Numerical tests on some viscoelastic flows

-multiscale approach

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Outline

Introduction

Multiscale approach

Numeric

Governing equations

$$\begin{cases} Re(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \alpha \Delta \mathbf{u} + \nabla \cdot \boldsymbol{\sigma} \\ \nabla \cdot \mathbf{u} = 0 \end{cases} \tag{1}$$

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

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Two approaches describing the elastic stress

Macro: constitutive law (Oldroyd-B model):

$$\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{C} - \nabla \mathbf{u} \cdot \mathbf{C} - \mathbf{C} \cdot (\nabla \mathbf{u})^T = \frac{1}{We}(\mathbf{I} - \mathbf{C}) \tag{2}$$

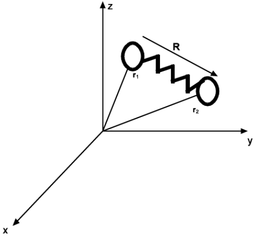
where $\mathbf{C} = \frac{1-\alpha}{We}(\boldsymbol{\sigma} - \mathbf{I})$, $We = \lambda \frac{U}{L}$ is Weissenberg number, λ is relaxation time.

Results do not converge for high We.

Micro: molecular theory

End to end dumbbell

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



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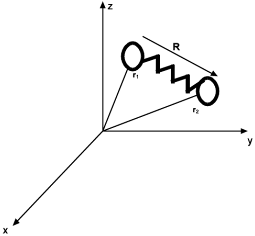

Spring force: $\mathbf{F}(\mathbf{R}) = \mathbf{R}$ (Hooke law)

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, μ_s solvent viscosity, a radius of bead.

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Newton's second law

$$-\zeta(\dot{\mathbf{r}}_1 - \mathbf{v}(\mathbf{r}_1, t)) + \mathbf{F}(\mathbf{R}) + \mathbf{B}_1 = 0, \tag{3}$$

$$-\zeta(\dot{\mathbf{r}}_2 - \mathbf{v}(\mathbf{r}_2, t)) - \mathbf{F}(\mathbf{R}) + \mathbf{B}_2 = 0. \tag{4}$$

$$\dot{\mathbf{R}} = \nabla \mathbf{v} \cdot \mathbf{R} - \frac{2}{\zeta}\mathbf{F}(\mathbf{R}) + \sqrt{\frac{4kT}{\zeta}}\frac{d\mathbf{W}_t}{dt}. \tag{5}$$

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Probability distribution function $\psi(\mathbf{x}, \mathbf{R}, t)$:
at a position $\mathbf{x}$ and time t, the probability of a dumbbell vector that stays between $\mathbf{R}$ and $\mathbf{R} + d\mathbf{R}$.

$$\iint \psi(\mathbf{x}, \mathbf{R}, t)d\mathbf{R} = 1.$$

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Fokker-Planck equation

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \nabla_{\mathbf{R}} \cdot ((-\nabla \mathbf{u} \cdot \mathbf{R} + \frac{1}{2We}\mathbf{F}(\mathbf{R}))\psi) + \frac{1}{2We}\Delta_{\mathbf{R}}\psi \quad (6)$$

Relation between micro and macro

$$\boldsymbol{\sigma} = \frac{1-\alpha}{We}(-\mathbf{I} + \iint \mathbf{R} \otimes \mathbf{R}\psi d\mathbf{R}).$$

$$\iint \mathbf{R} \otimes \mathbf{R} \times (6) d_{\mathbf{R}} \Rightarrow (2).$$

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

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Multiscale system

$$\begin{cases} Re(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \alpha \Delta \mathbf{u} + \nabla \cdot \boldsymbol{\sigma} \\ \nabla \cdot \mathbf{u} = 0 \\ \boldsymbol{\sigma} = \frac{1-\alpha}{We}(-\mathbf{I} + \iint \mathbf{R} \otimes \mathbf{R}\psi d\mathbf{R}) \\ \frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \nabla_{\mathbf{R}} \cdot ((-\nabla \mathbf{u} \cdot \mathbf{R} + \frac{1}{2We}\mathbf{R})\psi) + \frac{1}{2We}\Delta_{\mathbf{R}}\psi \end{cases} \tag{7}$$

1. **Navier-Stokes**

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2. **Fokker-Planck**: space splitting
$\frac{\partial\psi}{\partial t} + \mathbf{u}\cdot\nabla\psi = \nabla_{\mathbf{R}}\cdot((-\nabla\mathbf{u}\cdot\mathbf{R} + \frac{1}{2We}\mathbf{F}(\mathbf{R}))\psi) + \frac{1}{2We}\Delta_{\mathbf{R}}\psi$

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

$$\frac{\partial\psi}{\partial t} + \mathbf{u}\cdot\nabla\psi = 0 \tag{8}$$

Upwind in physical space.

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

$$\frac{\psi^* - \psi^n}{\Delta t} = \nabla_{\mathbf{R}}\cdot((-\nabla\mathbf{u}\cdot\mathbf{R} + \frac{1}{2We}\mathbf{F}(\mathbf{R}))\psi^*) + \frac{1}{2We}\Delta_{\mathbf{R}}\psi^* \tag{9}$$

The configuration space is infinite!

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

$$\frac{\partial \phi}{\partial t} = b_0(\boldsymbol{\kappa}, \theta) L_0 \phi - b_1(\boldsymbol{\kappa}, \theta)\frac{\partial \phi}{\partial \theta} + L_1\phi, \qquad (10)$$

where L_0 and L_1 are linear operators,
$b_0 = \kappa_{11}\cos 2\theta + \frac{\kappa_{12}+\kappa_{21}}{2}\sin 2\theta$, $L_0\phi = -4r(1-r)^2[-s(1-\eta)^{-1}\phi + \frac{\partial\phi}{\partial\eta}]$,
$b_1 = -\kappa_{11}\sin 2\theta + \frac{\kappa_{12}+\kappa_{21}}{2}\cos 2\theta + \frac{\kappa_{21}-\kappa_{12}}{2}$,
$L_1\phi = c_1\phi + c_2\frac{\partial\phi}{\partial\eta} + c_3\frac{\partial^2\phi}{\partial\eta^2} + c_4\frac{\partial^2\phi}{\partial\theta^2}$
$c_1 = \frac{1}{We}[1+2s(1-\eta)^{-1}(-3r^4+2r^3-r)+8r^4(r-1)^2 s(s-1)(1-\eta)^{-2}]$,
$c_2 = \frac{2}{We}(3r^4-2r^2+r) - \frac{16}{We}r^4(r-1)^2 s(1-\eta)^{-1}$,
$c_3 = \frac{8}{We}r^4(r-1)^2$, $c_4 = \frac{1}{2We}(\frac{r}{1-r})^2$, $\boldsymbol{\kappa} = \nabla\mathbf{u}$,
$\psi(t,\mathbf{x},\mathbf{R}) = (1-\eta)^s\phi(t,\mathbf{x},\eta,\theta)$, $s = 2, \eta = 2(1-r)^2 - 1$.

Pseudo-spectral method

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

$$\phi(t, \mathbf{x}, \eta, \theta) = \sum_{i=0}^{1} \sum_{l=i}^{N_\theta} \sum_{k=1}^{N_\eta} \phi_{kl}^{i} h_k(\eta) \Phi_{il}(\theta), \qquad (11)$$

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

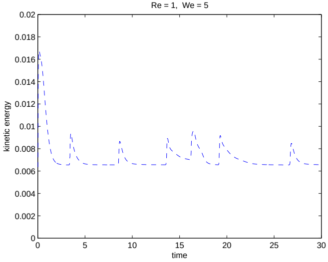
$$\bar{\phi}^{*} = [\mathbf{I} - \Delta t(\mathbf{M}_0 + \mathbf{M}_1 + \mathbf{M}_2)]^{-1} \bar{\phi}^{n}, \qquad (12)$$

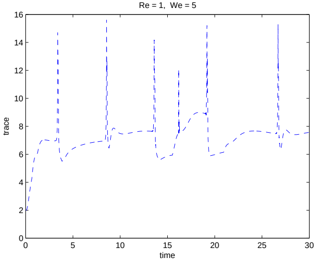
where $\bar{\phi}^{n}$ is the vector of the expansion coefficients ϕ_{kl}^{i} at time $t_n = n\Delta t$.

$$\mathbf{M}_0, \mathbf{M}_1, \mathbf{M}_2 \cdots$$

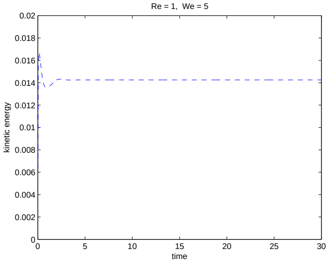
$$
\begin{cases}
Re(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}) = -\nabla p + \alpha\Delta\mathbf{u} + \nabla\cdot\boldsymbol{\sigma} \\
\nabla\cdot\mathbf{u} = 0 \\
\boldsymbol{\sigma} = (tr\mathbf{C})\mathbf{C} \\
\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{C} - \nabla\mathbf{u}\cdot\mathbf{C} - \mathbf{C}\cdot(\nabla\mathbf{u})^T = \frac{1}{We}(tr\mathbf{C})\mathbf{I} - \frac{1}{We}(tr\mathbf{C})^2\mathbf{C} + \epsilon\Delta\mathbf{C}
\end{cases}
$$

and $\frac{\partial \mathbf{C}}{\partial \mathbf{n}} = 0$ on the boundary.





Slight modification $tr\mathbf{C} \longrightarrow \max(tr\mathbf{C})$.



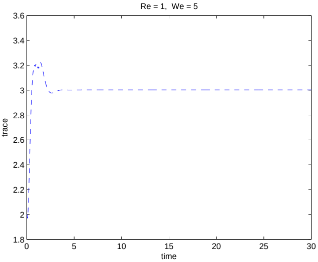


Table: L2-error of σ

mesh points	$\|\|\sigma_1 - \sigma_1(256)\|\|_{L_2}$	EOC	$\|\|\sigma_3 - \sigma_3(256)\|\|_{L_2}$	EOC
32	0.0636		0.4466	
64	0.0559	0.1858	0.3165	0.4969
128	0.0355	0.6538	0.1643	0.9457

Convergent!

Thank you for your attention!