Simulation of “Extreme Fluids”

Examples, Challenges and Simulation Techniques for Flow Problems with Complex Rheology

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What are „Extreme“ Fluids?

Complex rheology with „extreme“ changes of viscosity:

- Dependence of shear rate, pressure and temperature
  - Generalized Newtonian, resp., non-Newtonian rheology
- Viscoelastic effects
  - Extra-Polymer stress („turbulence“)
- Many interacting objects in the fluid
  - Suspensions as particulate flow
- Special discretization/stabilization required
- Special solution techniques required
- Special software techniques required

Black Box???
Realization in FeatFlow

**HPC features:**
- Moderately parallel
- GPU computing
- Open source

**Non-Newtonian flow module:**
- Generalized Newtonian model (Power-law, Carreau,...)
- Viscoelastic 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*

**Numerical features:**
- Higher order (Q2P1) 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

**Hardware-oriented Numerics**

**Engineering aspects:**
- Geometrical design
- Modulation strategy
- Optimization

**Here:** FEM-based tools for the accurate simulation of (multiphase) flow problems, particularly with complex rheology

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Example: Screw Extruder (I)

- Numerical simulation of \textit{(twin)screw extruders} for \textit{polymer processing}
- \textit{Non-Newtonian rheological} models (shear \& temperature dependent) with \textit{non-isothermal} conditions (cooling from outside, heat production)
- \textit{Analysis} of the influence of local characteristics on the global product quality, prediction of hotspots and maximum shear rates
- \textit{Optimization} of torque acting on the screws, energy consumption

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Example: Screw Extruder (II)

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Example: Screw Extruder (III)

Combination of screw segments

Twin-screw-element library

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• **Generalized Navier-Stokes equations**

\[
\rho \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) u = -\nabla p + \nabla \cdot \sigma, \quad \nabla \cdot u = 0,
\]

\[
\rho c_p \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \Theta = k_1 \nabla^2 \Theta + k_2 D : D,
\]

\[
D(u) = \frac{1}{2} \left( \nabla u + (\nabla u)^T \right).
\]

\[
\sigma = \sigma_s + \sigma_p.
\]

• **Viscous stress**

\[
\sigma_s = 2 \eta_s (\dot{\gamma}, \Theta, p) D, \quad \dot{\gamma} = \sqrt{\text{tr} \left( D(u)^2 \right)}.
\]

• **Elastic stress**

\[
\mathbf{f}_1(L, \sigma_p) \sigma_p + \Lambda \nabla \sigma_p + F_2(\sigma_p, D) + F_3(\sigma_p) = 2\eta_p D(u).
\]
Constitutive Models (I)

- Viscous stress

\[
\sigma_s = 2 \eta_s (\dot{\gamma}, \Theta, p) D, \quad \dot{\gamma} = \sqrt{\text{tr}(D(u)^2)}. 
\]

- Power Law model

\[
\eta_s (\dot{\gamma}, \Theta, p) = \eta_0 (\varepsilon + \dot{\gamma}^2)^{\left(\frac{r}{2}-1\right)}, \quad (\eta_0 > 0, \ r > 1).
\]

- Generalized Cross model

\[
\eta_s (\dot{\gamma}, \Theta, p) = \eta_\infty + \frac{(\eta_0 - \eta_\infty)}{(1 + (\lambda \dot{\gamma})^{r_1})^r} \exp(\alpha p + (a_1 + \frac{a_2}{a_3 + \Theta})), \\
(\eta_0 > \eta_\infty \geq 0, \ r > 1, \ \lambda > 0).
\]
Constitutive Models (II)

- Generalized upper convective constitutive model

\[
f_1(L_k, \text{tr}(\sigma_p), \Lambda, \eta_p)\sigma_p + \Lambda \sigma_p + F_2(\sigma_p, D) + F_3(\sigma_p) = 2\eta_p D(u),
\]

\[
\nabla \sigma_p := \frac{\partial \sigma_p}{\partial t} + u \cdot \nabla \sigma_p - \nabla u \cdot \sigma_p - \sigma_p \cdot \nabla u^T.
\]

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<th>(f_1)</th>
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<td>(\Lambda = \Lambda(\dot{\gamma}), \eta_p = \eta_p(\dot{\gamma}))</td>
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<td>PTT</td>
<td>(f_1(\eta_p, \text{tr}(\sigma_p), \Lambda))</td>
<td>(\xi(D\sigma_p + \sigma_p D))</td>
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<td>Pom-Pom</td>
<td>(f_1(\text{tr}(\sigma_p), \Lambda))</td>
<td>(F_2(G, \sigma_p, \Lambda))</td>
<td>(F_3(G, \sigma_p^2, \alpha))</td>
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</tbody>
</table>
Constitutive Models (III)

- **Exemplary model: White-Metzner**

\[
\sigma_p + \Lambda(\dot{\gamma})\sigma_p = 2\eta_p(\dot{\gamma}, \Theta, p)D(u), \quad \dot{\gamma} = \sqrt{2D(u) : D(u)}
\]

- **Larson:**

\[
\Lambda(\dot{\gamma}) = \frac{\Lambda}{1 + a\Lambda \dot{\gamma}} \quad \eta_p(\dot{\gamma}, \Theta, p) = \frac{\eta_p}{1 + a\Lambda \dot{\gamma}}
\]

- **Cross:**

\[
\Lambda(\dot{\gamma}) = \frac{\Lambda}{1 + (\dot{\gamma})^{-n}} \quad \eta_p(\dot{\gamma}, \Theta, p) = \frac{\eta_p}{1 + (k\dot{\gamma})^{-m}}
\]

- **Carreau-Yasuda:**

\[
\Lambda(\dot{\gamma}) = \Lambda\left[1 + (\dot{\gamma})^{b}\right]^{\frac{n-1}{b}} \quad \eta_p(\dot{\gamma}, \Theta, p) = \eta_p\left[1 + (k\dot{\gamma})^{a}\right]^{\frac{m-1}{a}}
\]
Numerical Challenges

• Discretizations have to handle the following challenges points
  ➢ Stable FEM spaces for velocity/pressure and velocity/stress interpolation \( \tilde{Q}_2 / P_1^{\text{disc}} \) or \( \tilde{Q}_1 / \tilde{Q}_1 / P_0 \) or \( \tilde{Q}_2 / \tilde{Q}_2 / P_1^{\text{disc}} \)
  ➢ Special treatment of the convective terms: edge-oriented/interior penalty (EO-FEM), TVD/FCT
  ➢ High Weissenberg number problem (HWNP): LCR (Reformulation)
  ➢ Locally adapted meshes due to steep gradients: GDM

• Solvers have to deal with different sources of nonlinearity
  ➢ Nonlinearity: Newton method
  ➢ Strong coupling of equations: monolithic multigrid approach

• Complex geometries (and meshes)
  ➢ FBM + distance based Level Set FEM for free interfaces
**Problem Reformulation (I)**

**Elastic stress** \( \rightarrow (u, p, \sigma_p) \)

\[
\rho \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) u = -\nabla p + 2 \nabla \cdot \eta_s D + \nabla \cdot \sigma_p, \quad \nabla \cdot u = 0
\]

(1) \[
f_1(L, \sigma_p) \sigma_p + \Lambda \sigma_p + F_2(\sigma_p, D) + F_3(\sigma_p) = 2\eta_p D(u)
\]

**Conformation stress** \( \rightarrow (u, p, \sigma_c) \) is positive definite by design !!

Replace \( \sigma_p \) in (1) with \( \sigma_p = \frac{\eta_p}{\Lambda} (\sigma_c - I) \) \( \rightarrow \) special discretization: TVD

\[
\rho \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) u = -\nabla p + 2 \nabla \cdot \eta_s D + \frac{1}{\Lambda} \nabla \cdot \eta_p \sigma_c, \quad \nabla \cdot u = 0,
\]

(2) \[rown \sigma_c + F_4(\sigma_c, u) = 0
\]
Problem Reformulation (II)

\[ \sigma_c(t) = \int_{-\infty}^{t} \frac{1}{We^2} \exp\left(\frac{-(t-s)}{We}\right) F(s, t) F(s, t)^T \, ds \]

Positive by design, so we can take its logarithm

2 Observations:
- positive definite \(\rightarrow\) special discretizations like FCT/TVD
- exponential behaviour \(\rightarrow\) approximation by polynomials???
**Problem Reformulation (III)**

**Driven Cavity:**
as $We$ number changes from $We=0.5$ to $We=1.5$, the stress value jumps significantly

Old Formulation Vs Lcr

- $We=0.5$  - $We=1.5$

**Cutline of Stress_11 component at $y=1.0$**
Problem Reformulation (IV)

• **Experience:**
  - Stresses grow exponentially
  - Conformation tensor is positive by design

• **Fattal and Kupferman:**
  - Take the logarithm as a new variable \( \sigma_{LCR} = \log \sigma_c \) using the eigenvalue decomposition
    \[
    \sigma_{LCR} = R \log(\lambda_{\sigma_c}) R^T
    \]
  - Decompose the velocity gradient inside the stretching part
    \[
    \nabla u = B + \Omega + N\sigma_c^{-1}
    \]

Remark for PTT only
\[
L = B + \Omega + N\sigma_c^{-1}, \quad L = \nabla u - \xi D
\]

**LCR can be applied to all upper convective models**
Problem Reformulation (V)

\[ f_1(L, \sigma_p) \sigma_p + \Lambda \sigma_p + F_2(\sigma_p, D) + F_3(\sigma_p) = 2\eta_p D(u) \]

\[ \nabla \sigma_c + F_4(\sigma_c, u) = 0 \]

\[ \nabla u = \Omega + B + N\sigma_c^{-1} \]

\[ \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \sigma_c - (\Omega \sigma_c - \sigma_c \Omega) + 2B\sigma_c = \frac{1}{\Lambda} \left( I - \sigma_c \right) \]

\[ \sigma_c = \exp \sigma_{LCR} \]

\[ \sigma_{LCR} = R \log(\lambda_{\sigma_c}) R^T \]

\[ \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \sigma_{LCR} - (\Omega \sigma_{LCR} - \sigma_{LCR} \Omega) - 2B = F_4(\sigma_{LCR}, u). \]
Full Set of Equations

- **Generalized Newtonian (VP)**
  \[
  \rho \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) u = -\nabla p + \nabla \cdot \left( 2\eta_s(\dot{\gamma}, \Theta, p)D(u) \right) + \frac{1}{\Lambda} \nabla \cdot \eta_p e^{\sigma_{LCR}}, \quad \nabla \cdot u = 0,
  \]

- **Non-isothermal effect (T)**
  \[
  \rho c_p \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \Theta = k_1 \nabla^2 \Theta + k_2 D : D,
  \]

- **LCR equation (S)**
  \[
  \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) \sigma_{LCR} - (\Omega \sigma_{LCR} - \sigma_{LCR} \Omega) - 2B = F_4(\sigma_{LCR}, u).
  \]

\[\text{Referred to all upper convective constitutive models}\]
Exemplary Viscoelastic Models

Oldroyd-B/UCM

\[ F_4 = \frac{1}{\Lambda} (e^{-\sigma_{LCR}} - I) \]

Giesekus

\[ F_4 = \frac{1}{\Lambda} \left( e^{-\sigma_{LCR}} - I - \alpha \varepsilon^{\sigma_{LCR}} - (e^{-\sigma_{LCR}} - I)^2 \right) \]

FENE-P/-CR

\[ F_4 = \frac{1}{\Lambda} f(R)(e^{-\sigma_{LCR}} - I) \quad \text{or} \quad F_4 = \frac{1}{\Lambda} \left( e^{-\sigma_{LCR}} - f(R)I \right) \]

White-Metzner

\[ F_4 = \frac{1}{\Lambda(\dot{\gamma})} \left( e^{-\sigma_{LCR}} - I \right) \]

Linear PTT

\[ F_4 = \frac{1}{\Lambda} \left( 1 + \varepsilon(\text{tr}(e^{\sigma_{LCR}} - 3))(e^{-\sigma_{LCR}} - I) \right) \]

Exponential PTT

\[ F_4 = \frac{1}{\Lambda} \exp(\varepsilon(\text{tr}(e^{\sigma_{LCR}} - 3))(e^{-\sigma_{LCR}} - I)) \]

Pom-Pom

\[ F_4 = -\frac{1}{\Lambda} \left( [f(\sigma_{LCR}) - 2\alpha]e^{\sigma_{LCR}} + \alpha e^{2\sigma_{LCR}} + (\alpha - 1)I \right) \]
FEM Discretization

- High order $Q_2/Q_2/P_1^{disc}$ for velocity-stress-pressure

- Advantages:
  - Inf-sup stable for velocity and pressure
  - High order: good for accuracy
  - Discontinuous pressure: good for solver & physics

- Disadvantages:
  - Stabilization for same spaces for stress-velocity
  - a single d.o.f. belongs to four elements (in 2D)

Compatibility condition between the stress and velocity spaces via EO-FEM
Variational Formulations

- **Standard Navier-Stokes bilinear forms**

\[
a(u, v) = \int_{\Omega} \frac{1}{\Delta t} u \cdot v \, d\Omega + \int_{\Omega} 2\eta_s D(u) : D(v) \, d\Omega
\]

\[
b(p, v) = -\int_{\Omega} p \, \nabla \cdot v \, d\Omega
\]

- **Nonsymmetric bilinear forms due to LCR**

\[
c(\sigma_{LCR}, v) = \int_{\Omega} \exp(\sigma_{LCR}) : D(v) \, d\Omega
\]

\[
\tilde{c}(\tau, u) = -2\int_{\Omega} B(\nabla u, \sigma_c) : \tau \, d\Omega
\]
Variational Formulations

- **Nonlinear tensor variational form due to LCR**
  \[ d(\sigma_{LCR}, \tau) = \int_{\Omega} \left( \frac{1}{\Delta t} + (u \cdot \nabla) \right) \sigma_{LCR} : \tau \, dx \]
  \[ - \int_{\Omega} (\Omega \sigma_{LCR} - \sigma_{LCR} \Omega) : \tau \, dx - \int_{\Omega} F_4(\sigma_{LCR}, u) : \tau \, dx \]

- **Nonsymmetric bilinear forms due to LCR**
  \[ e(\Theta, \Phi) = \int_{\Omega} \left( \frac{1}{\Delta t} + u \cdot \nabla \right) \Theta \Phi \, dx + \int_{\Omega} k \nabla \Theta \cdot \nabla \Phi \, dx \]
  \[ - \int_{\Omega} 2\eta_s [D(u) : D(u)] \Phi \, dx - \int_{\Omega} D(u) : \exp(\sigma_{LCR}) \Phi \, dx \]

- **Source term**
  \[ l(u, \sigma_{LCR}, \Theta, p) \]
Problem Formulation

- Set \( X := \left[ H^1_0(\Omega) \right]^2 \times \left[ L^2(\Omega) \right]^4 \times H^1(\Omega), \ Q := L^2_0(\Omega) \)

\[ \tilde{u} := (u, \sigma_{LCR}, \Theta) \quad \tilde{A} := \begin{bmatrix} A & C & 0 \\ \tilde{C}^T & D & 0 \\ E_{fD} & E_{\sigma_{LCR}} & E \end{bmatrix} \]

- Find \((\tilde{u}, p) \in X \times Q\) such that

\[ \langle K(\tilde{u}, p), (\tilde{v}, q) \rangle = \langle l(\tilde{v}, q) \rangle \quad \forall (\tilde{v}, q) \in X \times Q \]

\[ K = \begin{bmatrix} \tilde{A} & \tilde{B} \\ B^T & 0 \end{bmatrix} \]

(Non-)Classical saddle point problem
Compatibility Conditions

- Compatibility condition

\[
\begin{align*}
\sup_{u \in [H_0^1(\Omega)]^3} \int_\Omega \nabla \cdot u \ q \ dx & \geq \beta_1 \| q \|_{0, \Omega} \quad \forall q \in L_0^2(\Omega) \\
\sup_{\sigma \in [L^2(\Omega)]^4} \int_\Omega \sigma : \nabla u \ dx & \geq \beta_2 \| u \|_{1, \Omega} \quad \forall u \in [H_0^1(\Omega)]^2
\end{align*}
\]
• Edge-oriented stabilization for

- Equal order finite element interpolation for velocity and stress

- Convective dominated problem

\[ \langle J \tilde{u}, \tilde{v} \rangle = \sum_{\text{edge } E} \max(\gamma u \eta_p h_E, \gamma \tilde{u} h_E^2) \int_E [\nabla \tilde{u}][\nabla \tilde{v}] ds \]

with \( \tilde{u} = (u, \sigma, \Theta) \), \( \tilde{v} = (v, \tau, \Phi) \) and \([\nabla \tilde{u}][\nabla \tilde{v}] = \sum_i [\nabla \tilde{u}_i][\nabla \tilde{v}_i] \)

Then: Efficient Newton-type and multigrid solvers can be „easily“ applied
Nonlinear Solver

- Damped Newton results in the solution of the form

\[ R(x) = 0, \quad x = (u, \sigma_{LCR}, \Theta, p) \]

\[ x^{l+1} = x^l + \omega^l \left[ \frac{\partial R(x^l)}{\partial x} \right]^{-1} R(x^l) \]

- Inexact Newton: Jacobian is approximated using finite differences

\[ \left[ \frac{\partial R(x^l)}{\partial x} \right]_{ij} \approx \frac{R_j(x + \varepsilon e_i) - R_j(x - \varepsilon e_i)}{2\varepsilon} \]
Jacobian Matrix

- The Jacobian matrix takes the form

\[
J = \begin{bmatrix}
\frac{\partial R(x^n)}{\partial x} \\
\end{bmatrix} = \begin{bmatrix}
A & \tilde{B}^T \\
B & 0 \\
\end{bmatrix}
\]

- Generalized non-isothermal non-Newtonian problem

\[
A = \begin{bmatrix}
A_u & \tilde{C}^T & \tilde{H}^T \\
C & A_\sigma & 0 \\
H & 0 & A_\phi \\
\end{bmatrix}
\]

Modified saddle point problem
• Monolithic multigrid solver

  ➢ Standard geometric multigrid approach

  ➢ Full $Q_2, P_1^{\text{disc}}$ restrictions and prolongations

  ➢ Local MPSC via Vanka-like smoother

\[
\begin{bmatrix}
\tilde{u}^{l+1} \\
p^{l+1}
\end{bmatrix} =
\begin{bmatrix}
\tilde{u}^l \\
p^l
\end{bmatrix} + \omega^l \sum_{T \in T_h} [J_{|T}]^{-1} \begin{bmatrix}
R_u(\tilde{u}^l, p^l) \\
R_p(\tilde{u}^l, p^l)
\end{bmatrix}_{|T}
\]

**Fully implicit Monolithic FEM-Multigrid Solver**

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Linear Solver

Vanka-like Smoother

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Algorithm 1: Smoothing steps

Input: Predefined constant: $\omega > 0$, Number of smoothing steps: NSM

1. for $j = 1$ to NSM do
2. for $K \in \Omega_h$ do
3. \[
    x_{I(K)} \leftarrow x_{I(K)} + \omega C_K^{-1}(b - Ax)_{I(K)}
\]
4. Return $x$
5. end
Dynamic ALE-Mesh Adaptation

Advantages:
• Constant mesh/data structure $\rightarrow$ GPU
• Increased resolution in regions of interest ("r-adaptivity")
• Anisotropic ‘umbrella’ smoother (with snapping/projection) or GDM
• Straightforward usage on general meshes in 2D / 3D

Quality of the method depends on the construction of the monitor function
• Geometrical description (solid body, interface triangulation)
• Field oriented description (steep gradients, fronts) $\rightarrow$ numerical stabilization

Validation: 2.5D Rising bubble – light setup
Testing: 3D Rising bubble - hard setup
Test: Oscillating Cylinder

- Measure Drag/Lift Coefficients for a sinusoidally oscillating cylinder
- Compare results for FBM, adapted FBM and adapted FBM + boundary projection/parametrization

Nodes concentrated near liquid-solid interface
Nodes projected and parametrized on boundary plus concentration of nodes near boundary

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Oscillating Cylinder Results

Drag Coefficient $C_D$ for Classic FBM, FBM+adapt, FBM+param+adapt.

- Classic FBM
- FBM+adapt
- FBM+param+adapt
Viscous Liquid Jets

J. M. Nóbrega et al.: The phenomenon of jet buckling: Experimental and numerical predictions

Corn syrup-air system

24x24x48 mesh

Interface triangulation:

$T_0$: ~100,000 triangles

$T_N$: ~300,000 triangles

$F_i = - \sum_{T \in T_h, \Omega} \sigma_{h} \cdot \nabla \alpha_{h,i} \, d\Omega$.

Rendering: Raphael Münster / Blender

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Benchmark Problem

- **Coarse grid and mesh information**

- **n.o.f. for different problems**

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<th>Level</th>
<th>n.o.f. u</th>
<th>n.o.f. p</th>
<th>n.o.f. T</th>
<th>n.o.f. S</th>
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### Newtonian Problem (VP)

#### Navier-Stokes Re=20

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<th>N/L</th>
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#### Level independent solver

*Stokes vs. Navier-Stokes*
### Power Law Problem (VP)

#### \( \varepsilon = 10^{-2}, r = 1.5 \)

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#### \( \varepsilon = 10^{-4}, r = 1.5 \)

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#### \( \varepsilon = 10^{-2}, r = 3 \)

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#### \( \varepsilon = 10^{-4}, r = 3 \)

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<td>13.77970</td>
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\[ \eta_s(\dot{\gamma}, \Theta, p) = \eta_0(\varepsilon + \dot{\gamma}^2)^{\frac{r-1}{2}}, (\eta_0 > 0, r > 1). \]
Cross Model Problem (VP)

\[ \eta_s(\dot{\gamma}, \Theta, p) = \eta_x + \frac{(\eta_0 - \eta_x)}{(1 + (\lambda \dot{\gamma})^\gamma)} \exp(\alpha p + (\frac{a_1 + a_2}{a_3 + \Theta})) \]

\[ \eta_x = 10^{-3}, \quad a_1 = a_2 = 0, \]

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\[ r = 0, \ r_i = 1, \ \alpha = 0.1, \ \eta_0 = 10^{-1} \]

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Level and model independent solver

S. Turek | Simulation of Extreme Fluidics
Cross Model problem (VTP)

Non heated cylinder

\[ \eta_s(\dot{\gamma}, \Theta, p) = \eta_\infty + \frac{(\eta_0 - \eta_\infty)}{(1 + (\dot{\gamma})^n)^r} \exp(\alpha p + (a_1 + \frac{a_2}{a_3 + \Theta})) \]

\[ \eta_\infty = 10^{-3}, \quad a_1 = 0, \quad a_3 = 1, \quad k_1 = k_2 = 10^{-2}, \]

\[ r = 0.1, \ r_1 = 1, \ \alpha = 0, \ \eta_0 = 10^{-1}, \ a_2 = 0. \]

### Level and model independent solver

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<thead>
<tr>
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\[ r = 0, \ r_1 = 1, \ \alpha = 0, \ \eta_0 = 10^{-2}, \ a_2 = 0. \]

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\[ r = 0.1, \ r_1 = 1, \ \alpha = 0, \ \eta_0 = 10^{-2}, \ a_2 = 1. \]

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Cross Model Problem (VTP)

Heated cylinder

\[ \eta_s(\dot{\gamma}, \Theta, p) = \eta_s + \frac{(\eta_0 - \eta_s)}{(1 + (\dot{\gamma}^+)^n)} \exp(\alpha p + (a_1 + \frac{a_2}{a_3 + \Theta})) \]

\[ \eta_s = 10^{-3}, r = 0.1, r_1 = 1, \alpha = 10^{-3}, a_1 = 0, a_2 = 1, a_3 = 1, \]

\[ \eta_s = 10^{-1}, k_1 = k_2 = 10^{-2}. \]

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\[ \eta_s = 10^{-3}, k_1 = k_2 = 10^{-2}. \]

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\[ \eta_s = 10^{-1}, k_1 = k_2 = 10^{-2}. \]

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\[ \eta_s = 10^{-1}, k_1 = k_2 = 10^{-3}. \]

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Level and model independent solver

S. Turek | Simulation of Extreme Fluidics
Barus Model Problem (VP)

- **Coarse grid and mesh information**

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\[ \eta_s(\dot{\gamma}, \Theta, p) = \eta_0 \exp^{\alpha p} \]

- \( \eta_0 = 0.105 \)
- \( \alpha = 0.1 \)
Barus Model Problem (VP)

Mesh1, \( r = 0.15 \)

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Mesh2, \( r = 0.25 \)

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Mesh3, \( r = 0.30 \)

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Level and parameter independent solver

S. Turek | Simulation of Extreme Fluidics
### Viscoelastic Fluids (VSP)

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**Oldroyd-B**

### Level independent solver

### Giesekus

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### Oldroyd-B

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**Oldroyd-B**

### Giesekus

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S. Turek | Simulation of Extreme Fluidics
Viscoelastic Fluids (VSP)

Lower We vs. higher We

S. Turek | Simulation of Extreme Fluidics
### Viscoelastic Fluids (VSP)

#### Lower We vs. higher We

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Flow around Cylinder Benchmark

Coarse grid and mesh information

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<td>944</td>
<td>22457</td>
</tr>
<tr>
<td>R3a3</td>
<td>1520</td>
<td>35715</td>
</tr>
<tr>
<td>R3a4</td>
<td>2672</td>
<td>62221</td>
</tr>
<tr>
<td>R3a5</td>
<td>4976</td>
<td>115223</td>
</tr>
</tbody>
</table>

Local refinement via hanging nodes
Flow around Cylinder Benchmark

- Planar flow around cylinder (Oldroyd-B)

![Graph showing drag coefficient versus We number](image)
### Flow around Cylinder Benchmark

- **Oldroyd-B**

<table>
<thead>
<tr>
<th>We</th>
<th>Drag</th>
<th>NL</th>
<th>We</th>
<th>Drag</th>
<th>NL</th>
<th>We</th>
<th>Drag</th>
<th>NL</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>130.366</td>
<td>8</td>
<td>0.8</td>
<td>117.347</td>
<td>4</td>
<td>1.5</td>
<td>125.665</td>
<td>4</td>
</tr>
<tr>
<td>0.3</td>
<td>123.194</td>
<td>4</td>
<td>1.0</td>
<td>118.574</td>
<td>6</td>
<td>1.7</td>
<td>129.494</td>
<td>4</td>
</tr>
<tr>
<td>0.5</td>
<td>118.828</td>
<td>4</td>
<td>1.2</td>
<td>120.919</td>
<td>5</td>
<td>1.9</td>
<td>133.754</td>
<td>4</td>
</tr>
<tr>
<td>0.6</td>
<td>117.779</td>
<td>4</td>
<td>1.3</td>
<td>122.350</td>
<td>4</td>
<td>2.0</td>
<td>136.039</td>
<td>5</td>
</tr>
<tr>
<td>0.7</td>
<td>117.321</td>
<td>4</td>
<td>1.4</td>
<td>123.936</td>
<td>4</td>
<td>2.1</td>
<td>138.438</td>
<td>5</td>
</tr>
</tbody>
</table>

- **Giesekus**

<table>
<thead>
<tr>
<th>We</th>
<th>Drag</th>
<th>Peak2</th>
<th>NL</th>
<th>We</th>
<th>Drag</th>
<th>Peak2</th>
<th>NL</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>96.943</td>
<td>924.45</td>
<td>14</td>
<td>60</td>
<td>85.859</td>
<td>12010.57</td>
<td>4</td>
</tr>
<tr>
<td>20</td>
<td>89.905</td>
<td>4204.51</td>
<td>12</td>
<td>70</td>
<td>85.365</td>
<td>13773.61</td>
<td>4</td>
</tr>
<tr>
<td>30</td>
<td>88.304</td>
<td>6318.79</td>
<td>5</td>
<td>80</td>
<td>84.937</td>
<td>15502.45</td>
<td>4</td>
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<tr>
<td>40</td>
<td>87.256</td>
<td>8311.32</td>
<td>5</td>
<td>90</td>
<td>84.585</td>
<td>17207.87</td>
<td>4</td>
</tr>
<tr>
<td>50</td>
<td>86.476</td>
<td>10199.1</td>
<td>4</td>
<td>100</td>
<td>84.287</td>
<td>18897.95</td>
<td>4</td>
</tr>
</tbody>
</table>

**Efficient continuation for increasing We numbers**

S. Turek | Simulation of Extreme Fluidics
Flow around Cylinder Benchmark

- Direct steady vs. non-steady approach for Giesekus

Drag values

Conformation stress - Peak 2

Time

Time
Flow around Cylinder Benchmark

- Axial stress w.r.t. X-curved: Oldroyd-B vs. Giesekus

\[ W_e = 0.7 \]

Lack of pointwise mesh convergence due to model (?)
3D Viscoelastic Flow Simulations

Flow past a sphere benchmark: R.G. Owens T. N. Phillips

<table>
<thead>
<tr>
<th>Resolution</th>
<th>$\max_1(\tau_{xx})$</th>
<th>$\max_2(\tau_{xx})$</th>
<th>$F^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>L2</td>
<td>20.80</td>
<td>2.082</td>
<td>5.6976</td>
</tr>
<tr>
<td>L3</td>
<td>19.29</td>
<td>2.081</td>
<td>5.6946</td>
</tr>
<tr>
<td>L4</td>
<td>18.72</td>
<td>2.086</td>
<td>5.6941</td>
</tr>
<tr>
<td>L5</td>
<td>18.52</td>
<td>2.087</td>
<td>5.6940</td>
</tr>
</tbody>
</table>

Authors

Lunsmann [4] - - 5.6937
Owens [5] 18.27 - 5.6963

<table>
<thead>
<tr>
<th>Resolution</th>
<th>$\max_1(\tau_{xx})$</th>
<th>$\max_2(\tau_{xx})$</th>
<th>$F^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>L2</td>
<td>50.31</td>
<td>5.041</td>
<td>5.4170</td>
</tr>
<tr>
<td>L3</td>
<td>39.01</td>
<td>5.061</td>
<td>5.4133</td>
</tr>
<tr>
<td>L4</td>
<td>36.43</td>
<td>5.104</td>
<td>5.4128</td>
</tr>
<tr>
<td>L5</td>
<td>35.65</td>
<td>5.118</td>
<td>5.4128</td>
</tr>
</tbody>
</table>

Authors

Lunsmann [4] 35.17 - 5.4123
Owens [5] 35.67 - 5.4117
Sahin [6] 34.73 5.12 -
3D Viscoelastic Flow Simulations

M. Sahin: 3D flow past a cylinder benchmark

Prediction of special viscoelastic flow features for increased We numbers

We=1.2

We=1.8

Separation line between the upper/lower streams
Non-Newtonian Multiphase Flow

Single phase validation on 2D benchmark “flow around a cylinder”

<table>
<thead>
<tr>
<th>level</th>
<th>Shear thining n=0.75</th>
<th>Shear thickening n=1.50</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Damanik*</td>
<td>Our results</td>
</tr>
<tr>
<td></td>
<td>C_D</td>
<td>C_L</td>
</tr>
<tr>
<td>1</td>
<td>3.20082</td>
<td>-0.01261</td>
</tr>
<tr>
<td>2</td>
<td>3.26433</td>
<td>-0.01342</td>
</tr>
<tr>
<td>3</td>
<td>3.27739</td>
<td>-0.01342</td>
</tr>
</tbody>
</table>

Viscosity distribution

Pseudo 2D rising bubble in Power-Law fluids  Droplet generation for Power-Law fluids

Mesh converged bubble shapes for n = 0.5, 1.0, 2.0

Jet formation  n=1.0

Dripping  n=0.5

Reference: Damanik et al.

S. Turek | Simulation of Extreme Fluidics
Material 1: Viscoelastic fluid described by the Oldroyd-B model

Material 2: Newtonian fluid

<table>
<thead>
<tr>
<th>Test case</th>
<th>$\rho_1$</th>
<th>$\rho_2$</th>
<th>$\mu_1$</th>
<th>$\mu_2$</th>
<th>$g$</th>
<th>$\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. Viscoelastic ($\Lambda = 10$)</td>
<td>10</td>
<td>0.1</td>
<td>10</td>
<td>1</td>
<td>9.8</td>
<td>0.245</td>
</tr>
<tr>
<td>2. Newtonian ($\Lambda = 0$)</td>
<td>10</td>
<td>0.1</td>
<td>10</td>
<td>1</td>
<td>9.8</td>
<td>0.245</td>
</tr>
<tr>
<td>3. Viscoelastic ($\Lambda = 10$)</td>
<td>10</td>
<td>0.1</td>
<td>2</td>
<td>1</td>
<td>9.8</td>
<td>0.245</td>
</tr>
<tr>
<td>4. Newtonian ($\Lambda = 0$)</td>
<td>10</td>
<td>0.1</td>
<td>2</td>
<td>1</td>
<td>9.8</td>
<td>0.245</td>
</tr>
</tbody>
</table>
Encapsulation Processes

- Numerical simulation of micro-fluidic drug encapsulation ("monodisperse compound droplets")
- Polymeric "bio-degradable" outer fluid with generalized Newtonian behaviour
- Optimization w.r.t. boundary conditions, flow rates, droplet size, geometry

In Pharmaceutics
- Controlled drug release
- Protection of chemically active ingredients (from both sides)
- Protection against shear stress in stirred reactors
- Protection against evaporation
- Taste or odor masking

Jet Configuration
- Core material is defined as the specific material that requires to be coated (liquid, emulsion, colloid or solid)
- Shell material is present to protect and stabilize the core (Alginate, Chitosan, Gelatin, Pectin, Waxes, Starch)
## Encapsulation Processes

<table>
<thead>
<tr>
<th>mgLS(^{(2)})-FBM-FEM flow module</th>
<th>Tasks related to code development</th>
<th>Tasks related to application</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Multiple Level Set fields for simulation of liquid core encapsulation - l/l/g</td>
<td>• Validation via experimental results</td>
<td></td>
</tr>
<tr>
<td>• Fictitious boundary method for particle encapsulation - s/l/g</td>
<td>• Modulation for monodisperse compound drops</td>
<td></td>
</tr>
</tbody>
</table>

**Ketoprofen/Ketoprofen Lysinate core**

**Alginate shell**

Preliminary simulation results for encapsulation of solid particles

Aqueous solutions of alginates have shear-thinning characteristics.
Robust numerical and algorithmic tools are available using

- Classical and Log Conformation Reformulation (LCR)
- Monolithic Finite Element Approach
- Edge Oriented stabilization (EO-FEM) and local GDM
- Fast Newton-Multigrid Solver with local MPSC smoother

for the simulation of nonlinear flow with (extreme) rheological behaviour

Advantages

- No CFL-condition restriction due to the fully implicit coupling
- Positivity preserving
- Higher order and local adaptivity
Compatibility Conditions for LCR

- The non-symmetric bilinear forms due to LCR

\[ \tau \in T_{PD} \subset \left[ L^2(\Omega) \right]^4 \] such that \( \tau \) is positive definite

\[ c(\tau, v) = \int_{\Omega} \exp(\tau) : D(v) \, d\Omega \]

\[ \geq \beta_2 \| \exp(\tau) \|_{0,\Omega} \| v \|_{1,\Omega} \]

\[ \geq \beta_2 \| \tau \|_{0,\Omega} \| v \|_{1,\Omega} \quad \forall \tau \in T_{PD}, \quad \forall v \in \left[ H^1_0(\Omega) \right]^2 \]

\[ \tilde{c}(\tau, u) = -2 \int_{\Omega} B(\nabla u, \sigma_c) : \tau \, d\Omega \]

\[ \geq \beta_2 \| \tau \|_{0,\Omega} \| v \|_{1,\Omega} \quad \forall \tau \in \left[ L^2(\Omega) \right]^4, \quad \forall v \in \left[ H^1_0(\Omega) \right]^2 \]
Higher Order Nonconforming FEM

- Larger FE space which allows high order approximation
- d.o.f.s belong to at most two elements which is good for parallelisation
- Coupling of different polynomial orders
  - Mortar condition: test space \( \approx \) order at slave side
  \[
  |E|^{-1} \int_{E_i} u_h|K_2 L_{E_i,k} \, ds = |E|^{-1} \int_{E_i} u_h|K_1 L_{E_i,k} \, ds, \quad 0 \leq k < 2
  \]
  - No hanging nodes
What are „Extreme Fluids“???