) = 2 \frac{\eta_p}{\Lambda} D(u)$,

    $\nabla \cdot u = 0, \quad \mu \cdot D(u) - \sigma = 0$

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

- discrete operators and nonlinear systems via FEM with $Q_2/P_1^{\text{disc}}/Q_2/Q_0$
"Tensor Diffusion" $\mu$ from PDE

- **approach III:** determine "Tensor Diffusion" $\mu$ from PDE
  - insert stress decomposition into constitutive equation for $\sigma$
    \[
    (u \cdot \nabla)[\mu \cdot D(u)] - \nabla u^T \cdot [\mu \cdot D(u)] - [\mu \cdot D(u)] \cdot \nabla u + \frac{1}{\Lambda} [\mu \cdot D(u)] = 2 \frac{\eta_p}{\Lambda} D(u)
    \]
  - suitable treatment of 2nd $u$-derivatives:
    \[
    (u \cdot \nabla)[\mu \cdot D(u)] = (u \cdot \nabla)[\mu \cdot D(u)] + (\nabla \cdot u) \cdot (\mu \cdot D(u)) = \nabla \cdot [(\mu \cdot D(u)) \otimes u]
    \]

  $\rightarrow$ monolithic **three-field** formulation in $(u, \mu, p)$
  - $- \frac{1}{2} \nabla \cdot (\mu \cdot D(u) + D(u) \cdot \mu^T) + \nabla p = 0$, $\nabla \cdot u = 0$
  - $\nabla \cdot [(\mu \cdot D(u)) \otimes u] - \nabla u^T \cdot [\mu \cdot D(u)] - [\mu \cdot D(u)] \cdot \nabla u + f(\Lambda, \eta_p, \mu, u) = 2 \frac{\eta_p}{\Lambda} D(u)$

- now, **non-vanishing velocity coupling** in momentum equation – even for "no-solvent"!
- potential benefit regarding numerical difficulties?
Potential benefits

- prototypical **Operator-Splitting** in iterative methods
  1. for given $\mu^n$ (e.g. $\mu = I$ for $n = 0$) determine $(u^{n+1}, p^{n+1})$ from „Tensor Stokes“-problem

\[-\frac{1}{2} \nabla \cdot (\mu^n \cdot D(u^{n+1}) + D(u^{n+1}) \cdot \mu^{nT}) + \nabla p^{n+1} = 0, \quad \nabla \cdot u^{n+1} = 0\]

*approach II* – four-field formulation in $(u, p, \sigma, \mu)$

2. for $u^{n+1}$, determine stress tensor $\sigma^{n+1}$ from **integral** or **differential** model

3. determine (tensor) viscosity $\mu^{n+1}$ via $\sigma^{n+1} = \mu^{n+1} \cdot D(u^{n+1})$

*approach III* – three-field formulation in $(u, p, \mu)$

2. for $u^{n+1}$, calculate $\mu^{n+1}$ from PDE
Potential benefits

- **monolithic** solution approach for „no-solvent“ (differential models only, single-mode)

→ diffusive operator introduced in „natural way“

**approach II** – four-field formulation in \((u, p, \sigma, \mu)\)

\[
\begin{pmatrix}
-T(\mu) & B & 0 & 0 \\
B^T & 0 & 0 & 0 \\
D & 0 & K(u) & 0 \\
0 & 0 & M & D(u)
\end{pmatrix}
\begin{pmatrix}
u \\ p \\ \sigma \\ \mu
\end{pmatrix} =
\begin{pmatrix}
r_u \\ r_p \\ r_\sigma \\ r_\mu
\end{pmatrix}
\]

**approach I** – pure \((u, p)\)-problem

\[
\begin{pmatrix}
-T(u) & B \\
B^T & 0
\end{pmatrix}
\begin{pmatrix}
u \\ p
\end{pmatrix} =
\begin{pmatrix}
r_u \\ r_p
\end{pmatrix}
\]

→ Operator-Splitting / standard Stokes-solvers applicable for all approaches
Proof of concept
\( \mu \) known analytically

- in the following, consider **fully developed channel flows**

\[
u = \begin{pmatrix} u \\ v \\ 0 \end{pmatrix}, \quad \frac{\partial u}{\partial x} = \frac{\partial v}{\partial x} = \frac{\partial v}{\partial y} = 0, \quad \frac{\partial}{\partial x} \sigma_{ij} = \frac{\partial}{\partial x} B_{ij} = 0 \text{ for } i, j \in \{1,2\}\]

- for **differential version** of UCM, parabolic velocity profile obtained
- corresponding stresses read

\[
\sigma_{\text{diff}} = \begin{pmatrix} 2 \Lambda \eta_p \left( \frac{\partial u}{\partial y} \right)^2 & \eta_p \frac{\partial u}{\partial y} \\ \eta_p \frac{\partial u}{\partial y} & 0 \end{pmatrix}, \quad D(u) = \frac{1}{2} \begin{pmatrix} 0 & \frac{\partial u}{\partial y} \\ \frac{\partial u}{\partial y} & 0 \end{pmatrix} \Rightarrow \mu_{\text{diff}}(u) = 2 \eta_p \begin{pmatrix} 1 & 2 \Lambda \frac{\partial u}{\partial y} \\ 0 & 1 \end{pmatrix}
\]

\( \Rightarrow \) tensor quantity relating \( \sigma \) to \( D(u) \) known analytically
**μ** known analytically

- In DFM, analytical solution of Finger tensors for $s \in [0, \infty[$ given
  
  $$
  B_{22}(s) = 1, \quad B_{12}(s) = s \frac{\partial u}{\partial y}, \quad B_{11}(s) = s^2 \left( \frac{\partial u}{\partial y} \right)^2 + 1
  $$

- Inserting into stress integral for UCM gives
  
  $$
  \sigma = \int_0^{\infty} \frac{\eta_p}{\Lambda^2} \exp \left( -\frac{s}{\Lambda} \right) (B(s) - I) ds = \left\{ 2 \int_0^{\infty} \frac{\eta_p}{\Lambda^2} \exp \left( -\frac{s}{\Lambda} \right) \left( \begin{array}{cc} s & s^2 \frac{\partial u}{\partial y} \\ 0 & \frac{\partial u}{\partial y} \end{array} \right) ds \right\} \left\{ \begin{array}{cc} 1 & \frac{\partial u}{\partial y} \\ 0 & 1 \end{array} \right\}
  $$

  \rightarrow \text{decomposition of the stress tensor } \sigma = \mu(u) \cdot D(u)

  $$
  \mu_{\text{int}}(u) = 2\eta_p \left( \begin{array}{cc} 1 & 2\Lambda \frac{\partial u}{\partial y} \\ 0 & 1 \end{array} \right) = \mu_{\text{diff}}(u)
  $$

- Similar to differential case: "Tensor Diffusion" known analytically
**μ** known „semi-analytically“ - PSM

- for fully developed channel flows, PSM reads

\[
\sigma = \int_0^\infty \frac{\eta_p}{\Lambda^2} \exp\left(-\frac{s}{\Lambda}\right) \frac{1}{1 + \gamma \left(s^2 \left(\frac{\partial u}{\partial y}\right)^2\right)} \begin{pmatrix}
 s^2 \left(\frac{\partial u}{\partial y}\right)^2 + 1 & s \frac{\partial u}{\partial y} \\
 s \frac{\partial u}{\partial y} & 1
\end{pmatrix} ds
\]

- similar to UCM, stress integral can be decomposed into

\[
\sigma = \begin{pmatrix}
 g \left(\frac{\partial u}{\partial y}\right) & h \left(\frac{\partial u}{\partial y}\right) \\
 0 & g \left(\frac{\partial u}{\partial y}\right)
\end{pmatrix} D(u) + \begin{pmatrix}
 f \left(\frac{\partial u}{\partial y}\right) & 0 \\
 0 & f \left(\frac{\partial u}{\partial y}\right)
\end{pmatrix}
\]

→ „Tensor Diffusion“ **μ** explicity modelled depending on \(\frac{\partial u}{\partial y}\)
µ known „semi-analytically“ - PSM

→ direct modelling of „Tensor Diffusion“ according to $\mu = \mu \left( \frac{\partial u}{\partial y} \right) \left( \frac{\partial u}{\partial y} \right) \approx \text{shear rate}$
• for 1D-flows, procedure in principle applicable for „all“ integral models
• isotropic part absorbed into pressure $P = p - f \left( \frac{\partial u}{\partial y} \right)$

→ „transform“ full viscoelastic integral model to generalized non-Newtonian model

$$- \nabla \cdot \left( \mu \left( \frac{\partial u}{\partial y} \right) \cdot D(u) \right) + \nabla P = 0, \quad \nabla \cdot u = 0$$

• complex rheology (arising from stress integral) hidden in „Tensor Diffusion“
• now: for PSM-channel flow solve only
  ▪ „generalized tensor-valued“ Stokes problem
  ▪ including non-vanishing tensor-valued viscosity (NEW!)
Poiseuille flow - PSM

- "wrong" initial parabolic velocity profile, evaluate "suitable" $\mu$
  
  \[ u_0 \rightarrow \mu_0 \Rightarrow u_1 \rightarrow \mu_1 \Rightarrow u_2 \ldots \]

→ pure *Stokes-like problem* gives viscoelastic solution from *integral model*
Flow around cylinder

- simulations via *four-field* formulation of „Tensor Stokes“-problem
- key feature: **monolithic Newton-multigrid approach**
- drag coefficient calculated via
  \[
  C_D(T) = \frac{2}{u_{\text{mean}}^2 R} \int_{E_c} \left( T_{xx} n_1 + T_{xy} n_2 \right) \frac{\partial \varphi}{\partial x} \, dx
  \]

→ specific total stress tensor problem-dependent:

\[
T_C = -\rho I + 2\eta_s D(u) + \sigma,
\]
\[
T_T = -\rho I + 2\eta_s D(u) + \frac{1}{2} (\mu \cdot D(u) + D(u) \cdot \mu^T)
\]

Oldroyd-B \((\eta_s = 0.59)\)  
Giesekus \((\alpha = 0.1, \eta_s = 0.59)\)

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- good agreement to original approach and reference
- appropriate solver behaviour
Conclusion
Summary

- original problem: nonlinear system in \((u, \sigma, p)\) for „no-solvent“ in 2D

\[
-2 \eta_s \nabla \cdot D(u) - \nabla \cdot \sigma + \nabla p = 0, \quad \nabla \cdot u = 0
\]

\[(u \cdot \nabla)\sigma - \nabla u^T \cdot \sigma − \sigma \cdot \nabla u + f(\Lambda, \eta_p, \sigma) = 2 \frac{\eta_p}{\Lambda} D(u) \text{ (or integral model)}\]

- introducing „Tensor Diffusion“ via \(\sigma = \mu \cdot D(u), \mu \in \mathbb{R}^{2\times2} \text{ or } \mathbb{R}^{3\times3}\)

- explicitly model (1D-flows, semi-analytically)

- four-field formulation (algebraic approach)

- three-field formulation (PDE approach)

- „Tensor Diffusion“ not known
- numerical calculation from algebraic equation/PDE
- validated, evaluated for complex test cases
- more numerical tests, detailed numerical analysis

currently most interesting for future work!
Outlook

- explicit (semi-analytical) model of „Tensor Diffusion“ \( \mu = \mu(u, D(u)) \)
- for 1D-flows, complex rheology can be hidden in \( \mu \left( \frac{\partial u}{\partial y} \right) \)
- generalization of direct modelling approach?
  → even for complex 2D-configurations: instead of nonlinear system...
    ...solve „Tensor Stokes“-problem in \((u, p)\) only
    \[
    - \frac{1}{2} \nabla \cdot (\mu(u) \cdot D(u) + D(u) \cdot \mu(u)^T) + \nabla p = 0,
    \quad \nabla \cdot u = 0
    \]

Can steady viscoelastic fluids be modelled as generalized non-Newtonian Stokes equations including a tensor-valued viscosity?