

The background of the slide is a high-angle aerial photograph of a large, densely populated city. A prominent blue river or canal cuts through the center of the city, with several bridges crossing it. The city is filled with a mix of traditional and modern architecture, including numerous skyscrapers and lower residential buildings. The surrounding landscape beyond the city boundaries appears more rural and green.

Energy dissipative characteristic schemes for the diffusive Oldroyd-B viscoelastic fluid

Bangwei She

Cooperation with

Prof. Mária Lukáčová Prof. Hirofumi Notsu

Institute of Mathematics, Czech Academy of Science

04.12.2015

What is viscoelastic fluid?

viscoelastic = viscous + elastic



High Weissenberg Effect

- Part I: Introduction
- Part II: Energy stability
- Part III: Numerical methods

Navier-Stokes

$$\begin{cases} \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \boldsymbol{\tau} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

ρ : density

\mathbf{u} : velocity

p : pressure

$\boldsymbol{\tau}$: shear stress

Newtonian fluids:

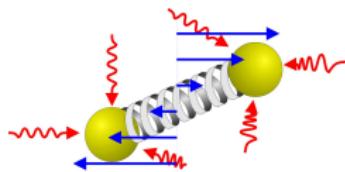
$$\boldsymbol{\tau} = 2\mu_0 \mathbf{D}(\mathbf{u}), \mathbf{D}(\mathbf{u}) = \frac{\nabla \mathbf{u} + (\nabla \mathbf{u})^T}{2}.$$

viscoelastic fluid is non-Newtonian:

$$\boldsymbol{\tau} = f(\mathbf{D}) \text{ is nonlinear}$$

Dilute theory

- Spring force: $\mathbf{F}(\mathbf{R}) = \mathbf{R}$ (Hooke law)
- Friction force from solvent: $\mathbf{f} = \zeta(\dot{\mathbf{r}} - \mathbf{v}(\mathbf{r}, t))$
- Stochastic force due to Brownian motion¹: $\mathbf{B}_i = \sqrt{2kT\zeta}d\mathbf{W}_i/dt$



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

Fokker-Planck equation

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

Fokker-Planck equation

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

Take the momentum of $\mathbf{R} \otimes \mathbf{R}$ and let $\boldsymbol{\sigma} = \int \psi \mathbf{R} \otimes \mathbf{R} d\mathbf{R}$

$$\frac{\delta \boldsymbol{\sigma}}{\delta t} = \frac{1}{We} (\mathbf{I} - \boldsymbol{\sigma}) + \eta \Delta \boldsymbol{\sigma}, \quad \frac{\delta \boldsymbol{\sigma}}{\delta t} := \frac{\partial \boldsymbol{\sigma}}{\partial t} + (\mathbf{u} \cdot \nabla) \boldsymbol{\sigma} - \nabla \mathbf{u} \boldsymbol{\sigma} - \boldsymbol{\sigma} (\nabla \mathbf{u})^T$$

Oldroyd-B model

$$(A) \begin{cases} Re \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot \boldsymbol{\tau} \\ \nabla \cdot \mathbf{u} = 0 \\ \frac{\partial \boldsymbol{\sigma}}{\partial t} + (\mathbf{u} \cdot \nabla) \boldsymbol{\sigma} - \nabla \mathbf{u} \boldsymbol{\sigma} - \boldsymbol{\sigma} (\nabla \mathbf{u})^T = \frac{1}{We} (\mathbf{I} - \boldsymbol{\sigma}) + \eta \Delta \boldsymbol{\sigma} \end{cases}$$

$$\boldsymbol{\tau} = \underbrace{2\alpha \mathbf{D}}_{viscous} + \underbrace{\frac{\beta}{We} \boldsymbol{\sigma}}_{elastic}$$

Re : Reynolds number We : Weissenberg number

$\boldsymbol{\sigma}$: conformation tensor, spd

$\alpha \in (0, 1)$: ratio of Newtonian viscosity in total viscosity ($\beta = 1 - \alpha$)

$\eta \geq 0$: diffusive parameter

Non-diffusive case: global in time existence is open

Renardy, 1990.

well-posedness for Dirichlet IBV

Guillope and Saut, 1990

Fernandez-Cara, Guillen, and Ortega, 2002.

local existence and global existence for small initial data

Lin, Liu and Zhang, 2005.

local existence and global existence for small solutions

Arada and Sequeira, 2003.

strong steady solutions in bounded domain

Diffusive case:

Constantin and Kliegl, 2012

regularity in 2D

Barrett and Boyaval, 2014

global existence of weak solutions in 2D

Early studies

- FE: Crochet and Keunings (1982), Keunings (1986), Keunings and Shipman (1986), Marchal and Crochet (1987)
- FV: Xue, Phan-Thien and Tanner (1998)
- FD-FE: Crochet, Davies and Walters (1984)
- FE-FV: Wapperom and Webster (1998,1999), Aboubacar, Matallah, and Webster (2002)

High Weissenberg Number Problem!

Logarithm transformation: Fattal and Kupferman (FD, 2004, 2005)

$$\psi = \ln \sigma$$

FE: Turek's group (2010, 2010); Pan's group (2007, 2007)

FV: Afonso, Oliveira, Pinho and Alves (2009)

Introduction

Some stability approaches

Square-root: Balci, Thomases, Renardy, Doering (2011)

$$\psi = \sigma^{1/2}$$

Kernel: Afonso, Pinho and Alves (2012)

$$\psi = \sigma^k, \psi = \log_a \sigma.$$

Euler-Lagrangian method:

FD: Trebotich, Colella, and Miller (2005)

FE: Lee and Xu (2006), Lee, Xu, and Zhang(2011,2011)

$$\begin{aligned}\frac{\delta \sigma}{\delta t} &= \frac{\partial \sigma}{\partial t} + (\mathbf{u} \cdot \nabla) \sigma - \nabla \mathbf{u} \cdot \sigma - \sigma \cdot (\nabla \mathbf{u})^T \\ &\approx \frac{\sigma^{n+1} - \mathbf{F}(\sigma^n \circ X)\mathbf{F}^T}{\Delta t}, \text{ where } \frac{d\mathbf{F}}{dt} = \nabla \mathbf{u} \mathbf{F}.\end{aligned}$$

Introduction

Logarithm transformation

For any matrix $\nabla \mathbf{u}$ and symmetric positive definite matrix σ :

$$\nabla \mathbf{u} = \mathbf{B} + \Omega + \mathbf{N}\sigma^{-1}.$$

\mathbf{N}, Ω are anti-symmetric, \mathbf{B} is symmetric and commutes with σ .

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

can be written as

$$\frac{\partial \sigma}{\partial t} + (\mathbf{u} \cdot \nabla) \sigma = \underbrace{\Omega \sigma - \Omega \sigma}_{\text{rotation}} + \underbrace{2\mathbf{B}\sigma}_{\text{stretch}} + \frac{1}{We} (\mathbf{I} - \sigma).$$

log-transform $\psi = \ln \sigma$

$$\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \underbrace{\Omega \psi - \psi \Omega}_{\text{rotation}} + \underbrace{2\mathbf{B}}_{\text{stretch}} + \frac{1}{We} (e^{-\psi} - \mathbf{I}).$$

Stretch: exponential to polynomial.

Is "High Weissenberg Number Problem" solved?

Motivation

- the log-transform + the diffusive model
- construct numerical scheme such that
 - stable for high We
 - convergent

Diffusive Oldroyd-B model with LCR:

$$(B) \begin{cases} \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \alpha \Delta \mathbf{u} + \frac{\beta}{We} \nabla \cdot (\mathbf{e}^\psi - \mathbf{I}) \\ \nabla \cdot \mathbf{u} = 0 \\ \frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = \boldsymbol{\Omega} \psi - \psi \boldsymbol{\Omega} + 2\mathbf{B} + \frac{1}{We} (\mathbf{e}^{-\psi} - \mathbf{I}) + \varepsilon \Delta \psi \end{cases}$$

Energy stability

Free-energy (Hu and Lelièvre, 2006)

$$F(\mathbf{u}, \boldsymbol{\sigma}) = Re \ Ke + \frac{\beta}{2We} \ En. \quad (1)$$

$$Ke = \frac{1}{2} \int_{\mathcal{T}} \mathbf{u}^2 \geq 0,$$

$$En = \int_{\mathcal{T}} \text{tr}(\boldsymbol{\sigma} - \ln \boldsymbol{\sigma} - \mathbf{I}) \geq 0.$$

Theorem 1

(*Energy estimate for the diffusive logarithmic Oldroyd-B model*)
Let (\mathbf{u}, p, ψ) be a smooth solution to system (B), supplied with the homogeneous Dirichlet boundary condition for velocity, and with the zero Neumann boundary condition for ψ . Further, we assume that initially e^ψ is a symmetric positive-definite tensor. The free energy satisfies:

$$\frac{d}{dt} F(\mathbf{u}, e^\psi) + \alpha \int_{\mathcal{T}} |\nabla \mathbf{u}|^2 + \frac{\beta}{2We} \int_{\mathcal{T}} \text{tr}(e^\psi + e^{-\psi} - 2\mathbf{I}) \leq 0. \quad (2)$$

From this estimate, we obtain that $F(\mathbf{u}, e^\psi)$ decreases in time exponentially fast to zero.

Energy stability

Proof of Theorem 1

Inner product of the Navier-Stokes equation with the velocity:

$$\frac{Re}{2} \frac{d}{dt} \int_{\mathcal{T}} \mathbf{u}^2 + \alpha \int_{\mathcal{T}} |\nabla \mathbf{u}|^2 + \frac{\beta}{We} \int_{\mathcal{T}} \nabla \mathbf{u} : e^\psi = 0 \quad (3)$$

$$(B)_3 : e^\psi$$

$$\frac{d}{dt} \int_{\mathcal{T}} \text{tr}(e^\psi) = 2 \int_{\mathcal{T}} \nabla \mathbf{u} : e^\psi + \frac{1}{We} \text{tr}(\mathbf{I} - e^\psi) + \varepsilon \int_{\mathcal{T}} \Delta \psi : e^\psi. \quad (4)$$

$$\frac{d}{dt} \psi : e^\psi = \frac{d}{dt} \text{tr}(e^\psi).$$

$$(\boldsymbol{\Omega}\psi - \psi\boldsymbol{\Omega}) : e^\psi = \text{tr}(\boldsymbol{\Omega}\psi e^\psi) - \text{tr}(\psi\boldsymbol{\Omega} e^\psi) = 0.$$

$$\nabla \mathbf{u} : e^\psi = \boldsymbol{\Omega} : e^\psi + \mathbf{B} : e^\psi + \mathbf{N} e^{-\psi} : e^\psi = \mathbf{B} : e^\psi.$$

Energy stability

Proof of Theorem 1

$$(3) + \frac{\beta}{2We} \times (4) \Rightarrow$$

$$\begin{aligned} & \frac{d}{dt} \int_{\mathcal{T}} \left(\frac{Re}{2} \mathbf{u}^2 + \frac{\beta}{2We} \text{tr}(e^\psi - \mathbf{I}) \right) + \int_{\mathcal{T}} \left(\alpha |\nabla \mathbf{u}|^2 + \frac{\beta}{2We^2} \text{tr}(e^\psi - \mathbf{I}) \right) \\ &= \frac{\varepsilon\beta}{2We} \int_{\mathcal{T}} \Delta \psi : e^\psi = -\frac{\varepsilon\beta}{2We} \int_{\mathcal{T}} \nabla \psi : \nabla e^\psi \leq 0. \end{aligned} \quad (5)$$

$$\frac{\partial e^\psi}{\partial x} \neq e^\psi \frac{\partial \psi}{\partial x}.$$

$$\psi = R \text{diag}(\lambda_i) R^T, \sigma = R \text{diag}(e^{\lambda_i}) R^T.$$

We cannot show

$$e^\psi - \mathbf{I} \geq 0$$

but

$$e^\psi - \psi - \mathbf{I} \geq 0.$$

Energy stability

Proof of Theorem 1

Taking the trace of $(B)_3$, $\frac{d}{dt} \int_{\mathcal{T}} \text{tr}(\psi) = \frac{1}{We} \text{tr}(e^{-\psi} - \mathbf{I}). \quad (6)$

$$\begin{aligned} \frac{d}{dt} \int_{\mathcal{T}} \left(\frac{Re}{2} \mathbf{u}^2 + \frac{\beta}{2We} \text{tr}(e^\psi - \psi - \mathbf{I}) \right) \\ + \int_{\mathcal{T}} \left(\alpha |\nabla \mathbf{u}|^2 + \frac{\beta}{2We^2} \text{tr}(e^\psi + e^{-\psi} - 2\mathbf{I}) \right) \leq 0. \end{aligned}$$

Poincaré inequality: $\int_{\mathcal{T}} \mathbf{u}^2 \leq C_p \int_{\mathcal{T}} |\nabla \mathbf{u}|^2.$

$$0 \leq \text{tr}(e^\psi - \psi - \mathbf{I}) \leq \text{tr}(e^\psi - \psi - \mathbf{I}) + \text{tr}(e^{-\psi} + \psi - \mathbf{I}) = \text{tr}(e^\psi + e^{-\psi} - 2\mathbf{I}).$$

$$\frac{d}{dt} F(\mathbf{u}, \boldsymbol{\sigma}) \leq -c F(\mathbf{u}, \boldsymbol{\sigma}) \leq 0 \quad (c = \min\left(\frac{2\alpha}{Re C_p}, \frac{1}{We}\right) > 0).$$

Apply the Gronwall inequality,

$$F(\mathbf{u}, \boldsymbol{\sigma}) \leq F(\mathbf{u}(t=0), \boldsymbol{\sigma}(t=0)) e^{-ct}.$$

Numerical methods

- Schemes
- Energy stability of the schemes

Characteristic method

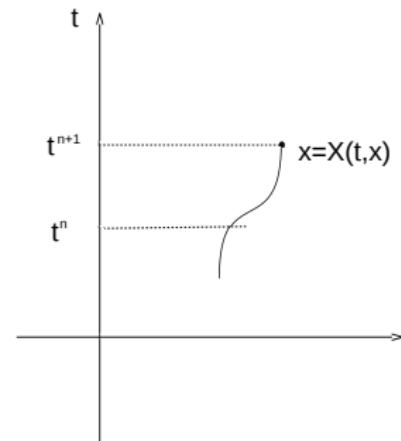
$$\begin{cases} \frac{d}{dt} X = \mathbf{u}(X, t), \quad \forall t \in [t^n, t^{n+1}], \\ X(t; x) = x. \end{cases}$$

Material derivative:

$$\begin{aligned} \frac{D\phi}{Dt} &= \frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi \\ &\approx \frac{\phi(X(t^{n+1}), t^{n+1}) - \phi(X(t^n), t^n)}{t^{n+1} - t^n} \end{aligned}$$

Nonlinear convection is avoided, symmetric coefficient matrix.

No CFL condition.



Numerical methods

Scheme 1: Pressure stabilized characteristic FEM

$$\begin{aligned} \frac{Re}{\Delta t}(\mathbf{u}_h^{n+1} - \mathbf{u}_h^n \circ X, \mathbf{v}_h) + 2\alpha(D(\mathbf{u}_h^{n+1}), D(\mathbf{v}_h)) \\ - (p_h^{n+1}, \nabla \cdot \mathbf{v}_h) - (\nabla \cdot \mathbf{u}_h^{n+1}, q_h) + s_h(p_h^{n+1}, q_h) = -\frac{\beta}{We}(e^{\psi_h^{n+1}}, \nabla \mathbf{v}_h) \end{aligned}$$

Stabilization $s_h(p, q) = -\delta \sum_K h_K^2 (\nabla p, \nabla q)_K$, $\delta > 0$.

$$\begin{aligned} \frac{1}{\Delta t}(\psi_h^{n+1} - \psi_h^n \circ X^n, \phi) + \varepsilon(\nabla \psi_h^{n+1}, \nabla \phi_h) \\ = (\Omega_h^{n+1} \psi_h^{n+1} - \psi_h^{n+1} \Omega_h^{n+1} + 2B_h^{n+1}, \phi_h) + \frac{1}{We}(e^{-\psi_h^{n+1}} - \mathbf{I}, \phi_h) \end{aligned}$$

$$\begin{aligned} X_h &\equiv \{\mathbf{v}_h \in C^0(\bar{\mathcal{T}}_h)^d; \mathbf{v}_h|_K \in \mathcal{P}^1(K)^d, \forall K \in \mathcal{T}_h\}, \quad V_h \equiv X_h \cap H_0^1(\mathcal{T})^d, \\ M_h &\equiv \{q_h \in C^0(\bar{\mathcal{T}}_h); q_h|_K \in \mathcal{P}^1(K), \forall K \in \mathcal{T}_h\}, \quad Q_h \equiv M_h \cap L_0^2(\mathcal{T}), \\ \Sigma_h &\equiv \{\phi_h \in C^0(\bar{\mathcal{T}}_h)^{d \times d}; \phi_h|_K \in \mathcal{P}^1(K)^{d \times d}, \forall K \in \mathcal{T}_h\}, \quad W_h \equiv \Sigma_h \cap H^1(\mathcal{T})^{d \times d}. \end{aligned}$$

Algorithm

Step-1 Given $\mathbf{u}_h^n, p_h^n, \psi_h^n$, set $\mathbf{u}_h^{n,0} = \mathbf{u}_h^n, \psi_h^{n,0} = \psi_h^n, p_h^{n,0} = p_h^n$.

Step-2 FOR $\ell = 0, 1, \dots$,

solve the equations with explicit RHS:

$$\frac{Re}{\Delta t}(\mathbf{u}_h^{n,\ell+1}, \mathbf{v}_h) + 2\alpha(D(\mathbf{u}_h^{n,\ell+1}), D(\mathbf{v}_h)) - (p_h^{n,\ell+1}, \nabla \cdot \mathbf{v}_h) - (\nabla \cdot \mathbf{u}_h^{n,\ell+1}, q_h)$$

$$+ s_h(p_h^{n,\ell+1}, q_h) = \frac{Re}{\Delta t}(\mathbf{u}_h^n \circ X, \mathbf{v}_h) - \frac{\beta}{We}(e^{\psi_h^{n,\ell}}, \nabla \mathbf{v}_h)$$

$$\frac{1}{\Delta t}(\psi_h^{n,\ell+1}, \phi_h) + \varepsilon(\nabla \psi_h^{n,\ell+1}, \nabla \phi_h) = (\Omega_h^{n,\ell} \psi_h^{n,\ell} - \psi_h^{n,\ell} \Omega_h^{n,\ell} + 2B_h^{n,\ell}, \phi_h)$$

$$+ \left(\frac{1}{\Delta t} \psi_h^n \circ X_1(\mathbf{u}_h^{n,\ell}, \Delta t), \phi_h \right) + \frac{1}{We}(e^{-\psi_h^{n,\ell}} - 1, \phi_h)$$

IF $\|\mathbf{w}_h^{n,\ell+1} - \mathbf{w}_h^{n,\ell}\| \leq \xi \|\mathbf{w}_h^{n,\ell}\|$ where $\mathbf{w}_h \in \{\mathbf{u}_h, p_h, \sigma_h\}$, ξ is small
break

ENDIF

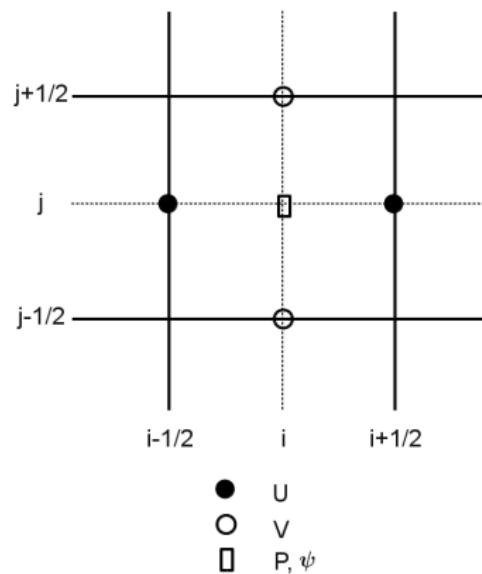
ENDFOR

Step-3 Update solution: $\mathbf{u}_h^{n+1} = \mathbf{u}_h^{n,\ell+1}, p_h^{n+1} = p_h^{n,\ell+1}, \psi_h^{n+1} = \psi_h^{n,\ell+1}$.

Numerical methods

Scheme 2: Characteristic-FD method

Staggered mesh



$$\begin{aligned} \frac{(\psi^{n+1} - \psi^n \circ \mathbf{X}^n)_{i,j}}{\Delta t} = & (\boldsymbol{\Omega}^{n+1} \psi^{n+1} - \psi^{n+1} \boldsymbol{\Omega}^{n+1} + 2\mathbf{B}^{n+1})_{i,j} \\ & + \frac{1}{We} (e^{-\psi_{i,j}^{n+1}} - \mathbf{I}) + \varepsilon \Delta_h \psi_{i,j}^{n+1}. \end{aligned} \quad (7a)$$

$$\begin{aligned} Re \frac{(U^{n+1} - U^n \circ \mathbf{X}^n)_{i+1/2,j}}{\Delta t} = & -Re \delta_x (U^{n+1})_{i+1/2,j}^2 - Re \delta_y (U^{n+1} V^{n+1})_{i+1/2,j} - (\delta_x p^{n+1})_{i+1/2,j} \\ & + \alpha \Delta_h U_{i+1/2,j}^{n+1} + (\delta_x \sigma_{11}^{n+1})_{i+1/2,j} + (\delta_y \sigma_{12}^{n+1})_{i+1/2,j}, \end{aligned} \quad (7b)$$

$$\begin{aligned} Re \frac{(V^{n+1} - V^n \circ \mathbf{X}^n)_{i,j+1/2}}{\Delta t} = & -Re \delta_x (U^{n+1} V^{n+1})_{i+1/2,j} - Re \delta_y (V^{n+1})_{i+1/2,j}^2 - (\delta_y p^{n+1})_{i,j+1/2} \\ & + \alpha \Delta_h V_{i,j+1/2}^{n+1} + (\delta_x \sigma_{21}^{n+1})_{i,j+1/2} + (\delta_y \sigma_{22}^{n+1})_{i,j+1/2}, \end{aligned} \quad (7c)$$

$$\nabla_h \cdot \mathbf{u}_{i,j}^{n+1} := \delta_x U_{i,j}^{n+1} + \delta_y V_{i,j}^{n+1} = 0. \quad (7d)$$

Numerical methods

Scheme 2: Characteristic-FD method for model (B)

Chorin projection

$$\mathbf{u}_t - \frac{\alpha}{Re} \Delta \mathbf{u} = -\mathbf{u} \cdot \nabla \mathbf{u} + \frac{1-\alpha}{Re} \frac{1}{We} \nabla \cdot \boldsymbol{\sigma}$$

$$\mathbf{u}_t = -\frac{1}{Re} \nabla p$$

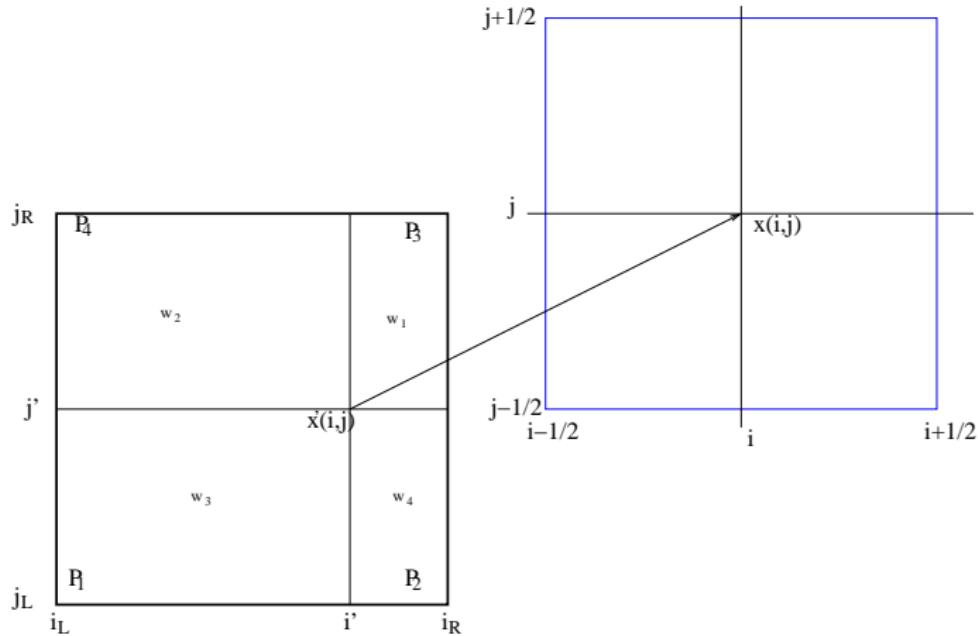
$$\frac{1}{\Delta t} (\mathbf{u}^{n+1} - \mathbf{u}^*) = -\nabla p^{n+1}$$

- a). $F = \nabla \cdot \mathbf{u}^*$
- b). $-\Delta p^{n+1} = -\frac{1}{\Delta t} F$
- c). $\mathbf{G} = \nabla p^{n+1}$
- d). $\mathbf{u}^{n+1} = \mathbf{u}^* - \Delta t \mathbf{G}.$

$$\nabla \cdot \mathbf{u}^{n+1} = \nabla \cdot (\mathbf{u}^* - \Delta t \mathbf{G}) = F - \Delta t \nabla \cdot (\nabla p^{n+1}) = 0.$$

Numerical methods

Characteristic path for Scheme 2



$$\psi^n \circ X^n = \psi^n(\mathbf{x}') = \sum w_k \psi(\mathbf{x}(P_k)), \quad \mathbf{x}' = \mathbf{x} - \mathbf{u} \Delta t.$$

Lemma 2

Let $(\mathbf{u}_h^n, p_h^n, \psi_h^n)_{0 \leq n \leq N_T}$ be a solution to the characteristic FEM scheme, supplied with homogeneous Dirichlet boundary condition for velocity, and with the zero Neumann boundary condition for ψ_h . Further, we assume that initially e^{ψ_h} is symmetric positive-definite. Then the free energy

$$F_h^n = F(\mathbf{u}_h^n, e^{\psi_h^n}) = \frac{Re}{2} \int_{\Omega} |\mathbf{u}_h^n|^2 + \frac{\beta}{2We} \int_{\Omega} \text{tr}(e^{\psi_h^n} - \psi_h^n - \mathbf{I})$$

satisfies

$$F_h^{n+1} + \Delta t \int_{\Omega} 2\alpha C_k |\nabla \mathbf{u}_h^{n+1}|^2 + \frac{\beta}{2We^2} \text{tr}(e^{\psi_h^n} + e^{-\psi_h^n} - 2\mathbf{I}) \leq F_h^n. \quad (8)$$

In particular, the sequence $(F_h^n)_{0 \leq n \leq N_T}$ is non-increasing.

Lemma 3

Let $(U_{i+1/2,j}^n, V_{i,j+1/2}^n, p_{i,j}^n, \psi_{i,j}^n)_{0 \leq n \leq N_T}$ be a solution of the discrete characteristic FD scheme, supplied with homogeneous Dirichlet boundary condition for velocity, and with the zero Neumann boundary condition for ψ . Further, we assume that initially e^ψ is symmetric positive-definite. Then the free energy

$$F_h^n = \frac{Re}{2} \left(\sum_{i=1}^{M-1} \sum_{j=1}^N (U_{i+1/2,j}^n)^2 + \sum_{i=1}^M \sum_{j=1}^{N-1} (V_{i,j+1/2}^n)^2 \right) + \frac{\beta}{2We} \sum_{i=1}^M \sum_{j=1}^N \operatorname{tr} (e^{\psi^n} - \psi^n - \mathbf{I})_{i,j}$$

satisfies

$$\begin{aligned} F_h^{n+1} + \alpha \Delta t & \left(\sum_{i=1}^{M-1} \sum_{j=1}^N |\nabla_h U_{i+1/2,j}^{n+1}|^2 + \sum_{i=1}^M \sum_{j=1}^{N-1} |\nabla_h V_{i,j+1/2}^{n+1}|^2 \right) \\ & + \frac{\Delta t \beta}{2We^2} \sum_{i=1}^M \sum_{j=1}^N \operatorname{tr} (e^{\psi^{n+1}} + e^{-\psi^{n+1}} - 2\mathbf{I})_{i,j} \leq F_h^n. \quad (9) \end{aligned}$$

In particular, the sequence $(F_h^n)_{0 \leq n \leq N_T}$ is non-increasing.

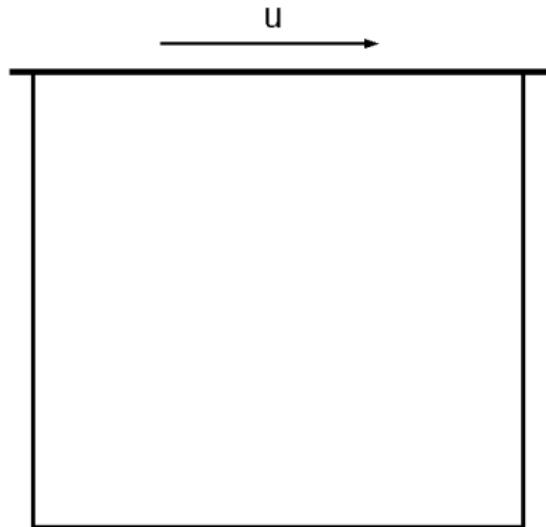
Numerical methods - test

Initial and boundary condition

Initial values $\mathbf{u} = \mathbf{0}, \sigma = \mathbf{I}$. Boundary conditions

$$\mathbf{u} = \begin{cases} (16x^2(1-x)^2, 0)^T, & \text{if } y = 1, x \in (0, 1), \\ \mathbf{0}, & \text{else.} \end{cases}$$

$$\frac{\partial \psi}{\partial \mathbf{n}} = 0.$$



Numerical methods - test

Non-diffusive models

Model (A): Standard-methods fail with $We > 1$

Model (B): Available for high We

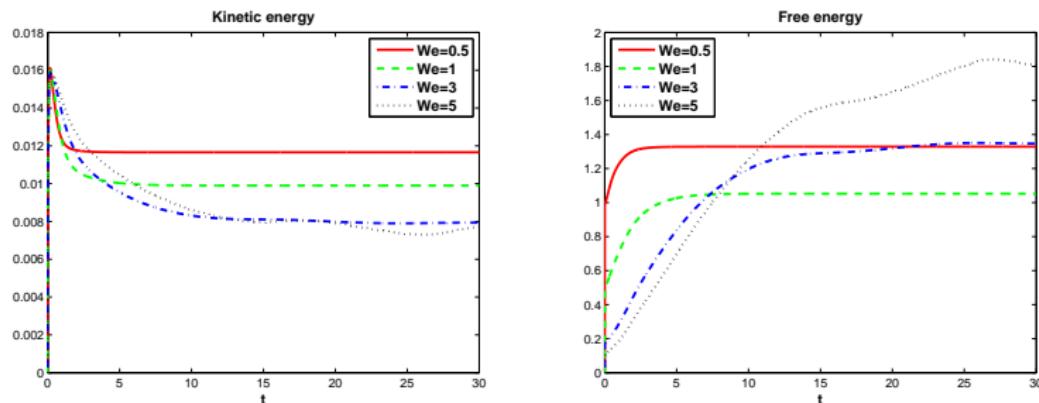
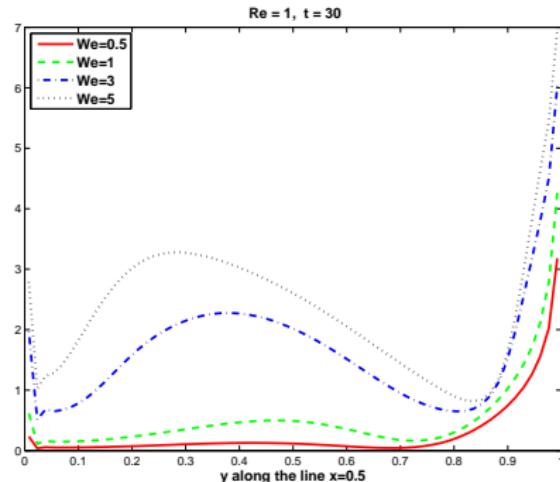


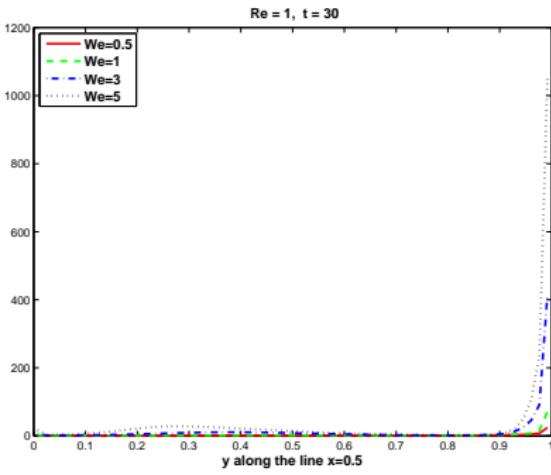
Figure : Kinetic and free energy.

Numerical methods - test

Non-diffusive model (B), $\varepsilon = 0$



(a) ψ_{11}



(b) σ_{11}

Figure : Conformation tensor component along the mid-line $x = 0.5$ at $t = 30$, $Re = 1$.

Numerical methods - test

Non-diffusive model (B), $\varepsilon = 0$

Table : L^2 -norm error with respect to mesh refinement of the non-diffusive Oldroyd-B model for σ_{11} : $\|\sigma_{11}(h) - \sigma_{11}(h/2)\|$.

mesh size h	We = 0.5	We = 1	We = 3
1/32	0.3502	1.5846	4.8967
1/64	0.5006	3.3141	10.8242
1/128	0.7181	5.3517	18.5389

Results do not converge !!

Numerical methods - test

Diffusive model

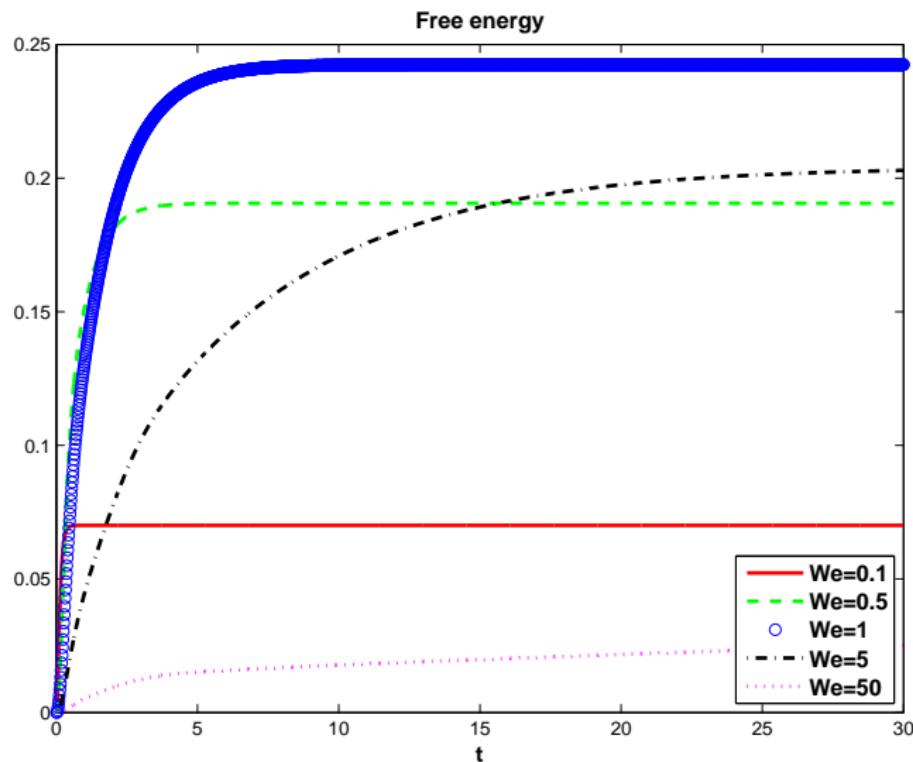


Figure : Free energy of the diffusive Oldroyd-B model (B), $\varepsilon = 0.01$.

Numerical methods - test

Diffusive model

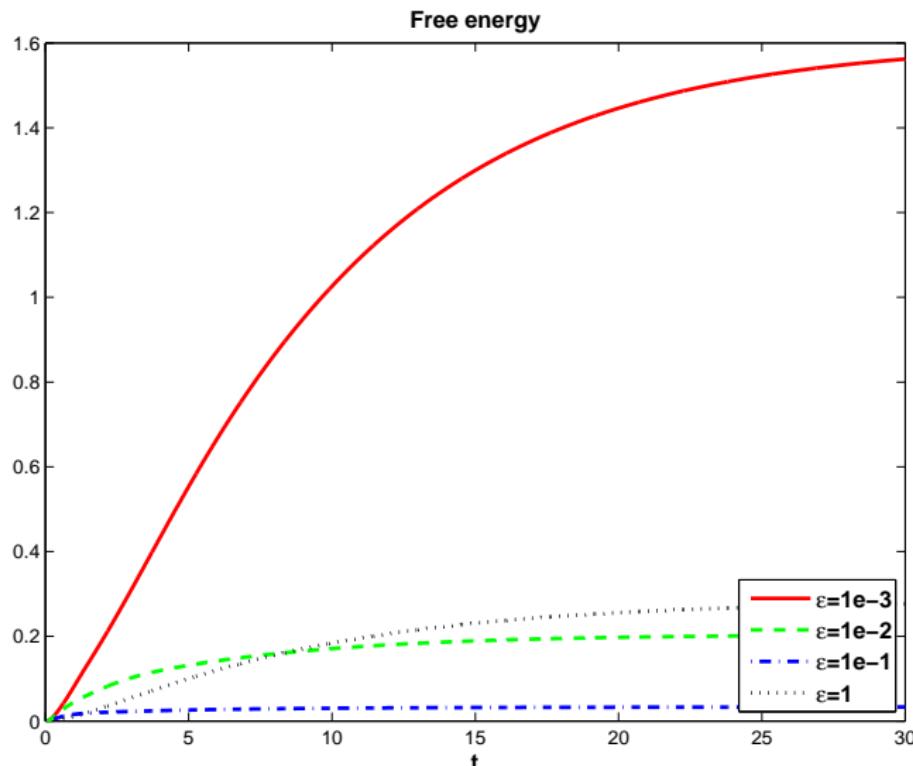


Figure : Free energy of the diffusive Oldroyd-B model, $We = 5$.

Numerical methods - test

Experimental Order of Convergence - Scheme 1

h	Error					
	$e(\mathbf{u}_h)$	$e(p_h)$	$e(\sigma_h)$	$e_1(u)$	$e_1(p_h)$	$e_1(\sigma_h)$
1/8	1.56e-02	1.84e-01	2.12e+00	5.85e-01	5.55e-01	3.15e+01
1/16	4.69e-03	9.74e-02	1.06e+00	3.19e-01	2.19e-01	1.86e+01
1/32	1.08e-03	3.07e-02	3.27e-01	1.51e-01	8.18e-02	8.05e+00
1/64	3.16e-04	1.21e-02	1.31e-01	7.54e-02	3.68e-02	4.12e+00
1/128	9.00e-05	4.61e-03	4.32e-02	3.85e-02	1.72e-02	1.98e+00
EOC						
1/8	1.73	0.91	0.99	0.88	1.34	0.76
1/16	2.11	1.67	1.70	1.07	1.42	1.21
1/32	1.78	1.34	1.32	1.01	1.15	0.97
1/64	1.81	1.39	1.60	0.97	1.10	1.05

Table : Error norms and EOC for diffusive Oldroyd-B model (B), $\varepsilon = 0.01$, We=5, computed by characteristic FEM scheme.

Numerical methods - test

Experimental Order of Convergence - Scheme 2

Error						
h	$e(\mathbf{u}_h)$	$e(p_h)$	$e(\sigma_h)$	$e_1(\mathbf{u}_h)$	$e_1(p_h)$	$e_1(\sigma_h)$
1/8	2.08e-02	3.76e-01	3.32e+00	2.26e-01	3.08e+00	3.42e+01
1/16	6.99e-03	1.89e-01	2.01e+00	9.11e-02	1.70e+00	2.13e+01
1/32	2.84e-03	8.78e-02	1.03e+00	3.80e-02	8.29e-01	1.02e+01
1/64	1.10e-03	3.16e-02	3.90e-01	1.35e-02	2.78e-01	3.71e+00
EOC						
1/8	1.58	0.99	0.72	1.31	0.86	0.68
1/16	1.30	1.11	0.97	1.26	1.03	1.06
1/32	1.37	1.47	1.40	1.49	1.57	1.46

Table : Error norms and EOC for diffusive Oldroyd-B model (B), $\varepsilon = 0.01$, We=5, computed by characteristic FD scheme.

- Energy stability for the diffusive Oldroyd-B model with LCR
- Numerical methods
 - Scheme 1: Characteristic FEM
 - Scheme 2: Characteristic FD
- Energy stability for the characteristic schemes on the discrete level
- Observed mesh convergence.

Thank you for your attention!

Appendix

For any symmetric positive-definite matrix $\sigma(t) \in (C^1([0, T)))^{\frac{d(d+1)}{2}}$, we have $\forall t \in [0, T]$:

$$\begin{aligned} \left(\frac{d}{dt} \sigma \right) : \sigma^{-1} &= \text{tr}(\sigma^{-1} \frac{d}{dt} \sigma) = \frac{d}{dt} \text{tr}(\ln \sigma), \\ \left(\frac{d}{dt} \ln \sigma \right) : \sigma &= \text{tr}(\sigma \frac{d}{dt} \ln \sigma) = \frac{d}{dt} \text{tr} \sigma. \end{aligned}$$

Since $\sigma(t) \in (C^1([0, T)))^{\frac{d(d+1)}{2}}$ is a symmetric positive-definite matrix, $\det \sigma$ is positive and $C^1([0, T])$. Thus, we get the classical Jacobi formula

$$\frac{d}{dt} \text{tr}(\ln \sigma) = \frac{d}{dt} \ln(\det \sigma) = (1/\det \sigma) \frac{d}{dt} \det \sigma = \text{tr}(\sigma^{-1} \frac{d}{dt} \sigma) = \left(\frac{d}{dt} \sigma \right) : \sigma$$

For the proof of the second equation, we set $\psi = \ln \sigma$ and then we can show

$$\left(\frac{d}{dt} \ln \sigma \right) : \sigma = \text{tr}(\sigma \frac{d}{dt} \ln \sigma) = \text{tr}(e^\psi \frac{d}{dt} \psi) = \text{tr}\left(\frac{d}{dt} e^\psi\right) = \frac{d}{dt} \text{tr} \sigma.$$

Appendix

Let $\sigma, \tau \in R^{d \times d}$ be symmetric positive-definite matrices, f_1 be an increasing function, and f_2 be a decreasing function, we have:

$$\begin{aligned}(\sigma - \tau) : (f_1(\sigma) - f_1(\tau)) &\geq 0, \\(\sigma - \tau) : (f_2(\sigma) - f_2(\tau)) &\leq 0, \\\nabla \sigma : \nabla \sigma^{-1} &\leq 0, \\\nabla(\ln \sigma) : \nabla \sigma &\geq 0.\end{aligned}$$