Nečas Center for Mathematical Modeling

MOdelling REvisited + MOdel REduction

ERC-CZ project LL1202 - MORE

MINISTRY OF EDUCATION, YOUTH AND SPORTS

Structured fluids

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Section 1

Foreword

NSEs

Incompressible Navier-Stokes equations

$$\boxed{\begin{gathered}\operatorname{div}\mathbf{v} = 0\\ \frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v}\otimes\mathbf{v}) = -\nabla p + \nu\Delta\mathbf{v}\end{gathered}}$$

Unknowns: $(\mathbf{v} = (v_1, v_2, v_3), p)$ $\nu > 0$

$$(\mathbf{a}\otimes\mathbf{b})_{ij} := a_i b_j$$

$$\operatorname{div}(\mathbf{v}\otimes\mathbf{v})_i = \sum_{j=1}^{3}\frac{\partial(v_i v_j)}{\partial x_j} = \sum_{j=1}^{3} v_j\frac{\partial v_i}{\partial x_j} = \mathbf{v}\cdot\nabla v_i$$

NSEs

Incompressible Navier-Stokes equations

$$\boxed{\begin{aligned} \operatorname{div} \mathbf{v} &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) &= -\nabla p + \nu \Delta \mathbf{v} \end{aligned}}$$

Unknowns: $(\mathbf{v}, p)$ $\nu > 0$

Compressible Navier-Stokes equations

$$\boxed{\begin{aligned} \frac{\partial \varrho}{\partial t} + \operatorname{div}(\varrho \mathbf{v}) &= 0 \\ \frac{\partial (\varrho \mathbf{v})}{\partial t} + \operatorname{div}(\varrho \mathbf{v} \otimes \mathbf{v}) &= -\nabla p(\varrho) + \nu \Delta \mathbf{v} + (\nu + \lambda) \nabla \operatorname{div} \mathbf{v} \end{aligned}}$$

Unknowns: $(\mathbf{v}, \varrho)$ $\nu > 0, \quad 2\nu + 3\lambda > 0$

Systems of PDEs of the **second** order

NSEs - rewritten

Incompressible Navier-Stokes equations

$$\boxed{\begin{aligned} \operatorname{div}\mathbf{v} &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v}\otimes\mathbf{v}) &= -\nabla p + \operatorname{div}\mathbb{S} \\ \mathbb{S} &= 2\nu\mathbb{D} =: \nu\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right) \end{aligned}}$$

Unknowns: $(\mathbf{v}, p, \mathbb{S})$ $\qquad \nu > 0$

Compressible Navier-Stokes equations

$$\boxed{\begin{aligned} \frac{\partial \varrho}{\partial t} + \operatorname{div}(\varrho\mathbf{v}) &= 0 \\ \frac{\partial (\varrho\mathbf{v})}{\partial t} + \operatorname{div}(\varrho\mathbf{v}\otimes\mathbf{v}) &= \operatorname{div}\mathbb{T} \\ \mathbb{T} &= -p(\varrho)\mathbb{I} + 2\nu\mathbb{D} + \lambda\operatorname{div}\mathbf{v}\mathbb{I} \end{aligned}}$$

Unknowns: $(\mathbf{v}, \varrho, \mathbb{T})$ $\qquad \nu > 0, \quad 2\nu + 3\lambda > 0$

Systems of PDEs of the **first** order

NSEs - rewritten again

Incompressible Navier-Stokes equations

$$\boxed{\begin{aligned}\frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) &= \operatorname{div} \mathbb{T} \\ \mathbb{T} - \frac{1}{3}(\operatorname{tr} \mathbb{T})\mathbb{I} &= 2\nu\mathbb{D}\end{aligned}}$$

Unknowns: $(\mathbf{v}, \mathbb{T})$ $\nu > 0$

$$m := \frac{1}{3} \operatorname{tr} \mathbb{T}$$

$$\mathbb{A}_\delta := \mathbb{A} - \frac{1}{3}(\operatorname{tr} \mathbb{A})\mathbb{I}$$

NSEs - rewritten again

Incompressible Navier-Stokes equations

$$\boxed{\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) &= \operatorname{div} \mathbb{T} \\ \mathbb{T} - \frac{1}{3}(\operatorname{tr} \mathbb{T})\mathbb{I} &= 2\nu\mathbb{D} \end{aligned}}$$

Unknowns: $(\mathbf{v}, \mathbb{T})$ $\qquad \nu > 0$

Compressible Navier-Stokes equations

$m := \frac{1}{3} \operatorname{tr} \mathbb{T} \qquad \mathbb{A}_\delta := \mathbb{A} - \frac{1}{3}(\operatorname{tr} \mathbb{A})\mathbb{I}$

$$\boxed{\begin{aligned} \frac{\partial \varrho}{\partial t} + \operatorname{div}(\varrho\mathbf{v}) &= 0 \\ \frac{\partial (\varrho\mathbf{v})}{\partial t} + \operatorname{div}(\varrho\mathbf{v} \otimes \mathbf{v}) &= \operatorname{div} \mathbb{T} \\ \mathbb{T}_\delta &= 2\nu\mathbb{D}_\delta \\ m + p(\varrho) &= (2\nu + 3\lambda) \operatorname{div} \mathbf{v} \end{aligned}}$$

Unknowns: $(\mathbf{v}, \varrho, \mathbb{S}, m)$ $\qquad \nu > 0, \quad 2\nu + 3\lambda > 0$

Physics vs Mathematics

• NSEs (physics): Navier (1821), St. Venant (1843), Poisson (1843), Stokes (1845)

• NSEs (mathematics): Oseen (1921), **Leray** (1934) 2d vs 3d, Padula (1986), DiPerna (1980-1989), PL Lions (1998), Feireisl (2004)

• Existence and smoothness of the Navier-Stokes equation (2000)

• Formulation of the mathematical models (much) ahead of the analysis of relevant PDEs problems

Newtonian vs Non-Newtonian

$$\boxed{\mathbb{S} = 2\nu\mathbb{D}}$$

$$\boxed{\mathbb{T} = -p(\varrho)\mathbb{I} + 2\nu\mathbb{D} + \lambda \operatorname{div} \mathbf{v}\mathbb{I}}$$

- $\boxed{\text{Newtonian fluids/Navier-Stokes fluids}}$

  linear relation between $\mathbb{T}$ and $\nabla \mathbf{v}$

- Non-Newtonian fluid is a fluid that is not Newtonian

- $\boxed{\text{non-Newtonian fluids/structured fluids/complex fluids}}$

- Are there Non-Newtonian fluids?

Section 2

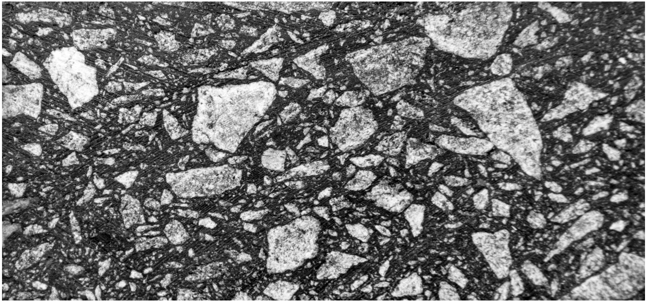
Complex fluids - examples

Asphalt concrete

- composite material
- consists of mineral aggregate bound with asphalt binder and compacted
- 2% of air voids $\Rightarrow$ almost incompressible
- viscoelastic behavior (Monismoth, Secor 1962)

Bovine eye

- transparent, colorless, gelatinous
- 98% of water, NaCl, hyaluronan
- maintains the shape of the eye, keeps a clear path to the retina
- viscoelastic behavior (Sharif-Kashani et al. 2011)



Asphalt concrete (cross-section through a sample 10cm x 5cm, grayscale image)

Materials - solid-like and fluid-like

Year	Event
1930	Plug trimmed off
1938	1st drop
1947	2nd drop
1954	3rd drop
1962	4th drop
1970	5th drop
1979	6th drop
1988	7th drop
2000	8th drop
2014	9th drop

Section 3

Non-Newtonian fluids and phenomena

Departures from behavior of Newtonian fluids

Non-Newtonian phenomena

1. Nonlinear relation between the stress and the shear rate
2. The presence of activation or deactivation criteria
3. The presence of the normal stress differences in simple shear flows
4. Stress Relaxation
5. (Nonlinear) Creep

Viscosity

Definition

Coefficient of proportionality between the shear stress and the shear-rate

Simple shear flow: $\mathbf{v}(x,y,z) = \begin{pmatrix} v(y) \\ 0 \\ 0 \end{pmatrix}$ $\quad \mathbb{D} = \frac{1}{2}\begin{pmatrix} 0 & v' & 0 \\ v' & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

Newton (1687):

> *The resistance arising from the want of lubricity in parts of the fluid,* **other things being equal**, *is* **proportional** *to the velocity with which the parts of the fluid are separated from one another.*

$$\mathbb{S}_{xy} = \mu v'(y)$$

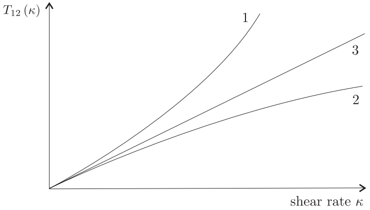
Experiments confirm the dependence on the shear-rate, pressure, concentration, ...

$$g(\mathbb{S}_{xy}, v'(y)) = 0$$

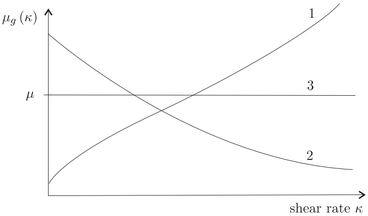
Nonlinear relation between stress and shear-rate

Generalized viscosity

$$\mu_g(\kappa) := \frac{\mathbb{S}_{xy}(\kappa)}{\kappa} \quad \text{where } \kappa = v'$$



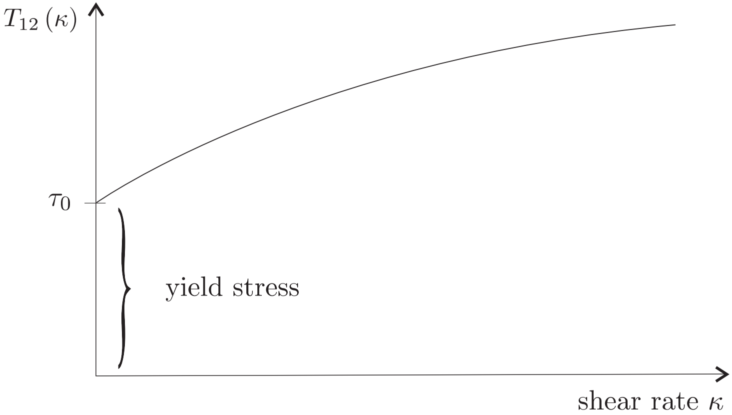
Shear thinning/thickening



Generalized viscosity

1. Viscosity increases with increasing shear-rate (shear thickening)
2. Viscosity decreases with increasing shear-rate (shear thinning)
3. Constant viscosity (Newtonian fluid - provided that the fluid does not exhibit other effects)

Presence of activation criteria (such as yield stress)



Bingham and Herschel-Bulkley fluids

Normal stress differences in simple shear flow

$$\boldsymbol{v}(x,y,z) = \begin{pmatrix} v(y) \\ 0 \\ 0 \end{pmatrix}$$

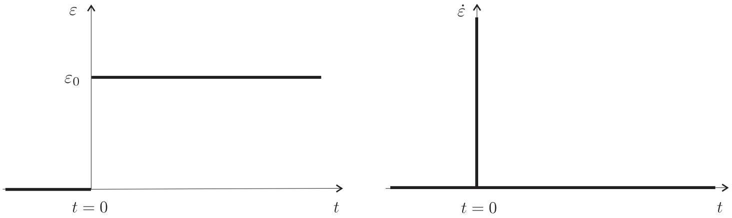
For the model $\mathbb{T} = -p\mathbb{I} + \nu(p, |\mathbb{D}|^2)\mathbb{D}$

$$\mathbb{T}_{11} - \mathbb{T}_{22} = -p + p = 0$$
$$\mathbb{T}_{22} - \mathbb{T}_{33} = -p + p = 0$$

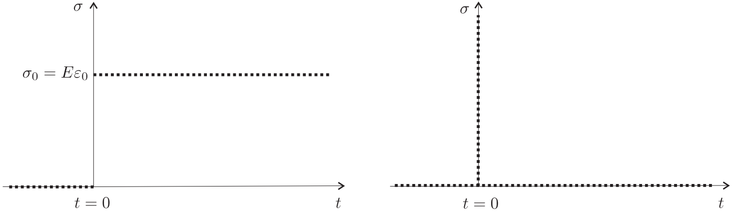
The presence of non-zero normal stress differences in simple shear flows is associated with the effects such as

- Die swell
- Delayed die swell
- Rod climbing

Stress relaxation

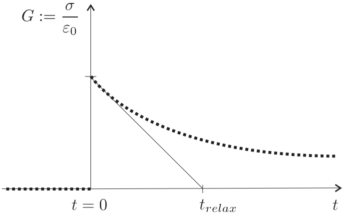


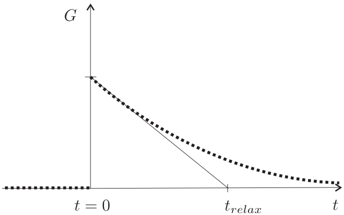
Sudden jump discontinuous change of deformation



Response at stress relaxation test for linear spring and linear dashpot

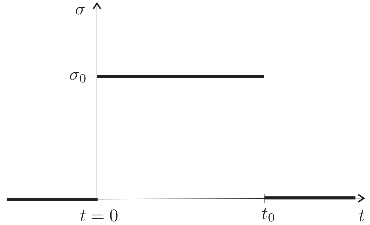
Stress relaxation



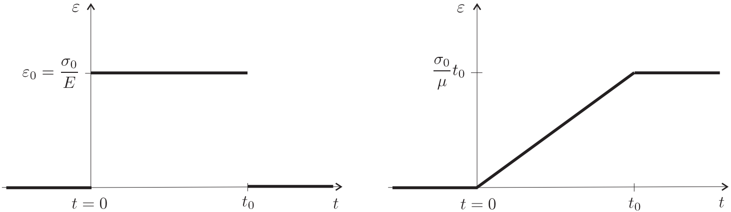


Response at stress relaxation test for natural materials: solid-like response (left) and fluid-like response (right)

(Non-linear) creep

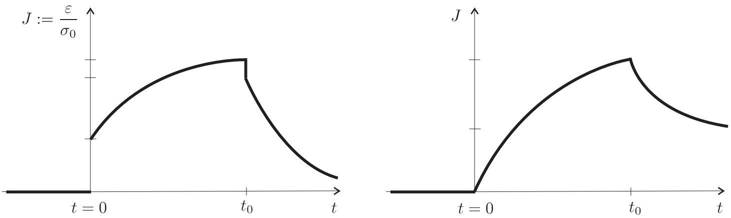


Sudden jump discontinuous change in the shear stress



Response at creep test for linear spring and linear dashpot

(Non-linear) creep



Response at creep test for natural materials: solid-like response (left) and fluid-like response (right)

Selected areas of application

Newtonian fluid is exception

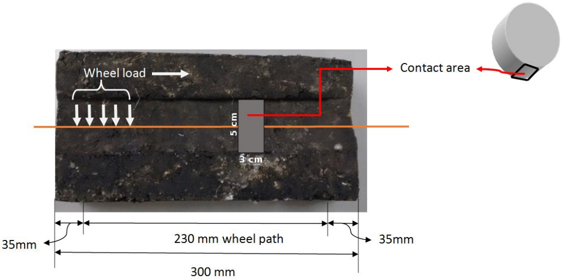
1. Food materials such as milk, oil, tomato products, products of granular type (such as rice)
2. Chemical suspensions, gels, paints, ...
3. Biological materials such as blood and synovial fluid
4. Geophysical materials such as rocks, soil, sand, clay, lava, the earth's mantle, glacier

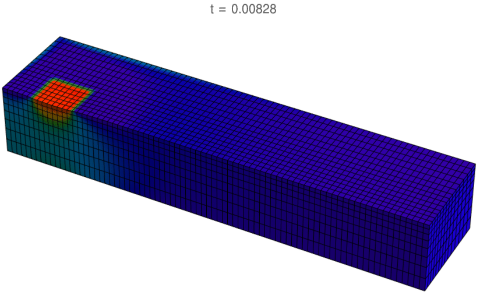
Section 4

The approach

Wheel tracker test of asphalt concrete

- asphalt concrete exhibits viscoelastic behavior
- "torture test" to check the abilities of the material
- done by the group of J. Murali Krishnan (IITM)
- brick dimensions $30 \times 13.8 \times 5\,\mathrm{cm}$
- time demanding simulation by K. Tůma
- 800 kPa, speed 1 km/h, 8 960 elements
- pressure distribution, deformation scaled $100\times$





Approach

- Continuum mechanics and thermodynamics - (microscopic or mesoscopic approach is impossible due to complicated microstructure and chemical processes involved)
- Experiment (good access) - Computer simulation (capable of performing in some cases)
- Steps
  - Experiment
  - One-dimensional (intuitively derived) mathematical model
  - Design of three-dimensional models
  - Identification of boundary conditions
  - Simulations
- Goal: real-world problem (as a highway Prague-Liberec) vs digital twin

Role of mathematics and mathematical physics

Aims

- How to describe complex phenomena?
- How to quantify the difference between the real process and outcome of simulation?
- How to achieve efficient computation?

Recent approaches in continuum thermodynamics

1. Implicit constitutive theory
2. Knowledge of mechanisms how the material stores the energy and how the material dissipates the energy is sufficient to determine the constitutive equations and boundary conditions
3. Concept of natural configuration associated to the current configuration of the body
4. Consequences towards the mixture theory

K.R. Rajagopal (since 1993)

Role and goals of analysis/1

Guaranteed error between the computed solution and the solution of infinite-dimensional PDE problem

1. proper definition of the infinite-dimensional object we approximate: definition of solution and its properties
2. definition/choice of appropriate distance function or measure associated to the considered problem
3. methods of discretization and their properties
4. methods of linearization and their properties
5. methods of solving linear problems and their properties
6. stability (with respect to perturbations - rounding errors, ..., stationary/periodic solution)

Z. Strakoš (since 2006)

Role and goals of analysis/2

Connections between infinite-dimensional problems and huge yet finite-dimensional problems

1. infinite-dimensional description can hep us to avoid artefacts/constants that may occur in finite-dimensional discretization
2. severe gap - inverse (solution) operator cannot be compact in the solution space while finite dimensional approximations are compact

Section 5

Viscous fluids and visco-elastic fluids

Unsteady flows of incompressible fluids

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

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

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

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

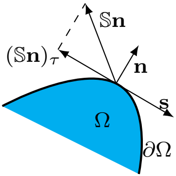
Energy balance $\mathbb{A} : \mathbb{B} := \sum_{i,j=1}^{3} A_{ij} B_{ij}$

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

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

Internal flows

$$\int_{\partial\Omega} (-\mathbb{S}) : (\mathbf{v} \otimes \mathbf{n}) = \int_{\partial\Omega} (-\mathbb{S})\mathbf{n} \cdot \mathbf{v} = \int_{\partial\Omega} \big((-\mathbb{S})\mathbf{v}\big)_\tau \cdot \mathbf{v}_\tau$$



Boundary conditions

- $\mathbf{v} \cdot \mathbf{n} = 0$ on $\partial\Omega$
- constitutive equation involving $\mathbf{v}_\tau$ and/or $(-\mathbb{S}\mathbf{n})_\tau$

$\mathbf{s} := (-\mathbb{S}\mathbf{n})_\tau$ $\qquad$ $\mathbf{z}_\tau := \mathbf{z} - (\mathbf{z} \cdot \mathbf{n})\mathbf{n}$

$$\int_{\partial\Omega} (-\mathbb{S}) : (\mathbf{v} \otimes \mathbf{n}) = \int_{\partial\Omega} (-\mathbb{S})\mathbf{n} \cdot \mathbf{v} = \int_{\partial\Omega} \big((-\mathbb{S}\mathbf{n})\big)_\tau \cdot \mathbf{v}_\tau$$

$\mathbf{v}_\tau = \mathbf{0}$	no slip boundary condition
$\mathbf{s} = \gamma_* \mathbf{v}_\tau$ with $\gamma_* > 0$	Navier's slip boundary condition
$\mathbf{s} = \mathbf{0}$	(perfect) slip boundary condition

Energy estimates and constitutive equations

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

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

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

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

- Energy equality valid for $t \in (0,T]$ $\qquad \mathbb{D} := \frac{1}{2}\left(\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}}\right)$

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

- To close the system

$$\boxed{\text{we add a material dependent relation involving } \mathbb{S} \text{ and } \mathbb{D}}$$

$$\boxed{\text{we add a material dependent relation involving } \mathbf{s} \text{ and } \mathbf{v}_\tau}$$

Constitutive equations

Classes of constitutive equations

$$\boxed{\begin{aligned} \operatorname{div}\mathbf{v} &= 0 \\ \frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v}\otimes\mathbf{v}) &= -\nabla p + \operatorname{div}\mathbb{S}, \qquad \mathbb{S} = \mathbb{S}^{\mathrm{T}} \end{aligned}}$$

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

`implicit algebraic equations`

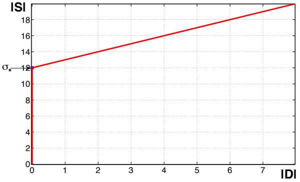
(2) $\mathbb{G}(\overset{*}{\mathbb{S}},\mathbb{S},\overset{*}{\mathbb{D}},\mathbb{D}) = \mathbb{O}$ $\qquad$ $\overset{*}{\mathbb{A}}$ an objective time derivative

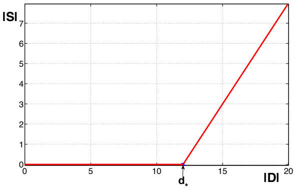
`rate type viscoelastic fluids`

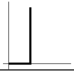
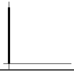
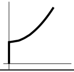
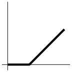
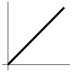
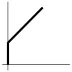
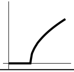
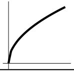
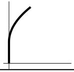
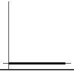
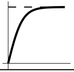
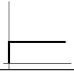
(3) $\mathbb{G}(\overset{*}{\mathbb{S}},\mathbb{S},\overset{*}{\mathbb{D}},\mathbb{D}) - \Delta\mathbb{S} = \mathbb{O}$

`rate type viscoelastic fluids with stress diffusion`

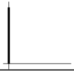
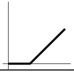
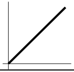
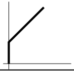
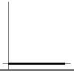
$\mathbb{S} = 2\nu\mathbb{D}$	Navier-Stokes
$2\nu(\vert\mathbb{S}\vert^2, \vert\mathbb{D}\vert^2)\mathbb{D} = 2\alpha(\vert\mathbb{S}\vert^2, \vert\mathbb{D}\vert^2)\mathbb{S}$	generalized viscosity
$2\nu\mathbb{D} = \dfrac{(\vert\mathbb{S}\vert - \sigma_*)^+}{\vert\mathbb{S}\vert}\mathbb{S}$	Bingham
$2\nu\dfrac{(\vert\mathbb{D}\vert - d_*)^+}{\vert\mathbb{D}\vert}\mathbb{D} = \mathbb{S}$	Euler/Navier-Stokes





Euler/limiting shear-rate 	limiting shear-rate 	rigid body 
Euler/shear-thickening 	shear-thickening 	rigid/shear-thickening 
Euler/Navier-Stokes 	Navier-Stokes 	Bingham = rigid/Navier-Stokes 
Euler/shear-thinning 	shear-thinning 	rigid/shear-thinning 
Euler 	limiting shear stress 	perfect plastic 
$\lvert\mathbb{D}\rvert \le \delta_* \iff \mathbb{S} = \mathbb{O}$	no activation	$\lvert\mathbb{S}\rvert \le \sigma_* \iff \mathbb{D} = \mathbb{O}$

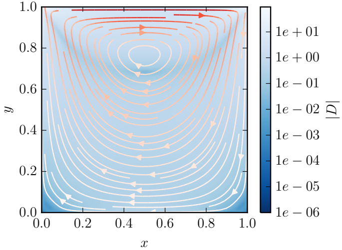
Summary of systematic classification of fluid-like responses
with corresponding $\lvert\mathbb{S}\rvert$ vs $\lvert\mathbb{D}\rvert$ diagrams.

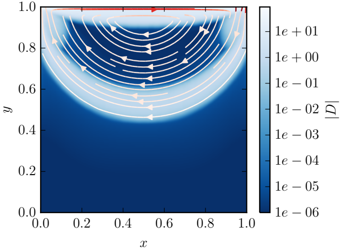
		no-slip 
slip/Navier's slip 	Navier's slip 	stick-slip 
slip 		
$\lvert \mathbf{v}_\tau \rvert \le \delta_* \iff \mathbf{s} = \underline{0}$	no activation	$\lvert \mathbf{s} \rvert \le \sigma_* \iff \mathbf{v}_\tau = \underline{0}$

Summary of systematic classification of boundary conditions
with corresponding $|\mathbf{s}|$ vs $|\mathbf{v}_\tau|$ diagrams.

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)

J. Blechta, J. Málek, K.R. Rajagopal: TODO to be completed (2018)

J. Blechta: Ph.D. Thesis (2018)

Formulation of the problem

PROBLEM

$$
\left.\begin{aligned}
\operatorname{div}\mathbf{v} &= 0\\
\partial_t\mathbf{v} + \operatorname{div}(\mathbf{v}\otimes\mathbf{v}) - \operatorname{div}\mathbb{S} &= -\nabla p\\
\mathbb{G}(\mathbb{S},\mathbb{D}) &= \mathbb{O}
\end{aligned}\right\}\ \text{in } Q_T
$$

$$
\mathbf{s} := -(\mathbb{S}\mathbf{n})_\tau \qquad \left.\begin{aligned}
\mathbf{v}\cdot\mathbf{n} &= 0\\
\mathbf{g}(\mathbf{s},\mathbf{v}_\tau) &= \mathbf{0}
\end{aligned}\right\}\ \text{on } \Sigma_T
$$

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

DATA

- $\Omega \subset \mathbb{R}^d$ bounded, open set with $\partial\Omega \in \mathcal{C}^{1,1}$ and $\mathbf{n} : \partial\Omega \to \mathbb{R}^d$
- $T > 0$ and $Q_T := (0,T)\times\Omega$, $\Sigma_T := (0,T)\times\partial\Omega$
- $\mathbf{v}_0$
- $\mathbb{G}$ and $\mathbf{g}$ - constitutive functions in the bulk and on the boundary

Large data and long time existence theory

Robust mathematical theory for a large class of constitutive equations and boundary conditions is available.

M. Bulíček, P. Gwiazda, J. Málek, A. Świerczewska-Gwiazda, *On unsteady flows of implicitly constituted incompressible fluids*, SIAM J. Math. Anal. **44** (2012) 2756–2801.

M. Bulíček, P. Gwiazda, J. Málek, K. R. Rajagopal, A. Świerczewska-Gwiazda, *On flows of fluids described by an implicit constitutive equation characterized by a maximal monotone graph*, Mathematical Aspects of Fluid Mechanics (Eds. J. C. Robinson, J. L. Rodrigo and W. Sadowski), London Mathematical Society Lecture Note Series (No. 402) (2012), Cambridge University Press, 23–51.

M. Bulíček, J. Málek *On unsteady internal fows of Bingham fuids subject to threshold slip on the impermeable boundary*, (Eds. H. Amann, Y. Giga, H. Okamoto, H. Kozono, M. Yamazaki), Recent Developments of Mathematical Fluid Mechanics, Birkhäuser/Springer, Basel, 2016, 135-156.

M. Bulíček, J. Málek, *Internal flows of incompressible fluids subject to stick-slip boundary conditions*, Vietnam Journal of Mathematics **45** (2017), 207–220.

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*, Nonlinear Analysis: Real World Applications 41 (2018) 152-178.

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

Impossibility to describe important phenomena

- normal stress differences
- stress relaxation
- nonlinear creep

exhibited by real fluid-like materials in many areas

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

$\overset{*}{\mathbb{A}}$ 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)

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

- Burgers (1939)

$$\boxed{\lambda_2 \overset{\triangledown\triangledown}{\mathbb{S}} + \lambda_1\overset{\triangledown}{\mathbb{S}} + \mathbb{S} = \eta_1\mathbb{D} + \eta_2\overset{\triangledown}{\mathbb{D}}}$$

- 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

$-$ Subtle issues regarding physical underpinnings

- ambiguity of objective derivatives
- the possibility of the derivation of the model at a purely macroscopic level (Oldroyd (1950))
- 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)

References - Surveys

J. Málek, **K. R. Rajagopal**: Mathematical Issues Concerning the Navier-Stokes Equations and Some of Its Generalizations, *Handbook of Mathematical Fluid Dynamics*, Volume 4 (Eds: S. Friedlander, D. Serre) (2006), Elsevier B. V., Amsterdam, 407–444.

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)

Section 6

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

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

$\boxed{\psi := e - \theta\eta}$ `Helmholtz free energy`

Restriction to isothermal processes

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

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

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

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

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

General thermodynamic framework

Constitutive equation for the Helmholtz free energy ψ:

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

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

$$\xi = \mathbb{T} : \mathbb{D} - \varrho \frac{d\psi}{dt} \overset{(2)}{=} \sum_{\alpha} J_\alpha A_\alpha \quad \text{with}$$

Constitutive equation for the rate of dissipation ξ:

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

leads to

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

General thermodynamic framework

Constitutive equation for the Helmholtz free energy ψ:

$$\boxed{\psi = \tilde{\psi}(y_1, \ldots, y_N)} \tag{2}$$

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

$$\xi = \mathbb{T} : \mathbb{D} - \varrho \frac{d\psi}{dt} \overset{(2)}{=} \sum_\alpha J_\alpha A_\alpha \quad \text{with}$$

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

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

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

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

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

`Compressible NS`

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

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

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

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

`Incompressible Navier-Stokes`

Elastic and Kelvin-Voigt incompressible solids

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

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

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

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

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

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

`Incompressible neo-Hokeean solid`

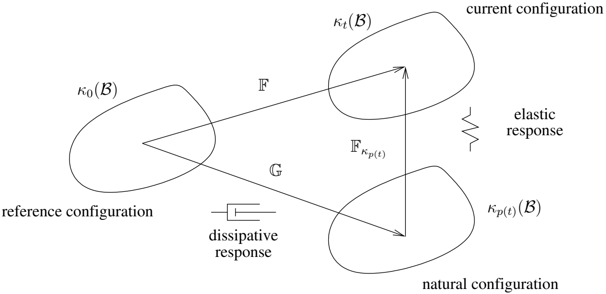
$$\boxed{\xi = 2\nu\mathbb{D} : \mathbb{D}} \quad \Longrightarrow \quad \boxed{\mathbb{T} = -p\mathbb{I} + \mu\mathbb{B} + 2\nu\mathbb{D}}$$

`Incompressible Kelvin-Voigt solid`

Second key idea - Natural configuration

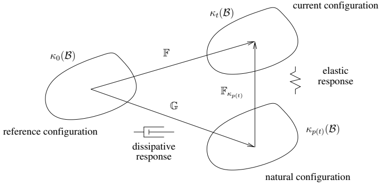
Natural configuration

- 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



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

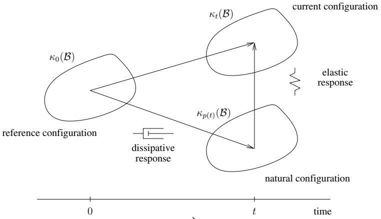
$$\frac{d\mathbb{B}_{\kappa_{p(t)}}}{dt} = \mathbb{L}\mathbb{B}_{\kappa_p(t)} + \mathbb{B}_{\kappa_p(t)}\mathbb{L}^{\mathrm{T}} - 2\mathbb{F}_{\kappa_{p(t)}} \mathbb{D}_{\kappa_{p(t)}} \mathbb{F}^{\mathrm{T}}_{\kappa_{p(t)}} \implies$$

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

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

Compressible and Incompressible responses/Maxwell & Oldroyd-B

Natural configuration provides more variants for imposing compressibility



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

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

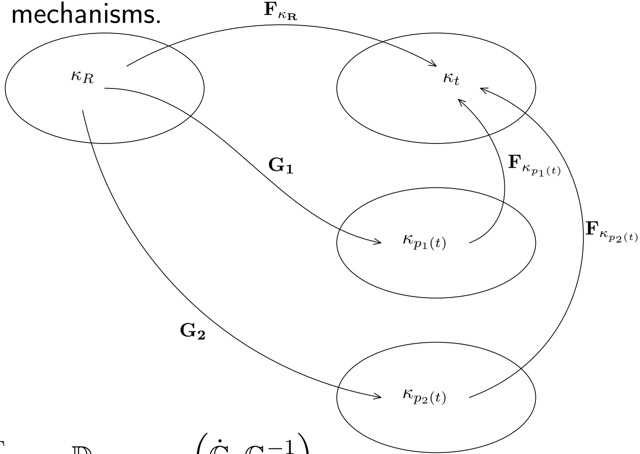
lead to Maxwell and Oldroyd-B fluid

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)

Two relaxation mechanisms

Experiments show that ashpalt and bovine eye has at least two different relaxation mechanisms.



$$\mathbb{B}_{\kappa_{p_1(t)}} = \mathbb{F}_{\kappa_{p_1(t)}} \mathbb{F}^{\mathrm{T}}_{\kappa_{p_1(t)}},\ \mathbb{D}_{\kappa_{p_1(t)}} = \left(\dot{\mathbb{G}}_1 \mathbb{G}_1^{-1}\right)_{\mathrm{sym}}$$
$$\mathbb{B}_{\kappa_{p_2(t)}} = \mathbb{F}_{\kappa_{p_2(t)}} \mathbb{F}^{\mathrm{T}}_{\kappa_{p_2(t)}},\ \mathbb{D}_{\kappa_{p_2(t)}} = \left(\dot{\mathbb{G}}_2 \mathbb{G}_2^{-1}\right)_{\mathrm{sym}}$$

Two constitutive relations for scalars are prescribed: Helmholtz free energy ψ, and rate of entropy production ξ.

Helmholtz free energy ψ – compressible neo-Hookean

$$\psi = \frac{G_1}{2\rho}\left(\operatorname{tr}\mathbb{B}_{\kappa_{p_1(t)}} - 3 - \ln\det\mathbb{B}_{\kappa_{p_1(t)}}\right) + \frac{G_2}{2\rho}\left(\operatorname{tr}\mathbb{B}_{\kappa_{p_2(t)}} - 3 - \ln\det\mathbb{B}_{\kappa_{p_2(t)}}\right)$$

Rate of entropy production ξ

$$0 \leq \tilde{\xi} = 2\mu|\mathbb{D}|^2 + 2G_1\tau_1\left|\mathbb{F}_{\kappa_{p_1(t)}}\mathbb{D}_{\kappa_{p_1(t)}}\right|^2 + 2G_2\tau_2\left|\mathbb{F}_{\kappa_{p_2(t)}}\mathbb{D}_{\kappa_{p_2(t)}}\right|^2$$

Derivation of isothermal model

Step 1. Take the $\frac{\mathrm{d}}{\mathrm{d}t}$ derivative of $\psi(\mathbb{B}_{\kappa_{p_1(t)}}, \mathbb{B}_{\kappa_{p_2(t)}})$.

Step 2. Use the reduced TD identity $\xi = \mathbb{T}\cdot\mathbb{D} - \rho\dot{\psi}$.

Step 3. Compare $\xi = \tilde{\xi}$.

$$\boxed{\begin{gathered}\mathbb{T} = -p\mathbb{I} + 2\mu\mathbb{D} + G_1(\mathbb{B}_{\kappa_{p_1(t)}} - \mathbb{I}) + G_2(\mathbb{B}_{\kappa_{p_2(t)}} - \mathbb{I}) \\ \overset{\triangledown}{\mathbb{B}}_{\kappa_{p_1(t)}} + \frac{1}{\tau_1}(\mathbb{B}_{\kappa_{p_1(t)}} - \mathbb{I}) = \mathbb{O} \\ \overset{\triangledown}{\mathbb{B}}_{\kappa_{p_2(t)}} + \frac{1}{\tau_2}(\mathbb{B}_{\kappa_{p_2(t)}} - \mathbb{I}) = \mathbb{O}\end{gathered}}$$

Equivalent to a standard Burgers model

$$\mathbb{T} = -p\mathbb{I} + 2\mu\mathbb{D} + \mathbb{S}$$

$$\overset{\triangledown\triangledown}{\mathbb{S}} + \left(\frac{1}{\tau_1} + \frac{1}{\tau_2}\right)\overset{\triangledown}{\mathbb{S}} + \frac{1}{\tau_1\tau_2}\mathbb{S} = 2\left(\frac{G_1}{\tau_2} + \frac{G_2}{\tau_1}\right)\mathbb{D} + 2(G_1 + G_2)\overset{\triangledown}{\mathbb{D}}$$

Rate-type fluids with stress diffusion

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

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

J. Málek, V. Průša, T. Skřivan, E. Süli: Thermodynamics of viscoelastic rate type fluids with stress diffusion, Physics of Fluids 30, 023101 (2018)

Summary

Thermodynamic approach

- 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, Burgers)
- compressible rate-type fluids (`Málek, Průša (2017)`)
- capable of developing models where different energy mechanisms take place
  - Navier-Stokes-Fourier (NSF) fluids (compressible and incompressible)
  - Korteweg NSF fluids (compressible and incompressible)
  - Cahn-Hilliard NSF fluids
  - boundary conditions (constitutive equations on the surfaces)

Why is knowledge of thermodynamical underpinnings important?

- important for theoretical analysis (function spaces, distance function)
- E. Feireisl for compressible NSF fluids

Energy estimates and specification of ψ and ξ

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

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

- 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

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

- Updated energy equality

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

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Thank you for your attention.

Comments

- EMS
  - EMS Council meeting, Prague, June 24-25
  - Applied Mathematics Committee (member since January 2018)
    - topics (Mathematical biology, Mathematics in HPC, EU-MATHS-IN, Big Data Analysis)
  - Pavel Exner, Volker Mehrmann
- ESSAM Schools in Kácov
- Nečas Center, EU.MATHS.IN.CZ - unify effort at national level
- Industry 4.0 (mentors - students; Tim Boll)