Numerical tests on some viscoelastic flows
-multiscale approach

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Outline

Introduction

Multiscale approach

Numeric
Governing equations

\[
\begin{align*}
\left\{ \begin{array}{l}
Re\left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \alpha \Delta \mathbf{u} + \nabla \cdot \sigma \\
\nabla \cdot \mathbf{u} = 0
\end{array} \right.
\end{align*}
\] (1)

\( \mathbf{u}, p, \sigma, \alpha, Re = \rho \frac{UL}{\mu} \) are velocity, pressure, elastic stress, and portion of Newtonian viscosity in total viscosity, Reynolds number.
Introduction
viscoelastic flow

Governing equations

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Two approaches describing the elastic stress

Macro: constitutive law (Oldroyd-B model):

\[
\frac{\partial C}{\partial t} + (u \cdot \nabla)C - \nabla u \cdot C - C \cdot (\nabla u)^T = \frac{1}{We} (I - C)
\]

(2)

where \( C = \frac{1-\alpha}{We} (\sigma - I) \), \( We = \lambda \frac{U}{L} \) is Weissenberg number, \( \lambda \) is relaxation time.

Results do not converge for high \( We \).

Micro: molecular theory
End to end dumbbell

Assumption:
a chain of beads and spring,
dilute,
zero-mass.

\[^{1}\text{H. C. Öttinger, Stochastic Processes in Polymeric Fluids: Tools and Examples for Developing Simulation Algorithms.}\]
End to end dumbbell

Assumption:
a chain of beads and spring, dilute, zero-mass.

Spring force: \( \mathbf{F}(\mathbf{R}) = \mathbf{R} \) (Hooke law)

Stochastic force\(^1\): \( \mathbf{B}_i = \sqrt{2kT\zeta} d\mathbf{W}_i / dt \)

Friction force: \( \mathbf{f} = \zeta (\dot{\mathbf{r}} - \mathbf{v}(\mathbf{r}, t)) \)

\( k \) Boltzmann constant, \( T \) absolute temperature, \( \zeta = 6\pi \mu_s a \) friction coefficient, \( \mu_s \) solvent viscosity, \( a \) radius of bead.

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\(^1\)H. C. Öttinger, Stochastic Processes in Polymeric Fluids: Tools and Examples for Developing Simulation Algorithms.
Newton’s second law

\[-\zeta(\dot{r}_1 - v(r_1, t)) + F(R) + B_1 = 0, \quad (3)\]

\[-\zeta(\dot{r}_2 - v(r_2, t)) - F(R) + B_2 = 0. \quad (4)\]

\[\dot{R} = \nabla v \cdot R - \frac{2}{\zeta} F(R) + \sqrt{\frac{4kT}{\zeta}} \frac{dW_t}{dt}. \quad (5)\]
Newton’s second law

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\[
\dot{R} = \nabla v \cdot R - \frac{2}{\zeta} F(R) + \sqrt{\frac{4kT}{\zeta}} \frac{dW_t}{dt}. \quad (5)
\]

Probability distribution function \(\psi(x, R, t)\):

at a position \(x\) and time \(t\), the probability of a dumbbell vector
that stays between \(R\) and \(R + dR\).

\[
\iint \psi(x, R, t) dR = 1.
\]
Newton’s second law

\[-\zeta(\dot{r}_1 - v(r_1, t)) + F(R) + B_1 = 0,\]  
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\[\dot{R} = \nabla v \cdot R - \frac{2}{\zeta} F(R) + \sqrt{\frac{4kT}{\zeta}} \frac{dW_t}{dt}.\]  

Probability distribution function $\psi(x, R, t)$:

at a position $x$ and time $t$, the probability of a dumbbell vector that stays between $R$ and $R + dR$.

\[\int\int \psi(x, R, t) dR = 1.\]

Fokker-Planck equation

\[\frac{\partial \psi}{\partial t} + u \cdot \nabla \psi = \nabla_R \cdot \left(\left(-\nabla u \cdot R + \frac{1}{2We} F(R)\right) \psi\right) + \frac{1}{2We} \Delta_R \psi\]
The micro approach is equivalent to the Oldroyd-B model!
Multiscale approach

Relation between micro and macro

\[ \sigma = \frac{1 - \alpha}{\text{We}} (-I + \iint R \otimes R \psi dR). \]

\[ \iint R \otimes R \times (6) dR \Rightarrow (2). \]

The micro approach is equivalent to the Oldroyd-B model!

Multiscale system

\[
\begin{cases}
\text{Re}(\frac{\partial u}{\partial t} + u \cdot \nabla u) = -\nabla p + \alpha \Delta u + \nabla \cdot \sigma \\
\nabla \cdot u = 0 \\
\sigma = \frac{1 - \alpha}{\text{We}} (-I + \iint R \otimes R \psi dR) \\
\frac{\partial \psi}{\partial t} + u \cdot \nabla \psi = \nabla_R \cdot ((-\nabla u \cdot R + \frac{1}{2\text{We}} R)\psi) + \frac{1}{2\text{We}} \Delta_R \psi
\end{cases}
\]
1. Navier-Stokes
1. **Navier-Stokes**

2. **Fokker-Planck**: space splitting

\[
\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \nabla_R \cdot ((-\nabla \mathbf{u} \cdot \mathbf{R} + \frac{1}{2We} \mathbf{F}(\mathbf{R}))\psi) + \frac{1}{2We} \Delta_R \psi
\]

In physical space \(\mathbf{x} \in \Omega(\text{geometry})\) we have

\[
\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = 0 \quad (8)
\]

Upwind in physical space.

In configuration space \(\mathbf{R} \in (-\infty, +\infty) \times (-\infty, +\infty)\), we use an implicit scheme

\[
\frac{\psi^* - \psi^n}{\Delta t} = \nabla_R \cdot ((-\nabla \mathbf{u} \cdot \mathbf{R} + \frac{1}{2We} \mathbf{F}(\mathbf{R}))\psi^*) + \frac{1}{2We} \Delta_R \psi^* \quad (9)
\]
The configuration space is infinite!

\[ \mathbf{F} = \frac{\mathbf{R}}{1 - \frac{|\mathbf{R}|^2}{R_0^2}}, |\mathbf{R}| \in (0, R_0). \]
The configuration space is infinite!

FENE, A. Lozinski, C. Chauviere, \( \mathbf{F} = \frac{\mathbf{R}}{1 - \frac{|\mathbf{R}|^2}{R_0^2}} \), \(|\mathbf{R}| \in (0, R_0)\).

Idea:

polar coordinates \((\rho, \theta) = (|\mathbf{R}|, \arctan \frac{R_2}{R_1})\),
infinite plane to unit circle \( r = \frac{1}{\rho + 1} \).

\[
\frac{\partial \phi}{\partial t} = b_0(\kappa, \theta)L_0 \phi - b_1(\kappa, \theta)\frac{\partial \phi}{\partial \theta} + L_1 \phi,
\]

where \( L_0 \) and \( L_1 \) are linear operators,

\[
b_0 = \kappa_{11} \cos 2\theta + \frac{\kappa_{12} + \kappa_{21}}{2} \sin 2\theta, \quad L_0 \phi = -4r(1 - r)^2[-s(1 - \eta)^{-1} \phi + \frac{\partial \phi}{\partial \eta}],
\]

\[
b_1 = -\kappa_{11} \sin 2\theta + \frac{\kappa_{12} + \kappa_{21}}{2} \cos 2\theta + \frac{\kappa_{21} - \kappa_{12}}{2},
\]

\[
L_1 \phi = c_1 \phi + c_2 \frac{\partial \phi}{\partial \eta} + c_3 \frac{\partial^2 \phi}{\partial \eta^2} + c_4 \frac{\partial^2 \phi}{\partial \theta^2}
\]

\[
c_1 = \frac{1}{We} [1 + 2s(1 - \eta)^{-1}(-3r^4 + 2r^3 - r) + 8r^4(r - 1)^2s(s - 1)(1 - \eta)^{-2}],
\]

\[
c_2 = \frac{2}{We} (3r^4 - 2r^2 + r) - \frac{16}{We} r^4(r - 1)^2s(1 - \eta)^{-1},
\]

\[
c_3 = \frac{8}{We} r^4(r - 1)^2, \quad c_4 = \frac{1}{2We} \left(\frac{r}{1-r}\right)^2, \quad \kappa = \nabla \mathbf{u},
\]

\[
\psi(t, \mathbf{x}, \mathbf{R}) = (1 - \eta)^s \phi(t, \mathbf{x}, \eta, \theta), \quad s = 2, \quad \eta = 2(1 - r)^2 - 1.
\]
Pseudo-spectral method

We look for an approximate solution to the Eq.(10) of the following form

\[
\phi(t, x, \eta, \theta) = \sum_{i=0}^{1} \sum_{l=i}^{N_\theta} \sum_{k=1}^{N_\eta} \phi_{kl} h_k(\eta) \Phi_{il}(\theta),
\]

(11)

where \( \Phi_{il}(\theta) = (1 - i) \cos(2l\theta) + i \sin(2l\theta) \),
\( N_\theta, N_\eta \) number of discretization points,
\( h_k(\eta) \) Lagrange interpolating polynomial,
\( \eta_m (m = 1, \cdots, N_\eta) \) Gauss-Legendre points \( \eta \in (-1, 1) \).

\[
\bar{\phi}^* = [I - \Delta t(M_0 + M_1 + M_2)]^{-1} \bar{\phi}^n,
\]

(12)

where \( \bar{\phi}^n \) is the vector of the expansion coefficients \( \phi_{kl} \) at time \( t_n = n\Delta t \).

\( M_0, M_1, M_2 \cdots \)
Numeric test for Peterlin model

\[
\left\{
\begin{align*}
Re\left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) &= -\nabla p + \alpha \Delta u + \nabla \cdot \sigma \\
\nabla \cdot u &= 0 \\
\sigma &= (tr C) C \\
\frac{\partial C}{\partial t} + (u \cdot \nabla) C - \nabla u \cdot C - C \cdot (\nabla u)^T &= \frac{1}{We} (tr C) I - \frac{1}{We} (tr C)^2 C + \epsilon \Delta C
\end{align*}
\right.
\]

and \( \frac{\partial C}{\partial n} = 0 \) on the boundary.
Slight modification \( \text{tr} \mathbf{C} \rightarrow \max(\text{tr} \mathbf{C}) \).

Table: L2-error of \( \sigma \)

<table>
<thead>
<tr>
<th>mesh points</th>
<th>( | \sigma_1 - \sigma_1(256) |_{L_2} )</th>
<th>EOC</th>
<th>( | \sigma_3 - \sigma_3(256) |_{L_2} )</th>
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</tbody>
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Thank you for your attention!