

A NEW PERSPECTIVE ON THE STANDARD MODELS OF VISCOELASTIC FLUIDS (W.I.P.)

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STANDARD VISCOELASTIC FLUID MODELS

For an unknown divergence-free velocity $\mathbf{v} : Q \rightarrow \mathbb{R}^d$, pressure $p : Q \rightarrow \mathbb{R}$ and extra stress tensor $\mathbf{B} : Q \rightarrow \mathbb{R}_{\text{sym}}^{d \times d}$, consider the system

$$\begin{aligned} \partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} - \nu \Delta \mathbf{v} + \nabla p &= \operatorname{div}(\mu \mathbf{B}), \quad \nu, \mu > 0, \\ \partial_t \mathbf{B} + \mathbf{v} \cdot \nabla \mathbf{B} + \frac{1}{\tau} (\mathbf{B}^\alpha - \mathbf{B}^{\alpha-1}) &= (\nabla \mathbf{v}) \mathbf{B} + \mathbf{B} (\nabla \mathbf{v})^T, \quad \tau > 0, \alpha \geq 1. \end{aligned} \quad (\text{B})$$

- $\alpha = 1$ is the Oldroyd-B model (1950) and $\alpha = 2$ is the Giesekus model (1962).
- Equation (B) can be written as

$$\nabla \mathbf{B} + \frac{1}{\tau} (\mathbf{B}^\alpha - \mathbf{B}^{\alpha-1}) = 0,$$

where

$$\begin{aligned} \nabla \mathbf{B} &:= \partial_t \mathbf{B} + \mathbf{v} \cdot \nabla \mathbf{B} - (\nabla \mathbf{v}) \mathbf{B} - \mathbf{B} (\nabla \mathbf{v})^T \\ &= \underbrace{\partial_t \mathbf{B} + \mathbf{v} \cdot \nabla \mathbf{B} + \mathbf{B} \mathbf{W} - \mathbf{W} \mathbf{B}}_{\overset{\circ}{\mathbf{B}} \text{ Jaumann-Zaremba}} - (\mathbf{B} \mathbf{D} + \mathbf{D} \mathbf{B}) = \overset{\circ}{\mathbf{B}} - (\mathbf{B} \mathbf{D} + \mathbf{D} \mathbf{B}) \end{aligned}$$

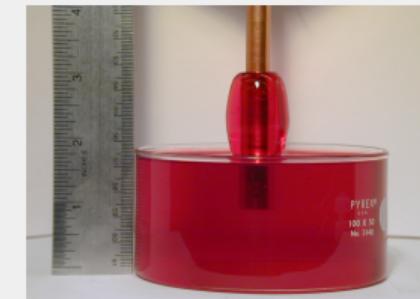
is the upper convected (Oldroyd) derivative and

$$\mathbf{D} := \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad \mathbf{W} := \frac{1}{2} (\nabla \mathbf{v} - (\nabla \mathbf{v})^T).$$

(DIS)ADVANTAGES OF THE OLDROYD-B/GIESEKUS MODELS

+ There are compelling arguments for considering equation (B) with $\overset{\nabla}{\mathbf{B}}$:

- ▶ $\overset{\nabla}{\mathbf{B}}$ is an objective derivative (rate), i.e.
$$\overset{\nabla}{\mathbf{B}}^*(t, x^*) = Q(t) \overset{\nabla}{\mathbf{B}}(t, x) Q(t)^T$$
 if $\overset{\nabla}{\mathbf{B}}^*(t, x^*) = Q(t) \mathbf{B}(t, x) Q(t)^T$
for any (non-stationary) rotation $Q(t)$ of the observer.
- ▶ When $\mathbf{B} = \mathbf{F}\mathbf{F}^T$, $\mathbf{F} = \partial_{\mathbf{x}}\chi(t, \mathbf{X})$ (solid mechanics) then $\overset{\nabla}{\mathbf{B}} = 0$.
- ▶ $\overset{\nabla}{\mathbf{B}}$ arises by downscaling certain microscopic models.
- ▶ Established in applications (polymeric fluids, rod climbing etc.).
- ▶ The Giesekus case $\alpha = 2$ (remarkably) admits a three-dimensional global weak solution for any initial data due to the recent result (Los et al. 2024).



- However, there are also drawbacks:

- ▶ $\overset{\nabla}{\mathbf{B}}$ is just one of really **many** objective derivatives.
- ▶ $\overset{\nabla}{\mathbf{B}}$ is **not corotational**. Cor. derivatives are **superior** in physics, analysis and numerics.
- ▶ In the Oldroyd-B case $\alpha = 1$, the a priori estimates are not sufficient for $(\nabla \mathbf{v})\mathbf{B} + \mathbf{B}(\nabla \mathbf{v})^T$.
- ▶ The equation is on the verge of being “ill-posed”, comparing just with $u' + u^\alpha = gu$, $g \in L^2$.

THE EQUIVALENCE RESULT

If done **properly**, the idea of multiplying the equation (B) by \mathbf{B}^{-1} leads to the following:

Theorem

Let $\mathbf{v} : Q \rightarrow \mathbb{R}^d$, $\mathbf{H} : Q \rightarrow \mathbb{R}_{\text{sym}}^{d \times d}$ be smooth and set

$\mathbf{B} = e^{2\mathbf{H}}$, so that $\mathbf{H} = \frac{1}{2} \log \mathbf{B}$ is the logarithmic (Hencky) strain.

Then \mathbf{B} solves the Oldroyd-B/Giesekus equation (B) if and only if \mathbf{H} solves

$$\partial_t \mathbf{H} + \mathbf{v} \cdot \nabla \mathbf{H} + \frac{1}{2\tau} (e^{2(\alpha-1)\mathbf{H}} - e^{2(\alpha-2)\mathbf{H}}) = \mathbf{D} - \mathbf{H} \Omega^{\log} + \Omega^{\log} \mathbf{H}, \quad (\mathbf{H})$$

where:

$\Omega^{\log} := \mathbf{W} - \sigma(\text{ad}_{\mathbf{H}})\mathbf{D}$ is the logarithmic spin,

$\text{ad}_{\mathbf{H}} X := \mathbf{H}X - X\mathbf{H}$, $X \in \mathbb{R}^{d \times d}$, is the commutator,

$\sigma(x) := \coth x - \frac{1}{x}$, $x \in \mathbb{R}$. is an odd function.

DEFINING $\sigma(\text{ad}_H)$

- The power series approach is problematic since \coth has poles on the imaginary axis, and so the formal power series of $\sigma(\text{ad}_H)$ may not converge.
- Instead, one can proceed more directly, using (pointwise) the Schur diagonalization

$$\mathbf{h} = Q^T \mathbf{H} Q, \quad \mathbf{h} = \text{diag}(h_i)_{i=1}^d, \quad Q^{-1} = Q^T.$$

- Then, for any function $f : \mathbb{R} \rightarrow \mathbb{R}$ we can put

$$f(\text{ad}_H)X := Q((f(h_i - h_j))_{ij} \odot (Q^T X Q)) Q^T, \quad X \in \mathbb{R}^{d \times d}.$$

- This resembles the Dalecki-Krein formula, but is not quite. In fact, the differences $h_i - h_j$ arise here as the eigenvalues of ad_H .
- One can verify that this definition is in alignment with the expected calculus (e.g. if f is holomorphic), in particular, that it is independent of the choice of Q . Moreover, there holds

$$f(\text{ad}_H)g(\text{ad}_H) = g(\text{ad}_H)f(\text{ad}_H) = (fg)(\text{ad}_H)$$

which is a key property in subsequent computations.

EXPLICIT FORMULAS

One may object that we still do not know **how to calculate** $\sigma(\text{ad}_H)\mathbf{D}$. To this end, thanks to the Caley-Hamilton theorem, we can prove the following **explicit** representation formulas:

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Lemma

$$\sigma(\text{ad}_H)\mathbf{D} = \frac{\sigma(\sqrt{\text{tr}^2 \mathbf{H} - 4 \det \mathbf{H}})}{\sqrt{\text{tr}^2 \mathbf{H} - 4 \det \mathbf{H}}} (\mathbf{H}\mathbf{D} - \mathbf{D}\mathbf{H}) \quad \text{if } d = 2,$$

and

$$\sigma(\text{ad}_H)\mathbf{D} = -P_2(\mathbf{H}\mathbf{D} - \mathbf{D}\mathbf{H}) + P_1(\mathbf{H}^2\mathbf{D} - \mathbf{D}\mathbf{H}^2) - P_0(\mathbf{H}^2\mathbf{D}\mathbf{H} - \mathbf{H}\mathbf{D}\mathbf{H}^2) \quad \text{if } d = 3,$$

where P_n are invariants of \mathbf{H} defined by

$$P_n := \frac{h_1^n \sigma(h_2 - h_3) + h_2^n \sigma(h_3 - h_1) + h_3^n \sigma(h_1 - h_2)}{(h_1 - h_2)(h_2 - h_3)(h_3 - h_1)}, \quad n = 0, 1, 2.$$

In fact, this holds analogously for any (odd) function. One can also note already here that $\sigma(\text{ad}_H)$ is a **bounded continuous** function of \mathbf{H} .

PROPERTIES OF THE MODEL (H)

The obtained logarithmic model has a number of remarkable properties.

$$\boxed{\begin{aligned}\partial_t \mathbf{H} + \mathbf{v} \cdot \nabla \mathbf{H} + \frac{1}{2\tau} (e^{2(\alpha-1)\mathbf{H}} - e^{2(\alpha-2)\mathbf{H}}) &= \mathbf{D} - \mathbf{H} \boldsymbol{\Omega}^{\log} + \boldsymbol{\Omega}^{\log} \mathbf{H}, \\ \boldsymbol{\Omega}^{\log} &= \mathbf{W} - \sigma(\text{ad}_{\mathbf{H}}) \mathbf{D}.\end{aligned}} \quad (\text{H})$$

The logarithmic derivative (*log*-rate)

$$\overset{\circ}{\mathbf{H}}{}^{\log} := \partial_t \mathbf{H} + \mathbf{v} \cdot \nabla \mathbf{H} + \mathbf{H} \boldsymbol{\Omega}^{\log} - \boldsymbol{\Omega}^{\log} \mathbf{H} \quad (1)$$

is objective and **corotational**. It is interesting to compare our approach with the theory of Xiao et al. (1998) for corotational derivatives (in context of the finite elastoplasticity), see



Xiao, H.; Bruhns, O. T. & Meyers, A. T. M.: *Strain rates and material spins*, Journal of Elasticity, 1998, 52, 1-41.

They argue that **every** objective corotational derivative arises through (1), where the spin tensor is

$$\boldsymbol{\Omega} = \mathbf{W} + \boldsymbol{\Gamma}(\mathbf{B}, \mathbf{D}) \quad \text{for some isotropic antisymmetric function } \boldsymbol{\Gamma}.$$

ADMISSIBLE SPIN TENSORS

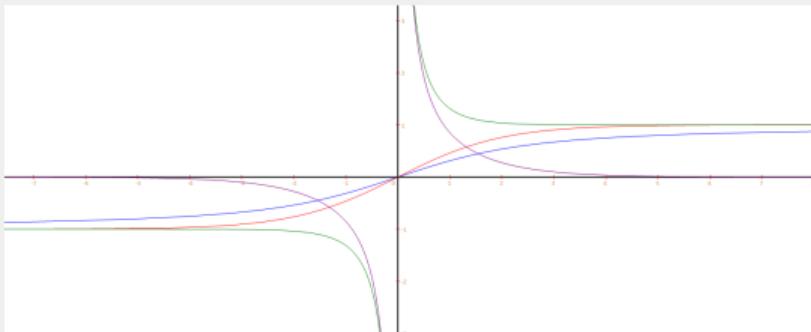
Xiao et al. further conclude that the spin tensor should be determined by a single **spin function** \tilde{h} and provide the representation in eigenprojections \mathbf{B}_i of the form

$$\Omega = \mathbf{W} + \sum_{i \neq j}^d \tilde{h}\left(\frac{b_i}{b_j}\right) \mathbf{B}_i \mathbf{D} \mathbf{B}_j \quad \text{for a continuous } \tilde{h} \text{ satisfying } \tilde{h}(z^{-1}) = -\tilde{h}(z).$$

We note that $\tilde{h}\left(\frac{b_i}{b_j}\right) = \tilde{h}(e^{2(h_i - h_j)}) = -f(h_i - h_j)$ for an **odd** function f . Thus, my approach gives an equivalent characterization of these admissible corotational derivatives via

$$\Omega = \mathbf{W} - f(\text{ad}_H)\mathbf{D} \quad \text{for a continuous } f \text{ satisfying } f(-x) = -f(x).$$

Virtually all the spin tensors encountered in practice can be recovered in this way:



0	\mathbf{W}	Jaumann-Zaremba
$\tanh \frac{x}{2}$	$\Omega^R = \dot{\mathbf{R}} \mathbf{R}^T$	angular velocity
$\text{csch } x$	Ω^L	Lagrangian twirl
$\coth x$	Ω^E	Eulerian twirl
$\underbrace{\coth x - x^{-1}}_{\sigma(x)}$	Ω^{\log}	Logarithmic spin

UNIQUE POSITION OF \mathbf{H} AND $\mathbf{\Omega}^{\log}$

- Within the solid mechanics, the dependence

$$\frac{d}{dt} \mathbf{H} \approx \mathbf{D} \quad (2)$$

had long been foreseen, but the fact that one has to take **precisely** $\frac{d}{dt} \mathbf{H} \equiv \mathbf{\dot{H}}^{\log}$ was shown only in 1991 (Th. Lehmann, Z.H. Guo and H.Y. Liang).

- In fact, in order to have only \mathbf{D} on the right-hand side of (2), one **has to select** the stress measure \mathbf{H} and the rate $\mathbf{\dot{H}}^{\log}$ **among all** possible stress measures **and** objective corotational rates. (Xiao et al. 1998)
- This shows that the choice of $\mathbf{H} = \frac{1}{2} \log \mathbf{B}$ as the stress measure and the choice of $\mathbf{\dot{H}}^{\log}$ as the objective derivative is quite special.

BACK TO FLUIDS

- In our **visco**elastic case, there is an additional damping term in the equation

$$\mathring{\mathbf{H}}^{\log} + \frac{1}{2\tau} (e^{2(\alpha-1)\mathbf{H}} - e^{2(\alpha-2)\mathbf{H}}) = \mathbf{D}$$

- We have basically two ways how to deal with it:

- 1) Use the Caley-Hamilton theorem for the matrix exponential: $e^{2\mathbf{H}} = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{H} + \alpha_2 \mathbf{H}^2$, where α_i are exponential-like functions of invariants of \mathbf{H} . Then deal with such nonlinearities.
- 2) **Linearize.**

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- 2) **Linearize.**

- Linearization merges the Oldroyd-B and Giesekus cases together, since

$$\frac{1}{2\tau} (e^{2(\alpha-1)\mathbf{H}} - e^{2(\alpha-1)\mathbf{H}}) = \frac{1}{\tau} \mathbf{H} + O(|\mathbf{H}|^2), \quad \mathbf{H} \rightarrow 0.$$

- Hence, the linearized model becomes simply

$$\overset{\circ}{\mathbf{H}}^{\log} + \frac{1}{\tau} \mathbf{H} = \mathbf{D}$$

SOME ARGUMENTS IN FAVOUR OF THE LINEARIZED MODEL

- Recently, Alrashdi & Giusteri (2024) provided a physical derivation of the model:

$$\nabla \mathbf{B} + \frac{1}{\tau} \mathbf{B} \log \mathbf{B} = 0.$$

- Now we know that its logarithmic counterpart is precisely $\mathbf{H}^{\log} + \frac{1}{\tau} \mathbf{H} = \mathbf{D}$!

- Note that

$$\mathbf{B} \log \mathbf{B} = \frac{1}{2}(\mathbf{B} - \mathbf{I}) + \frac{1}{2}(\mathbf{B}^2 - \mathbf{B}) + O(|\mathbf{B} - \mathbf{I}|^3) \quad \text{as} \quad \mathbf{B} \rightarrow \mathbf{I}.$$

- Moreover, Alrashdi & Giusteri provide convincing arguments in favor of including \mathbf{H} into the Cauchy stress tensor, instead of \mathbf{B} .
- The underlying Helmholtz free energies then are

$$\psi_{\mathbf{H}} = \frac{\mu}{2} |\mathbf{H}|^2 \quad \text{Linearized model;} \quad \psi_{\mathbf{B}} = \frac{\mu}{4} \text{tr}(e^{2\mathbf{H}} - \mathbf{I} - 2\mathbf{H}) \quad \text{Oldroyd-B.}$$

The choice $\psi_{\mathbf{H}}$ is somehow favoured and extensively studied in the works by Neff, using more specifically the decomposition

$$2\mu|\text{dev } \mathbf{H}|^2 + \kappa|\text{tr } \mathbf{H}|^2.$$

EXISTENCE OF WEAK SOLUTIONS

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} - \nu \Delta \mathbf{v} + \nabla p = \operatorname{div}(\mu \mathbf{H}).$$

$$\partial_t \mathbf{H} + \mathbf{v} \cdot \nabla \mathbf{H} + \frac{1}{\tau} \mathbf{H} - \lambda \Delta \mathbf{H} = \mathbf{D} + \operatorname{ad}_{\mathbf{H}}(\sigma(\operatorname{ad}_{\mathbf{H}}) \mathbf{D} - \mathbf{W}). \quad (3)$$

- The energy identity is

$$\frac{1}{2} \partial_t \int_{\Omega} (|\mathbf{v}|^2 + \mu |\mathbf{H}|^2) + \int_{\Omega} \left(\nu |\nabla \mathbf{v}|^2 + \frac{1}{\tau} |\mathbf{H}|^2 + \lambda |\nabla \mathbf{H}|^2 \right) = 0,$$

which provides sufficiently strong estimates to define everything in (3).

- Indeed, the only problematic term could be $\sigma(\operatorname{ad}_{\mathbf{H}}) \mathbf{D}$, but we have $|\sigma| \leq 1$ everywhere, and hence also $\sigma(\operatorname{ad}_{\mathbf{H}})$ is bounded and continuous w.r.t. to \mathbf{H} (thanks to C.H. formulas).
- Moreover, if $\lambda > 0$, then an approximation \mathbf{H}_n converges pointwise a.e., and thanks to the explicit formulas, we conclude that the right-hand side of (3) is weakly compact.
- $\lambda = 0$: Arguments by Lions & Masmoudi (2000) show that $\mathbf{H}_n \xrightarrow{L^2} \mathbf{H}$ if $\sigma = 0$. The crucial ingredient in their proof is testing with $\frac{\mathbf{H}}{1+\delta|\mathbf{H}|^2}$, which works regardless of σ .
- Note that the positive definiteness of \mathbf{B} is for granted; it follows from $\mathbf{B} = e^{2\mathbf{H}}$.

PROOF OF (B) \Leftrightarrow (H)

PROOF OF THE EQUIVALENCE, PT. I

In order to pass from $\partial_t \mathbf{H}$ to $\partial_t \mathbf{B} = \partial_t e^{2\mathbf{H}}$, for instance, one has to apply the operator $\frac{d\mathbf{B}}{d\mathbf{H}} = \frac{de^{2\mathbf{H}}}{d\mathbf{H}} : \mathbb{R}^{d \times d} \rightarrow \mathbb{R}^{d \times d}$, which can be given by the integral (Wilcox 1967):

$$\frac{d\mathbf{B}}{d\mathbf{H}} X = \int_0^1 e^{2(1-s)\mathbf{H}} X e^{2s\mathbf{H}} ds.$$

Since

$$\frac{d\mathbf{B}}{d\mathbf{H}} X \cdot Y = \int_0^1 e^{(1-s)\mathbf{H}} X e^{s\mathbf{H}} \cdot e^{(1-s)\mathbf{H}} Y e^{s\mathbf{H}} ds$$

(here $U \cdot V := \sum_{i,j}^d U_{ij} V_{ij}$, $|U| := \sqrt{U \cdot U}$), the operator $\frac{d\mathbf{B}}{d\mathbf{H}}$ is **symmetric and positive definite**, in particular its inverse $(\frac{d\mathbf{B}}{d\mathbf{H}})^{-1}$ exists. This we want to apply to the Oldroyd-B equation, but how to do it explicitly?

PROOF OF THE EQUIVALENCE, PT. II

There is also an alternative formula, well known in the theory of Lie groups:

$$\frac{d\mathbf{B}}{d\mathbf{H}} X = \mathbf{B} \left(\frac{1 - e^{-2 \operatorname{ad}_{\mathbf{H}}}}{\operatorname{ad}_{\mathbf{H}}} X \right) \quad \text{or} \quad \frac{d\mathbf{B}}{d\mathbf{H}} X = \left(\frac{e^{2 \operatorname{ad}_{\mathbf{H}}} - 1}{\operatorname{ad}_{\mathbf{H}}} X \right) \mathbf{B}.$$

Using our calculus for $f(\operatorname{ad}_{\mathbf{H}})$, it is now easy to express the inverse:

$$\left(\frac{d\mathbf{B}}{d\mathbf{H}} \right)^{-1} Y = \frac{\operatorname{ad}_{\mathbf{H}}}{1 - e^{-2 \operatorname{ad}_{\mathbf{H}}}} (\mathbf{B}^{-1} Y) \quad \text{or} \quad \left(\frac{d\mathbf{B}}{d\mathbf{H}} \right)^{-1} Y = \frac{\operatorname{ad}_{\mathbf{H}}}{e^{2 \operatorname{ad}_{\mathbf{H}}} - 1} (Y \mathbf{B}^{-1}).$$

We take advantage of this dichotomy to calculate what is

$$\left(\frac{d\mathbf{B}}{d\mathbf{H}} \right)^{-1} (\mathbf{B} \mathbf{D} + \mathbf{D} \mathbf{B}) \quad \text{and} \quad \left(\frac{d\mathbf{B}}{d\mathbf{H}} \right)^{-1} (\mathbf{B} \mathbf{W} - \mathbf{W} \mathbf{B}).$$

PROOF OF THE EQUIVALENCE, PT. III

As a consequence of the elementary identities

$$\frac{x}{1-e^{-x}} - \frac{x}{e^x-1} = x \quad \text{and} \quad \frac{x}{1-e^{-x}} + \frac{x}{e^x-1} = x \coth \frac{x}{2},$$

and the aforementioned calculus, we easily get

$$\left(\frac{d\mathbf{B}}{d\mathbf{H}} \right)^{-1} (\mathbf{B}\mathbf{W} - \mathbf{W}\mathbf{B}) = \text{ad}_{\mathbf{H}} \mathbf{W}, \quad \text{and} \quad \left(\frac{d\mathbf{B}}{d\mathbf{H}} \right)^{-1} (\mathbf{B}\mathbf{D} + \mathbf{D}\mathbf{B}) = (\text{ad}_{\mathbf{H}} \coth \text{ad}_{\mathbf{H}}) \mathbf{D}.$$

Finally, noting that

$$(\text{ad}_{\mathbf{H}} \coth \text{ad}_{\mathbf{H}}) \mathbf{D} = \mathbf{D} + \text{ad}_{\mathbf{H}} \sigma(\text{ad}_{\mathbf{H}}) \mathbf{D},$$

we see that indeed

$$\left(\frac{d\mathbf{B}}{d\mathbf{H}} \right)^{-1} (\nabla \mathbf{v} \mathbf{B} + \mathbf{B} (\nabla \mathbf{v})^T) = \mathbf{D} + \text{ad}_{\mathbf{H}} (\mathbf{W} + \sigma(\text{ad}_{\mathbf{H}}) \mathbf{D}) = \mathbf{D} + \mathbf{H} \Omega^{\log} - \Omega^{\log} \mathbf{H},$$

and hence we arrive at (H). □