

# Free-energy dissipative schemes for the Oldroyd-B model

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# The Model: Oldroyd-B

## A model for dilute polymer solutions: Oldroyd-B

Conservation of momentum:

$$\text{Re} \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + (1 - \varepsilon) \Delta \mathbf{u} + \text{div } \boldsymbol{\tau}$$

Conservation of mass:

$$\text{div } \mathbf{u} = 0$$

Constitutive equation (Maxwell fluid):

$$\frac{\partial \boldsymbol{\tau}}{\partial t} + (\mathbf{u} \cdot \nabla) \boldsymbol{\tau} - (\nabla \mathbf{u}) \boldsymbol{\tau} - \boldsymbol{\tau} (\nabla \mathbf{u})^T = -\frac{1}{\text{Wi}} \boldsymbol{\tau} + \frac{\varepsilon}{\text{Wi}} [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$$

$\mathbf{u}$  - velocity field,  $p$  - hydrostatic pressure,  $\boldsymbol{\tau}$  - extra-stress tensor

$\text{Re} = \frac{\rho UL}{\eta}$ ,  $\varepsilon = \frac{\eta_p}{\eta}$ ,  $\text{Wi} = \frac{\lambda U}{L} := \frac{t_{\text{elastic}}}{t_{\text{flow}}}$  (Weissenberg number)

# Local existence

Assume  $\mathbf{x} \in \Omega$  bounded in  $\mathbb{R}^d$  ( $d = 2$  or  $3$ ).

Provide initial data  $\mathbf{u}(t = 0), \tau(t = 0)$ .

Assume Homogeneous Dirichlet boundary conditions on  $\mathbf{u}$ .

**Local in time existence theorem for smooth enough initial data.**

**No global existence theorem.**

# Numerical difficulties

Problems as  $Wi \nearrow O(1)$ :

- Numerical instability causing divergence
- Results are mesh-dependent

Possible reasons:

- Analytical difficulties: apart from some cases, there may be no steady-state solution, or an unstable solution.
- Bad numerical scheme

**Goal:** write a "good" numerical scheme which verifies a free energy inequality.

**Consequence:** no spurious free energy is created.

**Analytical outputs:** global existence of discrete solutions.

# Conformation tensor

**Definition: conformation tensor**

$$\boldsymbol{\sigma} = \mathbf{I} + \frac{\text{Wi}}{\varepsilon} \boldsymbol{\tau}$$

$\boldsymbol{\sigma}$  is symmetric positive definite (spd)

Rewrite system: Oldroyd-B- $\boldsymbol{\sigma}$

$$\begin{aligned} \text{Re} \left[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] &= -\nabla p + (1 - \varepsilon) \Delta \mathbf{u} + \frac{\varepsilon}{\text{Wi}} \text{div } \boldsymbol{\sigma} \\ \text{div } \mathbf{u} &= 0 \\ \frac{\partial \boldsymbol{\sigma}}{\partial t} + (\mathbf{u} \cdot \nabla) \boldsymbol{\sigma} - (\nabla \mathbf{u})^T \boldsymbol{\sigma} - \boldsymbol{\sigma} (\nabla \mathbf{u}) &= -\frac{\boldsymbol{\sigma} - \mathbf{I}}{\text{Wi}} \end{aligned}$$

For a smooth solution with  $\boldsymbol{\sigma}(t=0)$  spd,  $\boldsymbol{\sigma}(t)$  is spd at all time.

# Improved stability of equations

Better numerical stability when using a logarithmic transformation of  $\sigma$  [Fattal, Kupferman]:

$$\psi = \ln \sigma$$

(well-defined since  $\sigma$  is spd.)

**Question:** does this improved stability show up in our analysis?

# A micro-macro model: Hookean dumbbells

The Oldroyd-B model is formally equivalent to the following micro-macro model:

## Hookean dumbbells

Navier-Stokes equations +

$$\begin{aligned}\boldsymbol{\tau} &= \frac{\varepsilon}{Wi} \left( \int_{\mathbb{R}^d} \mathbf{q} \otimes \mathbf{q} \psi(t, \mathbf{x}, \mathbf{q}) d\mathbf{q} - \mathbf{I} \right) \\ \frac{\partial \psi}{\partial t} + (\mathbf{u} \cdot \nabla) \psi &= \operatorname{div}_{\mathbf{q}} \left( \left( (\nabla \mathbf{u}) \mathbf{q} - \frac{1}{2Wi} \mathbf{q} \right) \psi \right) + \frac{1}{2Wi} \Delta_{\mathbf{q}} \psi\end{aligned}$$

$\mathbf{q}$  - extension vector of dumbbells,  $\psi$  - distribution of the dumbbells.



# Entropy and kinetic energy

In the micro-macro context, it is natural to work with the entropy:

$$H(t) = \int_{\Omega} \int_{\mathbb{R}^d} \psi(t, \mathbf{x}, \mathbf{q}) \ln \frac{\psi(t, \mathbf{x}, \mathbf{q})}{\psi_{\infty}(\mathbf{q})}$$

where  $\psi_{\infty}(\mathbf{q}) = \frac{\exp(-|\mathbf{q}|^2)}{\int_{\mathbb{R}^d} \exp(-|\mathbf{q}|^2)}$  is the equilibrium distribution.

Compute and obtain a macroscopic quantity:

$$H(t) = \frac{1}{2} \int_{\Omega} \text{tr}(\boldsymbol{\sigma} - \ln \boldsymbol{\sigma} - \mathbf{I})$$

Define the kinetic energy:

$$E_{\text{kinetic}}(t) = \frac{\text{Re}}{2} \int_{\Omega} |\mathbf{u}|^2$$

## Definition: free energy

Let  $(\mathbf{u}, p, \boldsymbol{\sigma})$  be a smooth solution to Oldroyd-B- $\boldsymbol{\sigma}$ . Define

$$F(\mathbf{u}, \boldsymbol{\sigma}) = \underbrace{\frac{\text{Re}}{2} \int |\mathbf{u}|^2}_{\text{kinetic energy}} + \underbrace{\frac{\varepsilon}{2\text{Wi}} \int_{\Omega} \text{tr}(\boldsymbol{\sigma} - \ln \boldsymbol{\sigma} - \mathbf{I})}_{\text{entropy}}$$

$\boldsymbol{\sigma}$  spd  $\Rightarrow F \geq 0$  always.

# Free energy dissipation

## A free energy equality

Let  $(\mathbf{u}, p, \boldsymbol{\sigma})$  be a smooth solution to Oldroyd-B- $\boldsymbol{\sigma}$ , then:

$$\frac{d}{dt} F(\mathbf{u}, \boldsymbol{\sigma}) + \underbrace{(1 - \varepsilon) \int_{\Omega} |\nabla \mathbf{u}|^2 + \frac{\varepsilon}{2\text{Wi}^2} \int_{\Omega} \text{tr}(\boldsymbol{\sigma} + \boldsymbol{\sigma}^{-1} - 2\mathbf{I})}_{\text{dissipative terms} \geq 0} = 0$$

$\Rightarrow F$  decreases in time.

Consequence : there exists  $C > 0$  s.t.

$$F(\mathbf{u}, \boldsymbol{\sigma}) \leq F(\mathbf{u}(t=0), \boldsymbol{\sigma}(t=0)) \exp(-Ct)$$

Useful to characterize long-time asymptotics of solutions.  
[Jourdain, Le-Bris, Lelièvre, Otto 06].

## A remark: classical energy estimate

The classical energy estimate can be used, but to obtain exponential decay, the assumption  $\det \sigma(t = 0) > 1$  is needed.

# Numerical framework: finite elements

In order to work in the F.E. framework, we need a variational formulation.

Then we need to be able to recover the free energy equality.

# Variational formulation

A smooth solution to Oldroyd-B- $\sigma$  ( $\mathbf{u}, p, \sigma$ ) satisfies

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 & \underbrace{- p \operatorname{div} \mathbf{v} + q \operatorname{div} \mathbf{u}}_{\text{NS terms}} \\
 & \underbrace{\left( \frac{\partial \sigma}{\partial t} + \mathbf{u} \cdot \nabla \sigma \right) : \phi - ((\nabla \mathbf{u}) \sigma + \sigma (\nabla \mathbf{u})^T) : \phi + \frac{1}{\operatorname{Wi}} (\sigma - \mathbf{I}) : \phi}_{\text{constitutive eq. terms}},
 \end{aligned}$$

for all sufficiently smooth test functions  $(\mathbf{v}, q, \phi)$ .

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for all sufficiently smooth test functions  $(\mathbf{v}, q, \phi)$ .

The free energy equality is recovered with

$(\mathbf{v}, q, \phi) = (\mathbf{u}, p, \frac{\varepsilon}{2\operatorname{Wi}}(\mathbf{I} - \sigma^{-1})) \Rightarrow \sigma^{-1}$  is a test function.

## A "simple" choice of F.E.

Scott-Vogelius mixed finite element space for  $(\mathbf{u}_h, p_h)$ :

- $\mathbf{u}_h \in (\mathbb{P}_2)^2$
- $p_h \in \mathbb{P}_{1,disc}$

Good because  $\operatorname{div} \mathbf{u}_h(\mathbf{x}) = 0, \forall \mathbf{x} \in \Omega$ .

For meshes built in a certain way, this F.E. satisfies the Babuška-Brezzi inf-sup condition.

For  $\sigma_h$ , assume simply

- $\sigma_h \in (\mathbb{P}_0)^3 \implies \sigma_h^{-1}$  can be used as test function.

# Main challenges

- Discretize the advection term  $(\mathbf{u} \cdot \nabla)\sigma$ :
  - ① Method of characteristics
  - ② Discontinuous Galerkin method
- Recover a free energy dissipation.

# Discrete problem

$$0 = \int_{\Omega} (\text{stuff}_h^n)$$

Show local existence in time, then define

**Definition: discrete free energy**

The free energy for the solution  $(\mathbf{u}_h^n, p_h^n, \boldsymbol{\sigma}_h^n)$  is:

$$F_h^n = F(\mathbf{u}_h^n, \boldsymbol{\sigma}_h^n) = \frac{\text{Re}}{2} \int_{\Omega} |\mathbf{u}_h^n|^2 + \frac{\varepsilon}{2\text{Wi}} \int_{\Omega} \text{tr}(\boldsymbol{\sigma}_h^n - \ln \boldsymbol{\sigma}_h^n - \mathbf{I})$$

# Recovering a free energy dissipation (method of characteristics)

**The problematic terms are the time derivatives.**

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**1. Treatment of  $\mathbf{u}$  derivative:**

$\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u}\right) \cdot \mathbf{v}$  is discretized as  $\left(\frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{\Delta t} + \mathbf{u}_h^n \cdot \nabla \mathbf{u}_h^{n+1}\right) \cdot \mathbf{v}$ .



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Using as test function  $\mathbf{v} = \mathbf{u}_h^{n+1}$ :

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(since  $\operatorname{div} \mathbf{u}_h^n(\mathbf{x}) = 0, \forall \mathbf{x} \in \Omega$ ).

# Recovering a free energy dissipation (method of characteristics)

## 2. Treatment of $\sigma$ derivative:

$(\frac{\partial \sigma}{\partial t} + \mathbf{u} \cdot \nabla \sigma) : \phi$  is discretized as  $(\frac{\sigma_h^{n+1} - \sigma_h^n \circ X^n(t^n)}{\Delta t}) : \phi$  where

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

$\operatorname{div} \mathbf{u}_h^n(\mathbf{x}) = 0, \forall \mathbf{x} \in \Omega \Rightarrow X^n(t)$  is a mapping with constant Jacobian (= 1),  $\forall t \in [t^n, t^{n+1}]$ .

# Recovering a free energy dissipation (method of characteristics)

Lemma 1:

Let  $\sigma$  and  $\tau$  be two symmetric positive definite matrices. Then

$$\mathrm{tr}((\sigma - \tau)\tau^{-1}) = \mathrm{tr}(\sigma\tau^{-1} - \mathbf{I}) \geq \mathrm{tr}(\ln \sigma - \ln \tau),$$

# Recovering a free energy dissipation with the method of characteristics

Use as test function  $\phi = \mathbf{1} - (\sigma_h^{n+1})^{-1}$ , and use Lemma 1:



# Recovering a free energy dissipation with the method of characteristics

Use as test function  $\phi = \mathbf{I} - (\boldsymbol{\sigma}_h^{n+1})^{-1}$ , and use Lemma 1:

$$\int_{\Omega} (\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{\sigma}_h^n \circ X^n(t^n)) : (\mathbf{I} - (\boldsymbol{\sigma}_h^{n+1})^{-1})$$

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(since  $X^n$  has Jacobian equal to 1).

# A discrete free energy inequality

## Discrete free energy inequality

Let  $(\mathbf{u}_h^n, p_h^n, \boldsymbol{\sigma}_h^n)_{0 \leq n \leq N_T}$  be a solution to the discrete problem, such that  $\boldsymbol{\sigma}_h^n$  is spd. Then, the free energy of the solution  $(\mathbf{u}_h^n, p_h^n, \boldsymbol{\sigma}_h^n)$  satisfies:

$$F_h^{n+1} - F_h^n + \int_{\Omega} \frac{\operatorname{Re}}{2} |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 + \Delta t \int_{\Omega} (1 - \varepsilon) |\nabla \mathbf{u}_h^{n+1}|^2 + \Delta t \frac{\varepsilon}{2\operatorname{Wi}^2} \int_{\Omega} \operatorname{tr} (\boldsymbol{\sigma}_h^{n+1} + (\boldsymbol{\sigma}_h^{n+1})^{-1} - 2I) \leq 0.$$

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

**Same free energy inequality for the DG method**

# The log transformation

The same treatment can be applied to the log-transformed system. We obtain an equivalent free energy inequality:

## log free energy inequality

For a solution  $(\mathbf{u}_h^n, p_h^n, \psi_h^n)$ , the free energy is

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

and it satisfies

$$\begin{aligned} F_h^{n+1} - F_h^n + \int_{\Omega} \frac{\text{Re}}{2} |\mathbf{u}_h^{n+1} - \mathbf{u}_h^n|^2 + \Delta t \int_{\Omega} (1 - \varepsilon) |\nabla \mathbf{u}_h^{n+1}|^2 \\ + \Delta t \frac{\varepsilon}{2\text{Wi}^2} \int_{\Omega} \text{tr} \left( e^{\psi_h^{n+1}} + e^{-\psi_h^{n+1}} - 2\mathbf{I} \right) \leq 0. \end{aligned}$$

# We obtained a "good" scheme

As a consequence, we obtain some numerical stability:

- ① Global existence in time and uniqueness of discrete solutions for  $\Delta t$  small enough in the  $\sigma$  formulation.
- ② In the case of the log formulation, global existence for any  $\Delta t$ .



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**MERCI!**

# Properties needed to obtain free energy estimate

Advection discretized by:	Characteristics	DG
Requirements for $\mathbf{u}_h$ :	$\operatorname{div} \mathbf{u}_h = 0$ ( $\Rightarrow \det(\nabla_{\mathbf{x}} X^n) \equiv 1$ ) ( $\Rightarrow (\mathbf{u}_h \cdot \mathbf{n}) _{E_j}$ well defined )	$\int_{\Omega} q \operatorname{div} \mathbf{u}_h = 0,$ $\forall q \in \mathbb{P}_0$ and $(\mathbf{u}_h \cdot \mathbf{n}) _{E_j}$ well defined

**Table:** Summary of the arguments with  $(\mathbf{u}_h, p_h, \boldsymbol{\sigma}_h)$  or  $(\mathbf{u}_h, p_h, \boldsymbol{\psi}_h)$  in  $(\mathbb{P}_2)^d \times \mathbb{P}_{1, \text{disc}} \times (\mathbb{P}_0)^{\frac{d(d+1)}{2}}$

## Discretized problem (characteristics method)

For a given  $(\mathbf{u}_h^n, p_h^n, \boldsymbol{\sigma}_h^n)$ , find

$(\mathbf{u}_h^{n+1}, p_h^{n+1}, \boldsymbol{\sigma}_h^{n+1}) \in (\mathbb{P}_2)^2 \times \mathbb{P}_{1, disc} \times (\mathbb{P}_0)^3$  such that, for any test function  $(\mathbf{v}, q, \boldsymbol{\phi}) \in (\mathbb{P}_2)^2 \times \mathbb{P}_{1, disc} \times (\mathbb{P}_0)^3$ ,

$$\begin{aligned} 0 = \int_{\Omega} \operatorname{Re} \left( \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{\Delta t} + \mathbf{u}_h^n \cdot \nabla \mathbf{u}_h^{n+1} \right) \cdot \mathbf{v} - p_h^{n+1} \operatorname{div} \mathbf{v} + q \operatorname{div} \mathbf{u}_h^{n+1} \\ + (1 - \varepsilon) \nabla \mathbf{u}_h^{n+1} : \nabla \mathbf{v} + \frac{\varepsilon}{\operatorname{Wi}} \boldsymbol{\sigma}_h^{n+1} : \nabla \mathbf{v} \\ + \left( \frac{\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{\sigma}_h^n \circ X^n(t^n)}{\Delta t} \right) : \boldsymbol{\phi} - \left( (\nabla \mathbf{u}_h^{n+1}) \boldsymbol{\sigma}_h^{n+1} + \boldsymbol{\sigma}_h^{n+1} (\nabla \mathbf{u}_h^{n+1})^T \right) : \boldsymbol{\phi} \\ + \frac{1}{\operatorname{Wi}} (\boldsymbol{\sigma}_h^{n+1} - \mathbf{I}) : \boldsymbol{\phi}. \end{aligned}$$



# Discretized problem (DG)

For a given  $(\mathbf{u}_h^n, p_h^n, \boldsymbol{\sigma}_h^n)$ , find

$(\mathbf{u}_h^{n+1}, p_h^{n+1}, \boldsymbol{\sigma}_h^{n+1}) \in (\mathbb{P}_2)^2 \times \mathbb{P}_{1, \text{disc}} \times (\mathbb{P}_0)^3$  such that, for any test function  $(\mathbf{v}, q, \phi) \in (\mathbb{P}_2)^2 \times \mathbb{P}_{1, \text{disc}} \times (\mathbb{P}_0)^3$ ,

$$\begin{aligned} 0 = & \sum_{k=1}^{N_K} \int_{K_k} \operatorname{Re} \left( \frac{\mathbf{u}_h^{n+1} - \mathbf{u}_h^n}{\Delta t} + \mathbf{u}_h^n \cdot \nabla \mathbf{u}_h^{n+1} \right) \cdot \mathbf{v} - p_h^{n+1} \operatorname{div} \mathbf{v} + q \operatorname{div} \mathbf{u}_h^{n+1} \\ & + (1 - \varepsilon) \nabla \mathbf{u}_h^{n+1} : \nabla \mathbf{v} + \frac{\varepsilon}{\operatorname{Wi}} \boldsymbol{\sigma}_h^{n+1} : \nabla \mathbf{v} \\ & + \left( \frac{\boldsymbol{\sigma}_h^{n+1} - \boldsymbol{\sigma}_h^n}{\Delta t} \right) : \phi - \left( (\nabla \mathbf{u}_h^{n+1}) \boldsymbol{\sigma}_h^{n+1} + \boldsymbol{\sigma}_h^{n+1} (\nabla \mathbf{u}_h^{n+1})^T \right) : \phi \\ & + \frac{1}{\operatorname{Wi}} (\boldsymbol{\sigma}_h^{n+1} - \mathbf{I}) : \phi + \sum_{j=1}^{N_E} \int_{E_j} |\mathbf{u}_h^n \cdot \mathbf{n}| [\boldsymbol{\sigma}_h^{n+1}] : \phi^+ \end{aligned}$$

# Discretization of the advection term in the DG method

$$\left(\frac{\partial \sigma}{\partial t} + \mathbf{u} \cdot \nabla \sigma\right) : \phi \text{ is discretized as}$$
$$\left(\frac{\sigma_h^{n+1} - \sigma_h^n \circ X^n(t^n)}{\Delta t}\right) : \phi + \sum_{j=1}^{N_E} \int_{E_j} |\mathbf{u}_h^n \cdot \mathbf{n}| \llbracket \sigma_h^{n+1} \rrbracket : \phi^+$$