Multiscale simulation of polymeric fluids using massively parallel computers

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OUTLINE

1. Modeling equations for multiscale approach
2. Numerical discretization
3. Simulation result: 3D contraction flow
4. Computational complexity
MODELING OF POLYMERIC FLUIDS

Two different modeling approaches:

<table>
<thead>
<tr>
<th>overview</th>
<th>macroscopic</th>
<th>multiscale</th>
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<tbody>
<tr>
<td>cost</td>
<td>low</td>
<td>high</td>
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<td>modeling accuracy</td>
<td>low</td>
<td>high</td>
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<tr>
<td>drawbacks</td>
<td>num. instabilities</td>
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1 Le Bris and Lelièvre 2009
Position vector \( x \) in flow space \( \mathcal{O} \subset \mathbb{R}^3 \).

\( q = (q_1, \ldots, q_N) \) in configuration space \( \mathcal{D} \subset \mathbb{R}^{3N} \).
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Description of a polymer ensemble

- **Stochastic approach:** random field \( \mathbf{Q} = (Q_1, \ldots, Q_N) \) with \( \mathbf{Q} : (\mathbf{x}, t) \in \mathcal{O} \times \mathcal{T} \mapsto \mathbf{Q}(\mathbf{x}, t) \) as \( \mathcal{D} \)-valued random variable.

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\(^1\) Laso and Öttinger 1993
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- **Fokker-Planck ansatz:**\(^2\) probability density function of field \( \mathbf{Q} \)
  - \( \psi : (\mathbf{x}, \mathbf{q}, t) \in \mathcal{O} \times \mathcal{D} \times \mathcal{T} \subset \mathbb{R}^{3N+4} \mapsto \psi(\mathbf{x}, \mathbf{q}, t) \in \mathbb{R}^+ \).
  - \( \int_{\mathcal{D}} \psi(\mathbf{x}, \mathbf{q}, t) \, d\mathbf{q} = 1 \) for all \( (\mathbf{x}, t) \in \mathcal{O} \times \mathcal{T} \).

---

\(^1\)Laso and Öttinger 1993 \(,\) \(^2\)Lozinski and Chauvière 2003
COUPLING OF MICRO- AND MACROSCOPIC SCALE

- Elastic fluid behavior modeled with macroscopic stress tensor

\[ \tau_p : (x, t) \in \mathcal{O} \times \mathcal{T} \mapsto \tau_p(x, t) \in \mathbb{R}^{3 \times 3}. \]
COUPLING OF MICRO- AND MACROSCOPIC SCALE

- Elastic fluid behavior modeled with macroscopic stress tensor $\mathbf{\tau}_p : (\mathbf{x}, t) \in \mathcal{O} \times \mathcal{T} \mapsto \mathbf{\tau}_p(\mathbf{x}, t) \in \mathbb{R}^{3 \times 3}$.

- Kramers’ relation for stress tensor

$$\mathbf{\tau}_p(\mathbf{x}, t) = \begin{pmatrix} \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \end{pmatrix}(\mathbf{x}, t) = C \sum_{i=1}^{N} \left( \mathbb{E} [ \mathbf{Q}_i(\mathbf{x}, t) \otimes \mathbf{F}(\mathbf{Q}_i(\mathbf{x}, t))] - \mathbf{Id} \right)$$

- Expectation $\mathbb{E} [ \cdot ] = \int_{\mathcal{D}} \cdot \psi(\mathbf{x}, \mathbf{q}, t) \, d\mathbf{q}$ in configuration space $\mathcal{D}$.
- Spring force $\mathbf{F} : \mathcal{D}_i \subset \mathbb{R}^3 \to \mathbb{R}^3$.

---

1Kramers 1944
COUPLING OF MICRO- AND MACROSCOPIC SCALE

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- Kramers'\(^1\) relation for stress tensor
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  \tau_p(x, t) = \begin{pmatrix}
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  \end{pmatrix} (x, t) = C \sum_{i=1}^{N} \left( \mathbb{E} \left[ Q_i(x, t) \otimes F(Q_i(x, t)) \right] - \text{Id} \right)
  \]

- expectation \( \mathbb{E} [\cdot] = \int_D \cdot \psi(x, q, t) \, dq \) in configuration space \( D \).
- spring force \( F : D_i \subset \mathbb{R}^3 \to \mathbb{R}^3 \).

- Various spring force models \( F \) in the literature
  - **Hooke model**: \( F(Q_i) = Q_i \) \hspace{1cm} (linear)
  - **FENE model\(^2\)**: \( F(Q_i) = \frac{Q_i}{1-\|Q_i\|^2/b} \) with \( \|Q_i\|^2 \leq b \in \mathbb{R}^+ \) \hspace{1cm} (nonlinear)
  - **CPAIL model\(^3\)**: \( F(Q_i) = \frac{1-\|Q_i\|^2/(3b)}{1-\|Q_i\|^2/b} Q_i \) with \( \|Q_i\|^2 \leq b \in \mathbb{R}^+ \) \hspace{1cm} (nonlinear)

---

\(^1\)Kramers 1944, \(^2\)Warner 1972, \(^3\)Cohen 1991
**Stochastic multiscale system**

\[
\frac{DU(x, t)}{Dt} = -\nabla P(x, t) + \frac{\beta}{Re} \Delta U(x, t) + \frac{1}{Re} \nabla \cdot \tau_p(x, t) \quad (1)
\]

\[
\nabla \cdot U(x, t) = 0 \quad (2)
\]

\[
dQ(x, t) = \left[ -U(x, t)\nabla Q(x, t) + (\nabla U(x, t))^T Q(x, t) - \frac{1}{4De} A \cdot F(Q(x, t)) \right] dt + \sigma dW(t) \quad (3)
\]

\[
\tau_p(x, t) = C \sum_{i=1}^{N} (\mathbb{E}[Q_i(x, t) \otimes F(Q_i(x, t))] - \text{Id}) . \quad (4)
\]

for the unknown random fields \( U, P, Q, \tau_p \),
dimensionless parameters \( De, Re, \beta, \sigma \in \mathbb{R}^+ \)
+ initial and boundary conditions.

(1)+(2) Navier-Stokes equations *(macroscopic)*

(3) Stochastic PDE *(microscopic)*

(4) upscaling from micro- to macroscopic scale
**Stochastic approach for microscale**$^{1,2}$

- Approximation of random field $Q(x_k, t)$ at discrete points $x_k$ with 3$N$-dimensional **samples** $Q^{(j)}(x_k, t) \sim \psi(x_k, \cdot, t)$ for $j = 1, \ldots, M_s$.

---

$^1$Hulsen et al. 1997,  $^2$Laso and Öttinger 1993
STOCHASTIC APPROACH FOR MICROSCALE$^{1,2}$

- Approximation of random field $Q(x_k, t)$ at discrete points $x_k$ with $3N$-dimensional samples $Q^{(j)}(x_k, t) \sim \psi(x_k, \cdot, t)$ for $j = 1, \ldots, M_s$.
- Monte Carlo approximation of expectation

$$
\tau_p(x_k, t) = C \sum_{i=1}^{N} \left( \mathbb{E}[Q_i(x_k, t) \otimes F_i(Q_i(x_k, t))] - Id \right)
$$

$$
\approx C \sum_{i=1}^{N} \left( \frac{1}{M_s} \sum_{j=1}^{M_s} Q_i^{(j)}(x_k, t) \otimes F_i(Q_i^{(j)}(x_k, t)) - Id \right).
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**Stochastic Approach for Microscale**\(^1,2\)

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- Variance error in \(\tau_p\) is of order \(O(M_s^{-1/2})\).

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**Temporal Evolution of Microscopic Scale**

- Density $\psi$ only known at $t = 0$ for complex spring models.
- At $t = 0$ create stochastic samples using rejection sampling\(^1\).

\(^1\) von Neumann 1951
TEMPORAL EVOLUTION OF MICROSCOPIC SCALE

- Density $\psi$ only known at $t = 0$ for complex spring models.
- At $t = 0$ create stochastic samples using rejection sampling$^1$.
- For $t > 0$: Semi-implicit Euler-Maruyama scheme with 1. order accuracy in time.

Fokker-Planck approach

stochastic approach

---

$^1$ von Neumann 1951
Simulation: 3D contraction flow

- Applications: injection moulding, polymer processing, . . .
- Discretization in space with 3D flow solver *NaSt3dGPF*\textsuperscript{1,2,3} on a staggered grid of size $M_g$ with center $x_k$.

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\textsuperscript{1}Griebel et al. 1998, \textsuperscript{2}Croce et al. 2009 \textsuperscript{3}For non-profit use: http://wissrech.ins.uni-bonn.de
SIMULATION: 3D contraction flow

- Applications: injection moulding, polymer processing, ... 
- Discretization in space with 3D flow solver NaSt3dGPF\textsuperscript{1,2,3} on a staggered grid of size $M_g$ with center $x_k$.
- Dimensionless characteristic units:

  \begin{align*}
  &\textbf{Reynolds number:} \quad Re = \frac{2L \rho U}{\eta(\dot{\gamma})}, \\
  &\textbf{Deborah number:} \quad De = \frac{\lambda U}{L}
  \end{align*}

  $U$ average velocity, $\lambda$ relaxation time, $\eta(\dot{\gamma})$ viscosity, $\dot{\gamma}$ shear rate, $L$ characteristic length

\textsuperscript{1}Griebel et al. 1998, \textsuperscript{2}Croce et al. 2009 \textsuperscript{3}For non-profit use: http://wissrech.ins.uni-bonn.de
**Shear-thinning fluid in 4:1 contraction**

- Experimental measurements:
  - fluid: Glycerol + water + PAA (600ppm)
  - relaxation time: $\lambda = 32s$
  - experimental Deborah numbers: $De = 1, \ldots, 200$

**Figure:** Visualization of contraction flow\(^1\) with $Re = 2.37$, $De = 174$

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\(^1\) Sousa, Coelho, Oliveira and Alves 2011
**Shear-thinning fluid in 4 : 1 contraction**

- Experimental measurements:\(^1\)
  - fluid: Glycerol + water + PAA (600ppm)
  - relaxation time: \(\lambda = 32\) s
  - experimental Deborah numbers: \(De = 1, \ldots, 200\)
- For high Deborah number flows:
  - large corner vortices occur
  - streamline divergence
  - inverted streamline rotation
- Macroscopic approaches often suffer from numerical instabilities\(^2,^3\).

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**Figure:** Visualization of contraction flow\(^1\) with \(Re = 2.37, De = 174\)

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\(^1\) Sousa, Coelho, Oliveira and Alves 2011, \(^2\) Keunings 1986, \(^3\) Mangoubi et al. 2009
3D SIMULATION RESULTS

- 8 multiscale simulations.

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<td>Deborah number $De$</td>
<td>24.1, 108, 157</td>
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<tr>
<td>spring model FENE chain</td>
<td>1, 3, 5</td>
</tr>
<tr>
<td>spring segments $N$</td>
<td>1, 3, 5</td>
</tr>
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<td>$380 \times 64 \times 64$</td>
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<td>samples per cell $M_s$</td>
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$^1$ partial results in Griebel and R. 2014
**3D SIMULATION RESULTS**

- 8 multiscale simulations.
- All elastic effects reproduced in simulation.
- No stability issues occurred.

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**FIGURE**: Simulation of 5-segment chain with $De = 157$.

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**Figure**: Simulation of 5-segment chain with $De = 157$.

---

1 partial results in Griebel and R. 2014
COMPARISON OF EXPERIMENT AND SIMULATION

- **Velocity profiles** compared on the channel’s centerline (a).
- **Inverted 3D streamline rotation** compared to Newtonian flow (b+c).
- Simulation results correspond with experimental measurements.

(a) velocity profile $De=24$

(b) streamlines $De=1.0$

(c) streamlines $De=157$
Complexity of multiscale simulations

Clusters for multiscale simulations

<table>
<thead>
<tr>
<th></th>
<th>Atacama</th>
<th>JUROPA</th>
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</thead>
<tbody>
<tr>
<td># cores</td>
<td>1,248 CPUs</td>
<td>17,664 CPUs</td>
</tr>
<tr>
<td>memory</td>
<td>4,992 GB</td>
<td>52,992 GB</td>
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<tr>
<td>Linpack</td>
<td>≈ 21 TFlops/s</td>
<td>207 TFlops/s</td>
</tr>
<tr>
<td>installation</td>
<td>Mar 2014</td>
<td>access: 11/2013 - 10/2014</td>
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Institute for Numerical Simulation, University of Bonn
Jülich Supercomputing Centre, Jülich Research Centre
Complexity of multiscale simulations

- $M_g$ grid cells in space,
- $M_s$ samples per grid cell,
- spring model with $N$ segments.
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Solution approach

1. Parallelization
2. Model reduction:
   - proper generalized decomposition (PGD)
   - sparse grids

---

1Chinesta, Ammar, Leygue and Keunings 2011, 2Delaunay, Lozinski and Owens 2007
Sparse grid combination technique

- Approximation of full grid solution \( u_l \in V_l \) as a combination of coarse full grid solution spaces \( u_m \in V_m \).
- Multi-indices \( m, l \in \mathbb{N}^d \) denote discretization accuracy.

**Figure:** Combination technique (left), sparse grid (center) and full grid (right).

---

\(^{1}\) Griebel, Schneider, Zenger 1992, \(^{2}\) R. and Griebel, submitted to Appl Math & Comput
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- Approximation of full grid solution \( u_l \in V_l \) as a combination of coarse full grid solution spaces \( u_m \in V_m \).
- Multi-indices \( m, l \in \mathbb{N}^d \) denote discretization accuracy.
- Combination technique is intrinsically parallel.
- Existing multiscale solver can be reused.
- **Numerical result:** Computational effort reduced by one order of magnitude in shear and extensional flows.

**Figure:** Combination technique (left), sparse grid (center) and full grid (right).

---

Summary

1. Simulation of 3D contraction flow with multiscale model:
   - Results compared with experimental measurements from the literature.
   - Experimental phenomena could be reproduced.

Thank you for your attention!
Summary

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12. R. Keunings
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13. C. Mangoubi, M. Hulsen, R. Kupferman
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14. M. Griebel, A. Rüttgers
    Multiscale simulations of 3D viscoelastic flows in a square-square contraction
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