Nečas Center for Mathematical Modeling
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MINISTRY OF EDUCATION, YOUTH AND SPORTS

Viscoelastic rate type fluids with stress diffusion: thermodynamic and PDE analysis

Josef Málek
Nečas Center for Mathematical Modeling
and
Charles University, Faculty of Mathematics and Physics
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Miroslav Bulíček, Vít Průša and **Endré Süli**
K. R. Rajagopal and **Karel Tůma**
Tomáš Skřivan

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Section 1

Viscous fluids and visco-elastic fluids without/with stress diffusion

Unsteady flows of incompressible fluids

Governing equations $\Omega \subset \mathbb{R}^3$

$$\left.\begin{aligned} \operatorname{div} \mathbf{v} &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) &= -\nabla p + \operatorname{div} \mathbb{S} \\ \mathbb{S} &= \mathbb{S}^{\mathrm{T}} \end{aligned}\right\} \text{ in } (0,T) \times \Omega$$

$$\mathbf{v} = \mathbf{0} \qquad \} \text{ on } (0,T) \times \partial\Omega$$

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Energy balance

$$\tfrac{1}{2} \frac{\partial |\mathbf{v}|^2}{\partial t} + \operatorname{div} \left(\frac{|\mathbf{v}|^2}{2} \mathbf{v} + p\mathbf{v} - \mathbb{S}\mathbf{v} \right) + \mathbb{S} : \nabla \mathbf{v} = 0$$

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$$\boxed{\frac{d}{dt}\int_\Omega |\mathbf{v}|^2 + 2\int_\Omega \mathbb{S} : \nabla \mathbf{v} + \int_{\partial\Omega} (|\mathbf{v}|^2 + 2p)(\mathbf{v} \cdot \mathbf{n}) - 2\mathbb{S} : (\mathbf{v} \otimes \mathbf{n}) = 0}$$

Energy estimates and constitutive equations

- Governing equations $\qquad \Omega \subset \mathbb{R}^3$

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- Energy equality valid for $t \in (0,T]$

$$\boxed{\|\mathbf{v}(t)\|_2^2 + 2\int_0^t \int_\Omega \mathbb{S} : \mathbb{D} = \|\mathbf{v}_0\|_2^2} \qquad \mathbb{D} := \frac{1}{2}\left(\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}}\right)$$

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Constitutive equations

Classes of constitutive equations

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(1) $\mathbb{G}(\mathbb{S},\mathbb{D}) = \mathbb{O}$

`implicit algebraic equations`

(2) $\mathbb{G}(\overset{*}{\mathbb{S}},\mathbb{S},\overset{*}{\mathbb{D}},\mathbb{D}) = \mathbb{O}$ $\qquad$ $\overset{*}{\mathbb{A}}$ an objective time derivative

`rate type viscoelastic fluids`

(3) $\mathbb{G}(\overset{*}{\mathbb{S}},\mathbb{S},\overset{*}{\mathbb{D}},\mathbb{D}) - \Delta\mathbb{S} = \mathbb{O}$

`rate type viscoelastic fluids with stress diffusion`

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`rate type viscoelastic fluids with stress diffusion`

- Examples and physical features
- PDE analysis of IBVP (long time existence of large data weak solutions)

$\mathbb{G}(\mathbb{S},\mathbb{D}) = \mathbb{O}$ KR Rajagopal (2003)

$\mathbb{S} = 2\nu\mathbb{D}$	Navier-Stokes
$2\nu(\lvert\mathbb{S}\rvert^2, \lvert\mathbb{D}\rvert^2)\mathbb{D} = 2\alpha(\lvert\mathbb{S}\rvert^2, \lvert\mathbb{D}\rvert^2)\mathbb{S}$	generalized viscosity
$2\nu\mathbb{D} = \frac{(\lvert\mathbb{S}\rvert - \sigma_*)^+}{\lvert\mathbb{S}\rvert}\mathbb{S}$	Bingham
$2\nu\frac{(\lvert\mathbb{D}\rvert - d_*)^+}{\lvert\mathbb{D}\rvert}\mathbb{D} = \mathbb{S}$	Euler/Navier-Stokes
$2\nu(\theta)\frac{(\lvert\mathbb{D}\rvert - d(\theta))^+}{\lvert\mathbb{D}\rvert}\mathbb{D} = \frac{(\lvert\mathbb{S}\rvert - \sigma(\theta))^+}{\lvert\mathbb{S}\rvert}\mathbb{S}$	θ-activated fluids

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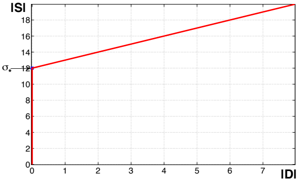

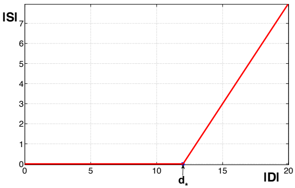

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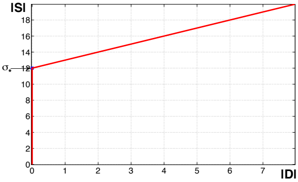
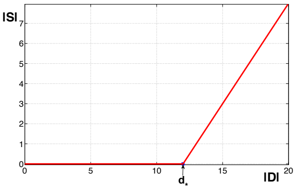
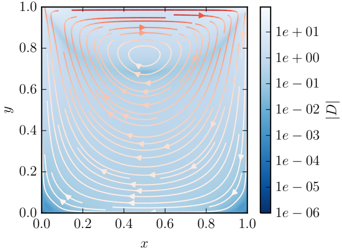


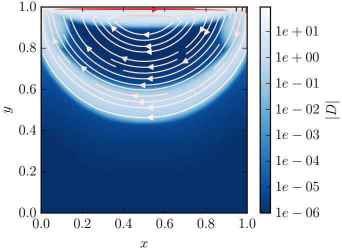


E. Maringová, J. Žabenský: On a Navier-Stokes-Fourier-like system capturing transitions between viscous and inviscid fluid regimes and between no-slip and perfect-slip boundary conditions, arXiv: 1705.00437 (2017)

Robustness of $\mathbb{G}(\mathbb{S}, \mathbb{D}) = \mathbb{O}$

$$2\nu\mathbb{D} = \frac{(|\mathbb{S}| - \sigma_*)^+}{|\mathbb{S}|}\mathbb{S}$$





J. Hron, J. Málek, J. Stebel, K. Touška: A novel view on computations of steady flows of Bingham fluids using implicit constitutive relations, MORE/2017/08 (2017)

Long-time and large-data theory for $\mathbb{G}(\mathbb{S}, \mathbb{D}) = \mathbb{O}$

- Well-posedness
  - 2d $\mathbb{S} = 2\nu\mathbb{D}$ Leray; Kiselev, Ladyzhenskaya
  - 3d $\mathbb{S} = 2(\nu + \nu_1|\mathbb{D}|^{r-2})\mathbb{D}$ for $r \geq 11/5$
    Ladyzhenskaya; Bulíček, Ettwein, Kaplický, Pražák

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- Existence theory
  - 3d $\mathbb{S} = 2\nu\mathbb{D}$ `Leray; Caffarelli, Kohn, Nirenberg`
  - 3d $\mathbb{S} = 2\nu(1 + |\mathbb{D}|^2)^{(r-2)/2}\mathbb{D}$ for $r \geq 9/5$
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  - 3d $\mathbb{S} = 2\nu(1 + |\mathbb{D}|^2)^{(r-2)/2}\mathbb{D}$ for $r > 6/5$
    `Diening, Růžička, Wolf; Breit, Diening, Schwarzacher`
  - 3d $\mathbb{G}(\mathbb{S},\mathbb{D}) = \mathbb{O}$ maximal, monotone, r-curve with $r > 6/5$
    `Bulíček, Gwiazda, Málek, Świerczewska-Gwiazda`

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Q: How large the class of fluids might be for which long-time and large-data existence of weak solutions can be established?

From viscous to elastic fluids through viscoelastic rate type fluids.

Insufficiency of $\mathbb{G}(\mathbb{S}, \mathbb{D}) = \mathbb{O}$

Impossibility to describe important phenomena

- nonlinear creep
- stress relaxation

exhibited by real fluid-like materials in many areas

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Popular choice

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Popular choice

rate type viscoelastic fluids

$\mathbb{G}(\overset{*}{\mathbb{S}}, \mathbb{S}, \overset{*}{\mathbb{D}}, \mathbb{D}) = \mathbb{O}$ - rate-type viscoelastic fluids

- capability of describing stress relaxation and nonlinear creep
- one possible direction towards the development of long-time and large-data mathematical theory for more complex fluid models

$\mathbb{G}(\overset{*}{\mathbb{S}}, \mathbb{S}, \overset{*}{\mathbb{D}}, \mathbb{D}) = \mathbb{O}$ - rate-type viscoelastic fluids

- capability of describing stress relaxation and nonlinear creep
- one possible direction towards the development of long-time and large-data mathematical theory for more complex fluid models

$\overset{*}{\mathbb{A}}$ generalizes $\frac{d}{dt}\mathbb{A} = \frac{\partial \mathbb{A}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbb{A}$ that is not objective

$$\overset{\triangledown}{\mathbb{A}} = \frac{d}{dt}\mathbb{A} - \mathbb{L}\mathbb{A} - \mathbb{A}\mathbb{L}^{\mathrm{T}} \qquad \mathbb{L} := \nabla \mathbf{v}$$

`upper-convected Oldroyd`

$$\overset{\circ}{\mathbb{A}} = \frac{d}{dt}\mathbb{A} - \mathbb{W}\mathbb{A} - \mathbb{A}\mathbb{W}^{\mathrm{T}} \qquad \mathbb{W} := (\mathbb{L} - \mathbb{L}^{\mathrm{T}})/2$$

`Jaumann-Zaremba (corotational)`

$$\overset{\square}{\mathbb{A}} = \overset{\circ}{\mathbb{A}} - a(\mathbb{D}\mathbb{A} - \mathbb{A}\mathbb{D}) \qquad a \in [-1, 1]$$

`Gordon-Schowalter`

Standard viscoelastic rate-type fluid models within $\mathbb{G}(\overset{*}{\mathbb{S}}, \mathbb{S}, \overset{*}{\mathbb{D}}, \mathbb{D}) = \mathbb{O}$

- Maxwell (1867)

$$\boxed{\tau \overset{\triangledown}{\mathbb{S}} + \mathbb{S} = 2\nu_1 \mathbb{D} \qquad \nu = 0} \qquad \tau = \frac{\nu_1}{E}$$

- Oldroyd-B (1950)

$$\boxed{\tau \overset{\triangledown}{\mathbb{S}} + \mathbb{S} = 2\nu\tau \overset{\triangledown}{\mathbb{D}} + 2(\nu_1 + \nu)\mathbb{D}} \qquad \tau = \frac{\nu_1}{E}$$

- Johnson-Segalman (1977)

$$\boxed{\tau \overset{\square}{\mathbb{S}} + \mathbb{S} = 2\nu\tau \overset{\square}{\mathbb{D}} + 2(a + \nu)\mathbb{D}} \qquad a \in [-1, 1]$$

$\pm$ of standard rate type fluids

+ $\mathbb{G}(\overset{*}{\mathbb{S}}, \mathbb{S}, \overset{*}{\mathbb{D}}, \mathbb{D}) = \mathbb{O}$ is capable of describing observed phenomena

+/- Mathematical theory available in some cases - first order PDE for $\mathbb{S}$

- 3d, Jaumann-Zaremba: Lions, Masmoudi (2000), Hu, Lelièvre (2007), Masmoudi (2011)
- survey: Le Bris, Lelièvre (2012)

– Subtle issues regarding physical underpinnings

- ambiguity of objective derivatives
- the possibility of the derivation of the model at a purely macroscopic level
- consistency of the models with second law of thermodynamics
- extension to compressible setting
- inclusion of thermal effects

Thermodynamical framework

Rajagopal and Srinivasa (2000) provided a simple, yet general method to solve some of these issues based on

- concept of the natural configuration
- the knowledge of constitutive equations for *two scalar quantities*: Helmholtz free energy (characterizing how the material stores the energy) and the rate of the entropy production (characterizing how the material dissipates the energy)

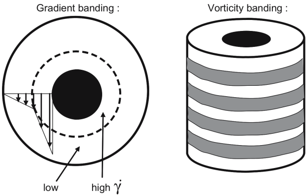
and

- derive new thermodynamically compatible classes of *non-linear* viscoelastic rate-type fluid model
- specify under what conditions models reduce to standard models

K. R. Rajagopal, A. R. Srinivasa: A thermodynamic framework for rate type fluid models, *Journal of Non-Newtonian Fluid Mechanics*, Vol. 88, pp. 207–227 (2000)

$\mathbb{G}(\overset{*}{\mathbb{S}}, \mathbb{S}, \overset{*}{\mathbb{D}}, \mathbb{D}) - \Delta\mathbb{S} = \mathbb{O}$

+ Both mathematical and physical
  - regularization (mathematical theory should be available)
    - steady flows: El-Kareh, Leal (1989)
    - 2d, Oldroyd: Barrett, Boyaval (2011)
    - 2d: Constantin+Kliegl (2012), Chupin+Martin (2015) Lukáčová, Mizerová, Nečasová (2015) Elgindi, Rousset (2016), Barrett, Süli (2017)
    - 3d, stronger regularization: Kreml, Pokorný, Šalom (2015)
  - instabilities: shear banding, vorticity banding - to determine thickness of bands



Dhont and Briels (2008)

Divoux et al. (2016)

– Subtle issues regarding physical underpinnings

- consistency of the models with the second law of thermodynamics
- specification of boundary conditions for $\mathbb{S}$
- extension to compressible setting
- inclusion of thermal effects
- PDE theory in 3d

Section 2

A thermodynamic approach towards derivation of a hierarchy of visco-elastic rate-type fluid models

First key idea

`Rajagopal and Srinivasa (2000, 2004)`

to specify the constitutive equations for two scalar quantities:

- Helmholtz free energy ψ that describes how the material stores the energy
- the rate of the entropy production ζ that describes how the material dissipates the energy

Governing equations

$$
\begin{aligned}
\frac{d\varrho}{dt} &= -\varrho \operatorname{div} \mathbf{v} \\
\varrho \frac{d\mathbf{v}}{dt} &= \operatorname{div} \mathbb{T}, \qquad \mathbb{T} = \mathbb{T}^{\mathrm{T}} \\
\varrho \frac{de}{dt} &= \mathbb{T} : \mathbb{D} - \operatorname{div} \mathbf{j}_e \\
\varrho \frac{d\eta}{dt} + \operatorname{div} \mathbf{j}_\eta &= \varrho\zeta \quad \text{ with } \zeta \geq 0
\end{aligned}
$$

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$$\boxed{\psi := e - \theta\eta}$$

Helmholtz free energy

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Helmholtz free energy

Restriction to isothermal processes

$$\mathbb{T} : \mathbb{D} - \varrho \frac{d\psi}{dt} - \operatorname{div}(\mathbf{j}_e - \theta \mathbf{j}_\eta) = \xi \quad \text{with } \xi := \theta\varrho\zeta \geq 0$$

Governing equations

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`Helmholtz free energy`

Restriction to isothermal processes

$$\mathbb{T} : \mathbb{D} - \varrho \frac{d\psi}{dt} - \operatorname{div}(\mathbf{j}_e - \theta \mathbf{j}_\eta) = \xi \quad \text{with } \xi := \theta\varrho\zeta \geq 0$$

If $\mathbf{j}_\eta = \frac{\mathbf{j}_e}{\theta}$ (not necessarily required here), then

$$\xi = \mathbb{T} : \mathbb{D} - \varrho \frac{d\psi}{dt} \quad \text{with } \xi \geq 0$$

Governing equations

$$\frac{d\varrho}{dt} = -\varrho \operatorname{div} \mathbf{v}$$
$$\varrho\frac{d\mathbf{v}}{dt} = \operatorname{div} \mathbb{T}, \qquad \mathbb{T} = \mathbb{T}^{\mathrm{T}}$$
$$\varrho\frac{de}{dt} = \mathbb{T} : \mathbb{D} - \operatorname{div} \mathbf{j}_e$$
$$\varrho\frac{d\eta}{dt} + \operatorname{div} \mathbf{j}_\eta = \varrho\zeta \quad \text{with } \zeta \geq 0$$

$$\psi := e - \theta\eta$$

`Helmholtz free energy`

Restriction to isothermal processes

$$\mathbb{T} : \mathbb{D} - \varrho\frac{d\psi}{dt} - \operatorname{div}(\mathbf{j}_e - \theta\mathbf{j}_\eta) = \xi \quad \text{with } \xi := \theta\varrho\zeta \geq 0$$

If $\mathbf{j}_\eta = \frac{\mathbf{j}_e}{\theta}$ (not necessarily required here), then

$$\xi = \mathbb{T} : \mathbb{D} - \varrho\frac{d\psi}{dt} \quad \text{with } \xi \geq 0$$

or for `incompressible` fluid when $\mathbb{T} = -p\mathbb{I} + \mathbb{S}$

$$\xi = \mathbb{S} : \mathbb{D} - \varrho\frac{d\psi}{dt} \quad \text{with } \xi \geq 0$$

Energy estimates and specification of ψ and ξ

- Energy equality valid for $t \in (0, T]$

$$\boxed{\|\mathbf{v}(t)\|_2^2 + 2\int_0^t \int_\Omega \mathbb{S} : \mathbb{D} = \|\mathbf{v}_0\|_2^2}$$

Energy estimates and specification of ψ and ξ

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$$\boxed{\|\mathbf{v}(t)\|_2^2 + 2\int_0^t \int_\Omega \mathbb{S} : \mathbb{D} = \|\mathbf{v}_0\|_2^2}$$

- Reduced thermodynamical identity

$$\boxed{\xi = \mathbb{S} : \mathbb{D} - \tfrac{d\psi}{dt} \qquad \text{with } \xi \geq 0}$$

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- Reduced thermodynamical identity

$$\boxed{\xi = \mathbb{S} : \mathbb{D} - \tfrac{d\psi}{dt} \qquad \text{with } \xi \geq 0}$$

- Specification of the constitutive equations of ψ and ξ

$$\boxed{\psi = \tilde{\psi}(\dots) \quad \xi = \tilde{\xi}(\dots)}$$

Energy estimates and specification of ψ and ξ

- Energy equality valid for $t \in (0, T]$

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- Reduced thermodynamical identity

$$\boxed{\xi = \mathbb{S} : \mathbb{D} - \tfrac{d\psi}{dt} \quad \text{with } \xi \geq 0}$$

- Specification of the constitutive equations of ψ and ξ

$$\boxed{\psi = \tilde{\psi}(\dots) \quad \xi = \tilde{\xi}(\dots)}$$

- Updated energy equality

$$\boxed{\|\mathbf{v}(t)\|_2^2 + \|\tilde{\psi}(\dots)(t)\|_1 + 2\int_0^t \int_\Omega \tilde{\xi}(\dots) = \|\mathbf{v}_0\|_2^2 + \|\tilde{\psi}_0(\dots)\|_1}$$

General thermodynamic framework

Constitutive equation for the Helmholtz free energy ψ:

$$\boxed{\psi = \tilde{\psi}(y_1, \ldots, y_N)} \tag{1}$$

By means of balance equations (mass, linear and angular momenta, energy) and kinematics one arrives at

$$\xi = \mathbb{T} : \mathbb{D} - \varrho \frac{d\psi}{dt} \stackrel{(1)}{=} \sum_{\alpha} J_\alpha A_\alpha \quad \text{with}$$

Constitutive equation for the rate of dissipation ξ:

$$\boxed{\xi = \sum_{\alpha} \gamma_\alpha |A_\alpha|^2}$$

leads to

$$J_\alpha = \gamma_\alpha A_\alpha \qquad \gamma_\alpha > 0$$

Compressible and incompressible Navier-Stokes fluids

$$\boxed{\psi = \psi_0(\varrho)} \qquad p_{\mathrm{th}}(\varrho) := \varrho^2 \psi_0'(\varrho)$$

$$\xi = \mathbb{T} : \mathbb{D} - \varrho \frac{d\psi}{dt} \quad \Longrightarrow \quad \boxed{\xi = \mathbb{T}_\delta : \mathbb{D}_\delta + (m + p_{\mathrm{th}}) \operatorname{div} \mathbf{v}}$$

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$$\boxed{\xi = 2\nu \mathbb{D}_\delta : \mathbb{D}_\delta + \frac{2\nu + 3\lambda}{3} |\operatorname{div} \mathbf{v}|^2}$$

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$$\boxed{\mathbb{T} = m\mathbb{I} + \mathbb{T}_\delta = -p_{\text{th}}\mathbb{I} + 2\nu\mathbb{D} + \lambda \operatorname{div} \mathbf{v}\, \mathbb{I}}$$

`Compressible NS`

Compressible and incompressible Navier-Stokes fluids

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`Compressible NS`

$$\operatorname{div} \mathbf{v} = 0$$

$$\xi = \mathbb{T}_\delta : \mathbb{D}_\delta \quad \text{with } \xi \geq 0$$

$$\boxed{\xi = 2\nu \mathbb{D}_\delta : \mathbb{D}_\delta}$$

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$$\boxed{\mathbb{T} = m\mathbb{I} + \mathbb{T}_\delta = m\mathbb{I} + 2\nu\mathbb{D}_\delta}$$

`Incompressible Navier-Stokes`

Elastic and Kelvin-Voigt incompressible solids

$$\boxed{\psi = \frac{\mu}{2\varrho}(\operatorname{tr}\mathbb{B} - 3)} \qquad \mathbb{B} := \mathbb{F}\mathbb{F}^{\mathrm{T}}$$

Elastic and Kelvin-Voigt incompressible solids

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Since $\frac{d\mathbb{F}}{dt} = \mathbb{L}\mathbb{F}$, we get

$$\frac{d\mathbb{B}}{dt} = \mathbb{L}\mathbb{B} + \mathbb{B}\mathbb{L}^{\mathrm{T}} \iff \overset{\triangledown}{\mathbb{B}} = \mathbb{O} \quad \text{and} \quad \frac{d}{dt}\operatorname{tr}\mathbb{B} = 2\mathbb{B} : \mathbb{D}$$

Elastic and Kelvin-Voigt incompressible solids

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Hence $\qquad \xi = \mathbb{T} : \mathbb{D} - \varrho\frac{d\psi}{dt}$ with $\xi \geq 0$

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$$\xi = (\mathbb{T} - \mu\mathbb{B}) : \mathbb{D} = (\mathbb{T}_\delta - \mu\mathbb{B}_\delta) : \mathbb{D} \quad \text{with } \xi \geq 0$$

Elastic and Kelvin-Voigt incompressible solids

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$$\boxed{\xi = 0} \quad \Longrightarrow \quad \boxed{\mathbb{T} = m\mathbb{I} + \mu\mathbb{B}_\delta = -p\mathbb{I} + \mu\mathbb{B}}$$

`Incompressible neo-Hokeean solid`

Elastic and Kelvin-Voigt incompressible solids

$$\boxed{\psi = \frac{\mu}{2\varrho}(\operatorname{tr}\mathbb{B} - 3)} \qquad \mathbb{B} := \mathbb{F}\mathbb{F}^{\mathrm{T}}$$

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`Incompressible neo-Hokeean solid`

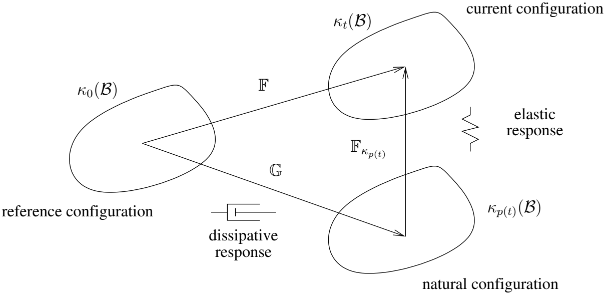
$$\boxed{\xi = 2\nu\mathbb{D} : \mathbb{D}} \quad \Longrightarrow \quad \boxed{\mathbb{T} = -p\mathbb{I} + \mu\mathbb{B} + 2\nu\mathbb{D}}$$

`Incompressible Kelvin-Voigt solid`

Second key idea - Natural configuration

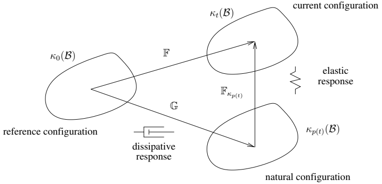
Natural configuration

- splits the deformation $\mathbb{F}$ into the elastic and dissipative parts $\mathbb{F}_{\kappa_{p(t)}}$ and $\mathbb{G}$



- $\boxed{\mathbb{F} = \mathbb{F}_{\kappa_{p(t)}} \mathbb{G}}$

Kinematics



- $\boxed{\mathbb{F} = \mathbb{F}_{\kappa_{p(t)}} \mathbb{G}}$
- $\mathbb{F}$, $\mathbb{G}$, $\mathbb{F}_{\kappa_{p(t)}}$ $\qquad \mathbb{B}_{\kappa_{p(t)}} := \mathbb{F}_{\kappa_{p(t)}} \mathbb{F}^{\mathrm{T}}_{\kappa_{p(t)}} \qquad \mathbb{C}_{\kappa_p(t)} := \mathbb{F}^{\mathrm{T}}_{\kappa_{p(t)}} \mathbb{F}_{\kappa_{p(t)}}$
- $\frac{d\mathbb{F}}{dt} = \mathbb{L}\mathbb{F} \implies \mathbb{L} = \frac{d\mathbb{F}}{dt}\mathbb{F}^{-1} \qquad \mathbb{D}, \mathbb{W}$
- $\mathbb{L}_{\kappa_{p(t)}} := \frac{d\mathbb{G}}{dt}\mathbb{G}^{-1} \qquad \mathbb{D}_{\kappa_{p(t)}}, \mathbb{W}_{\kappa_{p(t)}}$

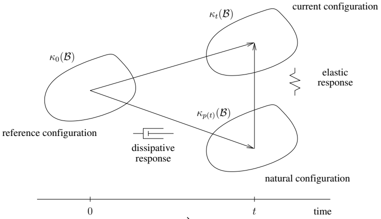
$$\frac{d\mathbb{B}_{\kappa_{p(t)}}}{dt} = \mathbb{L}\mathbb{B}_{\kappa_{p(t)}} + \mathbb{B}_{\kappa_{p(t)}}\mathbb{L}^{\mathrm{T}} - 2\mathbb{F}_{\kappa_{p(t)}}\mathbb{D}_{\kappa_{p(t)}}\mathbb{F}^{\mathrm{T}}_{\kappa_{p(t)}} \implies$$

$$\boxed{\overset{\triangledown}{\mathbb{B}}_{\kappa_{p(t)}} = -2\mathbb{F}_{\kappa_{p(t)}}\mathbb{D}_{\kappa_{p(t)}}\mathbb{F}^{\mathrm{T}}_{\kappa_{p(t)}}}$$

$$\boxed{\frac{d}{dt}\operatorname{tr}\mathbb{B}_{\kappa_{p(t)}} = 2\mathbb{B}_{\kappa_{p(t)}} : \mathbb{D} - 2\mathbb{C}_{\kappa_{p_i(t)}} : \mathbb{D}_{\kappa_{p(t)}}}$$

Compressible and Incompressible responses/Maxwell & Oldroyd-B

Natural configuration provides more variants for imposing compressibility



$$\psi = \frac{\mu}{2\rho}\left(\operatorname{tr}\mathbb{B}_{\kappa_{p(t)}} - 3 - \ln\det\mathbb{B}_{\kappa_{p(t)}}\right)$$

$$\xi = 2\nu\mathbb{D} : \mathbb{D} + 2\nu_1\mathbb{D}_{\kappa_{p(t)}}\mathbb{C}_{\kappa_p(t)} : \mathbb{D}_{\kappa_{p(t)}} = 2\nu|\mathbb{D}|^2 + 2\nu_1 \operatorname{tr}(\overset{\triangledown}{\mathbb{B}}_{\kappa_{p(t)}}\mathbb{B}^{-1}_{\kappa_{p(t)}}\overset{\triangledown}{\mathbb{B}}_{\kappa_{p(t)}})$$

lead to Maxwell and Oldroyd-B fluid

J. Málek, **K. R. Rajagopal**, **K. Tůma**: On a variant of the Maxwell and Oldroyd-B models within the context of a thermodynamic basis, *International Journal of Nonlinear Mechanics*, Vol. 76, pp. 42–47 (2015)

J. Málek, **V. Průša**: Derivation of equations of continuum mechanics and thermodynamics of fluids, *Handbook of Mathematical Analysis in Mechanics of Viscous Fluids*, (eds.Y. Giga, A. Novotný), Springer available online (2017)

Rate-type fluids with stress diffusion

$\mathbb{T} : \mathbb{D} - \varrho\dot{\psi} - \operatorname{div}(\mathbf{j}_e - \theta\mathbf{j}_\eta) = \xi$ with $\xi \geq 0$

Helmholtz free energy ψ – compressible neo-Hookean

$$\psi = \frac{\mu}{2\rho}\left(\operatorname{tr}\mathbb{B}_{\kappa_{p(t)}} - 3 - \ln\det\mathbb{B}_{\kappa_{p(t)}}\right) + \frac{\sigma}{2}|\nabla\operatorname{tr}\mathbb{B}_{\kappa_{p(t)}}|^2$$

Rate of entropy production ξ

$$0 \leq \tilde{\xi} = 2\nu|\mathbb{D}|^2 + 2\nu_1\mathbb{D}_{\kappa_{p(t)}}\mathbb{C}_{\kappa_p(t)} : \mathbb{D}_{\kappa_{p(t)}}.$$

Maxwell and Oldroyd-B model with stress difussion

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Maxwell and Oldroyd-B model with stress difussion

J. Málek, V. Průša, T. Skřivan, E. Süli: Thermodynamics of viscoelastic rate type fluids with stress diffusion, arXiv: 1706.06277 (2017)

Special class of rate-type fluids with stress diffusion

Simplification $[\mathbb{C}_{\kappa_{p(t)}}]_\delta = \mathbb{O} \implies [\mathbb{B}_{\kappa_{p(t)}}]_\delta = \mathbb{O}$

$$\mathbb{C}_{\kappa_p(t)} = \mathbb{B}_{\kappa_{p(t)}} = b\,\mathbb{I} \quad \text{where } b := \frac{\operatorname{tr}\mathbb{C}_{\kappa_p(t)}}{3} = \frac{\operatorname{tr}\mathbb{B}_{\kappa_p(t)}}{3}$$

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Simplification $[\mathbb{C}_{\kappa_p(t)}]_\delta = \mathbb{O} \implies [\mathbb{B}_{\kappa_{p(t)}}]_\delta = \mathbb{O}$

$$\mathbb{C}_{\kappa_p(t)} = \mathbb{B}_{\kappa_{p(t)}} = b\,\mathbb{I} \quad \text{where } b := \frac{\operatorname{tr}\mathbb{C}_{\kappa_p(t)}}{3} = \frac{\operatorname{tr}\mathbb{B}_{\kappa_p(t)}}{3}$$

Then

$$\frac{db}{dt} = -\frac{2}{3}\,b\,\operatorname{tr}\mathbb{D}_{\kappa_{p(t)}}$$

$$\xi = (\mathbb{T}_\delta + 9\sigma(\nabla b \otimes \nabla b)_\delta) : \mathbb{D} + (3\mu(b-1) - 18\sigma b\,\Delta b)\,\frac{\operatorname{tr}\mathbb{D}_{\kappa_{p(t)}}}{3}$$

Requiring that

$$\xi = 2\nu\mathbb{D} : \mathbb{D} + 2\nu_1(\operatorname{tr}\mathbb{D}_{\kappa_{p(t)}})^2 = 2\nu\mathbb{D} : \mathbb{D} + \frac{\nu_1}{2}\frac{1}{b^2}\left|\frac{db}{dt}\right|^2$$

$$\boxed{\begin{aligned} &\mathbb{T} = m\mathbb{I} + 2\nu\mathbb{D} - 9\sigma(\nabla b \otimes \nabla b)_\delta = -p\mathbb{I} + 2\nu\mathbb{D} - 9\sigma(\nabla b \otimes \nabla b) \\ &\quad \frac{\nu_1}{b}\frac{db}{dt} + 3\mu(b-1) - 18\sigma b\,\Delta b = 0 \end{aligned}}$$

Boundary conditions and energy estimates

$$\mathbb{S} : \mathbb{D} - \varrho\dot{\psi} - \operatorname{div}(\mathbf{j}_e - \theta\mathbf{j}_\eta) = \xi$$

Summary for the special choice $[\mathbb{B}_{\kappa_{p(t)}}]_\delta = \mathbb{O}$

$$\begin{aligned}\mathbf{j}_e - \theta\mathbf{j}_\eta &= 9\sigma\frac{db}{dt}\nabla b\\ \psi &= \frac{3\mu}{2}(b - 1 - \ln b) + \frac{9\sigma}{2}|\nabla b|^2\\ \xi &= 2\nu|\mathbb{D}|^2 + \frac{\nu_1}{2}\left|\frac{1}{b}\frac{db}{dt}\right|^2\end{aligned}$$

Energy estimates

$$\boxed{\begin{aligned}&\frac{\partial}{\partial t}\left(\frac{|\mathbf{v}|^2}{2} + \frac{3\mu}{2}(b - 1 - \ln b) + \frac{9\sigma}{2}|\nabla b|^2\right)\\ &\quad + 2\nu|\mathbb{D}|^2 + \frac{\nu_1}{2}\left|\frac{1}{b}\frac{db}{dt}\right|^2\\ &\quad + \operatorname{div}\left((\frac{3\mu}{2}(b - 1 - \ln b) + \frac{9\sigma}{2} + \frac{|\mathbf{v}|^2}{2})\mathbf{v} + \mathbb{T}\mathbf{v} + 9\sigma\frac{db}{dt}\nabla b\right) = 0\end{aligned}}$$

BCs: $\mathbf{v} = \mathbf{0}$ and $\nabla b \cdot \mathbf{n} = 0$ eliminates the contribution of the flux term to EEs

Section 3

Analysis of the simplified problem

Problem formulation

PDEs in $(0,T)\times\Omega$ $\qquad\qquad$ $\Omega\subset\mathbb{R}^d$

$$\operatorname{div}\mathbf{v} = 0$$
$$\frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v}\otimes\mathbf{v}) = -\nabla p + \Delta\mathbf{v} - \operatorname{div}(\nabla b\otimes\nabla b)$$
$$\frac{\partial b}{\partial t} + \operatorname{div}(b\mathbf{v}) + (b^2 - b) - b^2\Delta b = 0$$

Boundary and initial conditions

$$\mathbf{v} = \mathbf{0} \qquad \nabla b\cdot\mathbf{n} = 0 \qquad \text{on } (0,T)\times\partial\Omega$$
$$\mathbf{v}(0,\cdot) = \mathbf{v}_0 \qquad b(0,\cdot) = b_0 \qquad \text{in } \Omega$$

Energy estimates

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |\mathbf{v}|^2 + (b - 1 - \ln b) + |\nabla b|^2 \,\mathrm{d}x + \int_\Omega 2|\mathbb{D}|^2 + \left|\frac{1}{b}\frac{db}{dt}\right|^2 \,\mathrm{d}x = 0$$

Problem formulation

PDEs in $(0,T) \times \Omega$ $\qquad\qquad$ $\Omega \subset \mathbb{R}^d$

$$\operatorname{div} \mathbf{v} = 0$$

$$\frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) = -\nabla p + \Delta \mathbf{v} - \operatorname{div}(\nabla b \otimes \nabla b)$$

$$\frac{1}{b^2}\left(\frac{\partial b}{\partial t} + \nabla b \cdot \mathbf{v}\right) + (1 - b^{-1}) - \Delta b = 0$$

Boundary and initial conditions

$$\mathbf{v} = \mathbf{0} \qquad \nabla b \cdot \mathbf{n} = 0 \qquad \text{on } (0,T) \times \partial\Omega$$

$$\mathbf{v}(0,\cdot) = \mathbf{v}_0 \qquad b(0,\cdot) = b_0 \qquad \text{in } \Omega$$

Energy estimates

$$\frac{1}{2}\frac{d}{dt}\int_\Omega |\mathbf{v}|^2 + (b - 1 - \ln b) + |\nabla b|^2 \, \mathrm{d}x + \int_\Omega 2|\mathbb{D}|^2 + \frac{1}{b^2}\left|\frac{\partial b}{\partial t} + \nabla b \cdot \mathbf{v}\right|^2 \, \mathrm{d}x = 0$$

Existence result

Assumption on $(\mathbf{v}_0, b_0 > 0)$

$$\mathbf{v}_0 \in L^2_{0,\mathrm{div}}(\Omega), \quad b_0 \in W^{1,2}(\Omega), \quad b_0, b_0^{-1} \in L^\infty(\Omega)$$

Theorem (Bulíček, Málek, Pruša, Süli (2017))

Let $\Omega \subset \mathbb{R}^d$ *be a Lipschitz set. Then there exists a couple* $(\mathbf{v}, b)$*:*

$$\mathbf{v} \in L^\infty(0,T; L^2_{0,\mathrm{div}}) \cap L^2(0,T; W^{1,2}_{0,\mathrm{div}})$$

$$b \in L^\infty(0,T; W^{1,2}(\Omega)), \quad b, b^{-1} \in L^\infty(Q)$$

$$\partial_t b + \nabla b \cdot \mathbf{v} \in L^2(Q), \quad \Delta b \in L^2(Q)$$

s.t. for a.a. $t \in (0,T)$ *and all* $\mathbf{w} \in W^{1,2}_{0,\mathrm{div}} \cap W^{d+1,2}(\Omega)^d$*,* $w \in W^{1,2}(\Omega)$*:*

$$\langle \partial_t \mathbf{v}, \mathbf{w} \rangle + \int_\Omega (2\mathbb{D} - \nabla b \otimes \nabla b - \mathbf{v} \otimes \mathbf{v}) : \nabla \mathbf{w} \, \mathrm{d}x = 0$$

$$\int_\Omega \left(\frac{\partial_t b + \nabla b \cdot \mathbf{v}}{b^2} + \left(1 - \frac{1}{b}\right)\right) w + \nabla b \cdot \nabla w \, \mathrm{d}x = 0$$

Structure of the proof

$$T_n(s) := \min\{n, \max\{n^{-1}, s\}\} \text{ for } s \in \mathbb{R}.$$

Truncated system

$$\mathbf{v}^{n,\ell}(t,x) := \sum_{i=1}^{n} \alpha_i^{n,\ell}(t)\mathbf{w}_i(x), \qquad b^{n,\ell}(t,x) := \sum_{i=1}^{\ell} \beta_i^{n,\ell}(t) w_i(x)$$

$$\int_\Omega \partial_t \mathbf{v}^{n,\ell} \cdot \mathbf{w}_i - \mathbf{v}^{n,\ell} \otimes \mathbf{v}^{n,\ell} : \nabla \mathbf{w}_i + \mathbb{S}^{n,\ell} : \nabla \mathbf{w}_i \, \mathrm{d}x = 0$$

$$i = 1, \dots, n$$

$$\int_\Omega \frac{\partial_t b^{n,\ell} w_j}{(T_n(b^{n,\ell}))^2} + \frac{\nabla b^{n,\ell} \cdot \mathbf{v}^{n,\ell}}{(T_n(b^{n,\ell}))^2} w_j + (1 - (T_n(b^{n,\ell}))^{-1}) w_j \, \mathrm{d}x$$

$$+ \int_\Omega \nabla b^{n,\ell} \cdot \nabla w_j \, \mathrm{d}x = 0 \qquad j = 1, \dots, \ell$$

$$\mathbb{S}^{n,\ell} = 2\mathbb{D}^{n,\ell} - (\nabla b^{n,\ell} \otimes \nabla b^{n,\ell}), \quad 2\mathbb{D}^{n,\ell} = \nabla \mathbf{v}^{n,\ell} + (\nabla \mathbf{v}^{n,\ell})^T$$

- Galerkin both in $\mathbf{v}$ and b solved by Rothe's method
- $\ell \to \infty$, Galerkin in $\mathbf{v}$: maximum and minimum principle for b
- uniform estimates for $\mathbf{v}^n$, b^n mimicking the formal a priori info
- $n \to \infty$

Weak stability

$$
\begin{aligned}
\lim_{n\to\infty}\int_0^T \|\nabla b^n\|_2^2 \,\mathrm{d}t &= -\lim_{n\to\infty}\int_Q \frac{\partial_t b^n + \nabla b^n \cdot \mathbf{v}^n}{b^n} + (b^n - 1)\,\mathrm{d}x\,\mathrm{d}t \\
&= -\int_Q \frac{\partial_t b + \nabla b \cdot \mathbf{v}}{b} + (b-1)\,\mathrm{d}x\,\mathrm{d}t \\
&= \int_0^T \|\nabla b\|_2^2 \,\mathrm{d}t
\end{aligned}
$$

Summary

- Thermodynamic approach (`Rajagopal, Srinivasa (2000)`)
  - generates classes of the rate-type fluids satisfying the laws of thermodynamics
  - efficient even in a purely mechanical context for incompressible fluids (Maxwell, Oldroyd-B, Giesekus, Burgers)
  - compressible rate-type fluids (`Málek, Průša (2017)`)
  - capable of developing models where different energy mechanisms take place
- PDE analysis for a simplified model with stress diffusion
  - long-time and large data existence of weak solution in 3D
  - a simplified model shares many qualitative features with general viscoelastic rate-type models with stress diffusion
  - presence of stress diffusion in Eq. for $\mathbb{S}$ combined with the presence of Korteweg stress in Eq. for $\mathbf{v}$
  - non standard apriori estimates that would be difficult to find out without the thermodynamic approach presented

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Thank you for your attention.