

# Fluide d'Oldroyd B et second principe de la thermodynamique

## The Oldroyd B fluid and the second principle of thermodynamics

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Rencontre thématique du GDR GDM  
Jussieu, 22–24 novembre 2023

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# Overview

- ▶ Objective derivatives
- ▶ The Oldroyd B fluid
- ▶ Viscoelastic materials with internal variables
- ▶ Lagrangian Oldroyd B
- ▶ Oldroyd B and the second principle
- ▶ Oldroyd B-like models
- ▶ Conclusions

<https://arxiv.org/abs/2308.01211> or

<https://hal.sorbonne-universite.fr/hal-04166054>

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# General notation

Lagrangian description: uppercase. Eulerian description: lowercase. For instance,  $(x, t) = (\phi(X, t), t)$ ,  $v(x, t) = V(X, t) = \frac{\partial \phi}{\partial t}(X, t)$  and so on.

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- ▶ Deformation gradient  $F(X, t)$ , deformation rate  $H(X, t) = \frac{\partial}{\partial t} F(X, t)$ . Incompressible:  $J = \det F = 1$ .

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- ▶ Dynamics equation  $\rho \dot{v} - \text{div}_x \sigma = b$ .



# Objective derivatives

Frame-indifference: if  $\phi^*(X, t) = Q(t)\phi(X, t) + a(t)$  then

$$\sigma^*(x^*, t) = Q(t)\sigma(x, t)Q(t)^T.$$

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An objective derivative is a first order in time differential operator  $\hat{\diamond}$  such that

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A differential constitutive relation for the Cauchy stress of the form

$$\hat{\square}\sigma(x, t) = G(\sigma(x, t), d(x, t))$$

can then be frame-indifferent.

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The material derivative is not objective.

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# A characterization of objective derivatives

Unfortunately, there are infinitely many different objective derivatives. Consider those of the form  $\overset{\circ}{\sigma} = \dot{\sigma} + \text{Ob}(\sigma, h)$ , with  $\text{Ob}: \text{Sym}_3 \times \mathbb{M}_3 \rightarrow \text{Sym}_3$ .

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All functions  $\text{Ob}_s: \text{Sym}_3 \times \text{Sym}_3 \rightarrow \text{Sym}_3$  such that  $\text{Ob}_s(Q\sigma Q^T, QdQ^T) = Q\text{Ob}_s(\sigma, d)Q^T$  are known (*objective functions*), cf. Smith (1971). In particular, all symmetric-valued polynomials in  $(\sigma, d)$ .

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## Theorem

*Such an operator is objective if and only if*

$$\text{Ob}(\sigma, h) = \sigma w - w\sigma + \text{Ob}_s(\sigma, d).$$

*with  $w = \text{Skew}(h)$ ,  $d = \text{Sym}(h)$ , and  $\text{Ob}_s: \text{Sym}_3 \times \text{Sym}_3 \rightarrow \text{Sym}_3$  is an objective function.*

(Gurtin-Fried-Anand, 2010).

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Plenty of them.

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- ▶ The Zaremba-Jaumann derivative  $\overset{\square}{\sigma} = \dot{\sigma} + \sigma w - w\sigma$ ,  
with  $Ob_s = 0$ ,

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 $\overset{\Delta}{\sigma} = \dot{\sigma} + h^T\sigma + \sigma h$  with  $\text{Ob}_s(\sigma, d) = d\sigma + \sigma d$ ,

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Something special about Oldroyd B (incompressible case):

$$\overset{\nabla}{\sigma} = F \frac{\partial \Sigma}{\partial t} F^T,$$

where  $\Sigma$  is the second Piola-Kirchhoff stress. ( $\sigma = F\Sigma F^T$ ).

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Looks like this:

$$\sigma + \lambda_1 \overset{\nabla}{\sigma} = 2\eta(d + \lambda_2 \overset{\nabla}{d}),$$

$\eta > 0$  global viscosity,  $0 < \lambda_2 \leq \lambda_1$  relaxation times.

Frame-indifferent by design. Initial conditions?

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$$\Leftrightarrow \sigma = \sigma_s + \sigma_p, \quad \sigma_s = 2\eta_s d \quad \text{and} \quad \sigma_p + \lambda_1 \overset{\nabla}{\sigma}_p = 2\eta_p d,$$

$$\eta_s = \frac{\lambda_2}{\lambda_1} \eta \quad \text{and} \quad \eta_p = \left(1 - \frac{\lambda_2}{\lambda_1}\right) \eta.$$

$\sigma_s$ : Newtonian solvent stress with solvent viscosity  $\eta_s$ ,

$\sigma_p$ : polymer stress with polymer viscosity  $\eta_p$ .

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$$\Leftrightarrow \sigma = \sigma_s + \sigma_p, \quad \sigma_s = 2\eta_s d \quad \text{and} \quad \sigma_p + \lambda_1 \overset{\nabla}{\sigma}_p = 2\eta_p d,$$

$$\eta_s = \frac{\lambda_2}{\lambda_1} \eta \quad \text{and} \quad \eta_p = \left(1 - \frac{\lambda_2}{\lambda_1}\right) \eta.$$

$\sigma_s$ : Newtonian solvent stress with solvent viscosity  $\eta_s$ ,

$\sigma_p$ : polymer stress with polymer viscosity  $\eta_p$ .

Many different ways of deriving the Oldroyd B model. Here a phenomenological Lagrangian approach for testing its compatibility with the second principle of thermodynamics.

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1. Helmholtz free energy specific density

$$\hat{A}_m: \mathbb{M}_3^+ \times \mathbb{M}_3 \times \text{Sym}_3 \rightarrow \mathbb{R}.$$

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3. Flow rule  $\hat{K}: \mathbb{M}_3^+ \times \mathbb{M}_3 \times \text{Sym}_3 \rightarrow \text{Sym}_3$  used in ode

$$\frac{\partial B_i}{\partial t} = \hat{K}(F, H, B_i).$$

What about initial conditions?



# Viscoelastic materials with internal variables 2

Consequences of C-N procedure (*i.e.*, C-D inequality + constitutive assumptions + any deformation + chain rule):

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- ▶ No  $H$  in  $\hat{A}_m$ .
- ▶ Natural decomposition of the first PK stress

$$\hat{T}_R(F, H, B_i) = \hat{T}_{Rd}(F, H, B_i) + \frac{\partial \hat{A}_m}{\partial F}(F, B_i).$$

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- ▶ Constitutive law for the internal dissipation

$$\begin{aligned} \hat{D}_{\text{int}}(F, H, B_i) &= \hat{T}_{Rd}(F, H, B_i) : H \\ &\quad - \frac{\partial \hat{A}_m}{\partial B_i}(F, B_i) : \hat{K}(F, H, B_i). \end{aligned}$$

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Second principle, C-N version:  $\widehat{D}_{\text{int}}(F, H, B_i) \geq 0$  for all possible arguments. A constitutive restriction, equivalent to the second principle in this case.

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We will have to be less demanding for Oldroyd B.

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## List of ingredients for Oldroyd B:

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## List of ingredients for Oldroyd B:

Initial idea of Francfort & Lopez-Pamies (pers. comm. 2021): start with the neo-Hookean energy  $\widetilde{W}(C) = \frac{\mu}{2} \text{tr } C$ ,  $\mu > 0$ , where  $C = F^T F$ .  $\approx$  elastic polymer energy.

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Kinematically viscous stress: Newtonian solvent,

$$\widehat{T}_{\text{Rd}}(F, H, B_i) = 2\eta_s \text{Sym}(HF^{-1}) \text{cof } F.$$

= solvent part of the Cauchy stress  $\sigma_s = 2\eta_s d$ .

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What about the flow rule?

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# Oldroyd B: Lagrangian w. an internal variable 2

Decomposition of the 1st PK stress  $\leftrightarrow$  decomposition of the Cauchy stress  $\sigma = \sigma_s + \sigma_p$  with polymer part  $\sigma_p = \frac{\partial \hat{A}_m}{\partial F}(F, B_i) F^T$ , here,

$$\sigma_p = \mu F B_i F^T \text{ or } \Sigma_p = \mu B_i$$

when written with the 2nd PK polymer stress.

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Some reverse engineering  $\rightarrow (\frac{\partial B_i}{\partial t} = \hat{K}(F, H, B_i) \text{ and } \overset{\nabla}{\sigma} = F \frac{\partial \Sigma}{\partial t} F^T)$

$$\hat{K}(F, H, B_i) = -\frac{1}{\lambda_1} B_i + \frac{2\eta_p}{\mu\lambda_1} F^{-1} \text{Sym}(H F^{-1}) F^{-T}.$$

Then

$$\overset{\nabla}{\sigma}_p = -\frac{1}{\lambda_1} \sigma_p + \frac{2\eta_p}{\lambda_1} d$$

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*i.e., Oldroyd B!*

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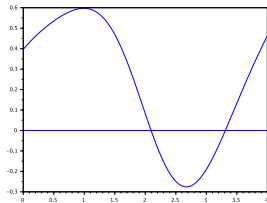
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# Oldroyd B and the second principle 1

From HLD-AR (2022), the naive Eulerian internal dissipation  $\sigma : d$  is not good:



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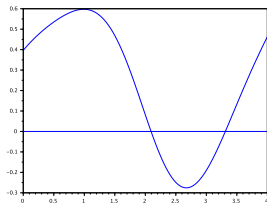
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Take  $\xi = \sigma_p$  as a Eulerian internal variable and see what happens.

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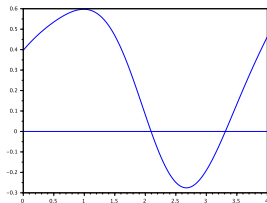
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Not good either: no free energy  $\hat{a}_m(\xi)$  making the nonnaive dissipation nonnegative (CN approach).

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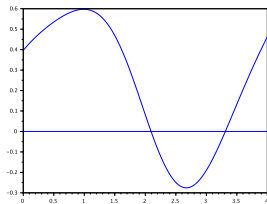
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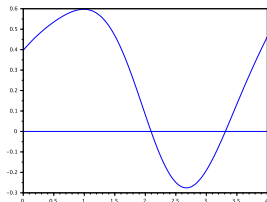
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Sketch of proof: given a deformation  $\phi$ , 1st order linear ode with constant coefficients for  $B_i \rightarrow$  Duhamel formula. Dissipation is  $\widehat{D}_{\text{int}}(F, H, B_i) = 2\eta_s \|d\|^2 + \frac{\mu}{2\lambda_1} B_i : C$ , and we show that  $B_i(t) : C(t) \geq 0$  for all  $t \geq 0$ .

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**Crucial remark:**  $\forall$  sym. positive semi-definite  $C, D$  in  $SL(3)$ ,  $C : D \geq 3$ .  
But  $B_i$  does not remain positive semidefinite for all times!

$(C : D \geq n(\det C)^{1/n}(\det D)^{1/n})$

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Role of indeterminate pressure?

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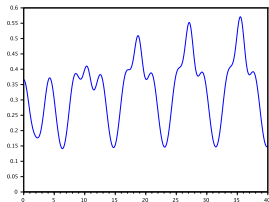
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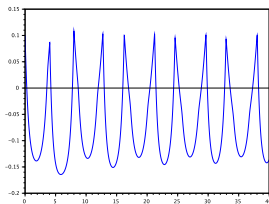
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Oldroyd B dissipation with positive definite initial  $\sigma_p$



Smallest eigenvalue of  $\sigma_p$

# Oldroyd B-likes, same Lagrangian approach

- ▶ Compressible Oldroyd B w. Truesdell derivative. At least one special case satisfies 2nd principle conditionally.

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$$\overset{\nabla}{\sigma}_p = -\frac{1}{\lambda_1 \mu_k} \sigma_p^{k+1} + \frac{2\eta_p}{\lambda_1} d.$$

→  $k = 0$ ,  $\mu_0 = 1$ : traditional, linear Oldroyd B,

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ZJ and Old A no 2nd principle with this free energy.

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- ▶ Traditional Oldroyd B fluid recast as a viscoelastic Lagrangian model w. internal variable, involving a neo-Hookean “polymer” energy and a Newtonian solvent.

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- ▶ Nontrivially satisfies a conditional version of the 2nd principle. Role of initial conditions.
- ▶ Fun compressible or nonlinear extensions, possibly of limited modeling interest.
- ▶ Zaremba-Jaumann and Oldroyd A fluids likewise recast but not thermodynamically sound.

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