Nečas Center for Mathematical Modeling



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PDE large data analysis for unsteady flows of non-Newtonian fluids

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Newtonian/Navier-Stokes fluids

• Newtonian fluids/Navier-Stokes fluids linear relation between \mathbb{T} and $\nabla \mathbf{v}$

- Non-Newtonian fluid is a fluid that is not Newtonian
- non-Newtonian fluids/structured fluids/complex fluids

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Section 1

Foreword

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

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

$$\nu > 0$$

$$(\mathbf{a} \otimes \mathbf{b})_{ij} := a_i b_j$$
$$\operatorname{div}(\mathbf{v} \otimes \mathbf{v})_i = \sum_{j=1}^3 \frac{\partial(v_i v_j)}{\partial x_j} = \sum_{j=1}^3 v_j \frac{\partial v_i}{\partial x_j} = \mathbf{v} \cdot \nabla v_i$$

$$\operatorname{div} \mathbf{v} = 0$$
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Compressible Navier-Stokes equations

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

Unknowns: (\mathbf{v}, ϱ) $\nu > 0, \quad 2\nu + 3\lambda > 0$ Systems of PDEs of the second order

$$\operatorname{div} \mathbf{v} = 0$$
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Systems of PDEs of the second order

NSEs - rewritten

Incompressible Navier-Stokes equations

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

 $\mathsf{Unknowns:}\;(\mathbf{v},p,\mathbb{S})$

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

Systems of PDEs of the first order

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 $\label{eq:constraint} {\sf Unknowns:} \ ({\bf v}, \varrho, \mathbb{T}) \qquad \qquad \nu > 0, \quad 2\nu + 3\lambda > 0$

Systems of PDEs of the first order

Incompressible Navier-Stokes equations

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

Unknowns: (\mathbf{v},\mathbb{T})

ν	> 1	0
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$$m := \frac{1}{3} \operatorname{tr} \mathbb{T}$$
$$\mathbb{A}_{\delta} := \mathbb{A} - \frac{1}{3} (\operatorname{tr} \mathbb{A}) \mathbb{I}$$

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• 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

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

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

- Non-Newtonian fluid is a fluid that is not Newtonian
- non-Newtonian fluids/structured fluids/complex fluids
- Are there Non-Newtonian fluids?

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 \mathbb{T} and $\nabla \mathbf{v}$

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Section 2

Complex fluids - examples

Asphalt concrete

Bovine eye

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

- 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 × 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

Non-Newtonian phenomena

- Nonlinear relation between the stress and the shear rate
- 2 The presence of activation or deactivation criteria
- Solution The presence of the normal stress differences in simple shear flows
- Stress Relaxation
- (Nonlinear) Creep

Viscosity

Definition

. . .

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

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



Shear thinning/thickening

Generalized viscosity

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

Presence of activation criteria (such as yield stress)



shear rate κ

Bingham and Herschel-Bulkley fluids

Normal stress differences in simple shear flow

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

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





Response at stress relaxation test for linear spring and linear dashpot



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

(Non-linear) creep



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)

Newtonian fluid is exception

- Food materials such as milk, oil, tomato products, products of granular type (such as rice)
- Ohemical suspensions, gels, paints,
- Biological materials such as blood and synovial fluid
- 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 $100\times$



- 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
 - Observation/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

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Aims

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

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
- 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

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

- 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
- **(**) stability (with respect to perturbations rounding errors,, stationary/periodic solution)
- connections between infinite-dimensional problems and huge yet finite-dimensional problems
- Z. Strakoš (since 2006)

Section 5

Highlights of Lecture 1

Incompressible Navier-Stokes equations

$$\operatorname{div} \mathbf{v} = 0$$
$$\frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) = -\nabla p + \operatorname{div} \mathbb{S}$$
$$\mathbb{S} = 2\nu \mathbb{D}$$

 $\mathsf{Unknowns:}\;(\mathbf{v},p,\mathbb{S})$

 $\nu > 0$, density

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

► NSEs (mathematics):

- Oseen (1921), **Leray** (1933/34) 2d vs 3d, Hopf (1951), Kiselev, Ladyzhenskaya (1957), Caffarelli, Kohn, Nirenberg (1982)
- DiPerna (1980-1989), PL Lions (1998), Feireisl (2004)
- Existence and smoothness of the Navier-Stokes equation (2000)
- ▶ Leray's program: long time nad large data existence of (weak) solution

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Section 6

Viscous fluids and visco-elastic fluids

Unsteady flows of incompressible fluids

Governing equations

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

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

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

$$\mathbb{S} = \mathbb{S}^{\mathrm{T}}$$

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

$$\mathbf{v}(0, \cdot) = \mathbf{v}_{0} \qquad \left. \right\} \text{ in } \Omega$$

Energy balance

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

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

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

Unsteady flows of incompressible fluids

Governing equations

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$$\frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) = -\nabla p + \operatorname{div} \mathbb{S} \qquad \left\{ \begin{array}{c} \operatorname{in} (0, T) \times \Omega \\ \mathbb{S} = \mathbb{S}^{\mathrm{T}} \\ \mathbf{v} \cdot \mathbf{n} = 0 \\ \mathbb{v}(0, \cdot) = \mathbf{v}_{0} \end{array} \right\} \text{ on } (0, T) \times \partial \Omega$$

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Internal flows

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

 $\mathbb{S}n$

 $(\mathbb{S}\mathbf{n})_{\tau}$

Boundary conditions

•
$$\mathbf{v} \cdot \mathbf{n} = 0$$
 on $\partial \Omega$

• constitutive equation involving \mathbf{v}_{τ} and/or $(-\mathbb{S}\mathbf{n})_{\tau}$

$$\mathbf{s} := (-\mathbb{S}\mathbf{n})_{\tau} \qquad \mathbf{z}_{\tau} := \mathbf{z} - (\mathbf{z} \cdot \mathbf{n})\mathbf{n}$$
$$\int_{\partial \Omega} (-\mathbb{S}) : (\mathbf{v} \otimes \mathbf{n}) = \int_{\partial \Omega} (-\mathbb{S})\mathbf{n} \cdot \mathbf{v} = \int_{\partial \Omega} \left((-\mathbb{S}\mathbf{n})_{\tau} \cdot \mathbf{v}_{\tau} \right)$$

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

Energy estimates and constitutive equations

• Governing equations

- -

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

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

$$\mathbb{D} := \frac{1}{2} \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}} \right)$$

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

• To close the system

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

Constitutive equations

Energy estimates and constitutive equations

• Governing equations

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

$$\mathbb{D} := \frac{1}{2} \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}} \right)$$

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

• To close the system

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

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

Constitutive equations

Energy estimates and constitutive equations

• Governing equations

1.

~

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

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

$$\mathbb{D} := \frac{1}{2} \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}} \right)$$

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

 \bullet To close the system

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

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

Constitutive equations

Classes of constitutive equations

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

higher order rate type viscoelastic fluids

Euler/limiting shear-rate		limiting shear- rate		rigid body	
Euler/shear- thickening		shear- thickening		rigid/shear- thickening	\geq
Euler/Navier- Stokes		Navier-Stokes		Bingham = rigid/Navier- Stokes	
Euler/shear- thinning		shear-thinning		rigid/shear- thinning	
Euler		limiting shear stress		perfect plastic	
$ \mathbb{D} \le \delta_* \iff 1$	$\mathbb{S} = \mathbb{O}$	no activation		$ \mathbb{S} \leq \sigma_* \iff$	$\mathbb{D} = \mathbb{O}$

 $\begin{array}{l} \mbox{Summary of systematic classification of fluid-like responses} \\ \mbox{with corresponding } |\mathbb{S}| \mbox{ vs } |\mathbb{D}| \mbox{ diagrams}. \end{array}$



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

Long time and large data existence theory

Ladyzhenskaya (1967-72), JL Lions (1969), Málek, Nečas, Ružička (1993-2000), Frehse, Málek, Steinhauer (1996-2003)



- L. Diening, M. Růžička, J. Wolf, Existence of weak solutions for unsteady motions of generalized Newtonian fluids, Ann. Sc. Norm. Super. Pisa Cl. Sci. (5) 9 (2010) 1–46.
- 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, 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.



J. Blechta, J. Málek, K.R. Rajagopal: On the classification of incompressible fluids and a mathematical analysis of the equations that govern their motions, a revised version considerd for publication in SIAM J. Math. Anal. (2019), arXiv: 1902.04853.



A. Abbatiello, E. Feireisl: On a class of generalized solutions to equations describing incompressible viscous fluids, arXiv: 1905.12732 (2019).

Tools: symmetric role of S and D; Lipschitz truncation of Bochner-Sobolev functions; maximal monotone responses; biting lemma

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

capability of describing stress relaxation and nonlinear creep

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

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

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)

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

Popular models within $\mathbb{G}(\overset{*}{\mathbb{S}},\mathbb{S},\overset{*}{\mathbb{D}},\mathbb{D})=\mathbb{O}$

• Maxwell (1867)

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

Oldroyd-B (1950)

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

• Johnson-Segalman (1977)

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



P. L. Lions, N. Masmoudi: Global solutions for some Oldroyd models of non-Newtonian flows, *Chinese Annals of Mathematics. Series B*, Vol. 21, pp. 131–146 (2000)



N. Masmoudi: Global existence of weak solutions to macroscopic models of polymeric flows, Journal de Mathématiques Pures et Appliquées. Neuvième Série, Vol. 96, pp. 502–520 (2011)

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

- + Both mathematical and physical
 - regularization (stabilization of numerical methods)
 - 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, Briels (2008), Divoux et al (2016)

- No 3d long-time and large-data theory for popular models with stress diffusion is available

A popular model within $\mathbb{G}(\mathbb{S},\mathbb{S},\mathbb{S},\mathbb{D},\mathbb{D},\mathbb{D})=\mathbb{O}$

▶ Burgers (1939)

$$\begin{aligned} \operatorname{div} \mathbf{v} &= 0\\ \frac{\partial \mathbf{v}}{\partial t} + \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) &= -\nabla p + \nu \Delta \mathbf{v} + \operatorname{div} \mathbb{S}\\ \overset{\nabla \nabla}{\mathbb{S}} + \lambda_1 \overset{\nabla}{\mathbb{S}} + \lambda_2 \mathbb{S} &= \eta_1 \mathbb{D} + \eta_2 \overset{\nabla}{\mathbb{D}} \end{aligned}$$

 $\overset{\nabla}{\mathbb{S}} := \tfrac{\partial \mathbb{S}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbb{S} - (\nabla \mathbf{v}) \mathbb{S} - \mathbb{S} (\nabla \mathbf{v})^{\mathrm{T}}$ the upper convected Oldroyd derivative

No mathematical theory is available

Asphalt concrete

Bovine eye

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

- 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)





Questions concerning physics

- consistency with the laws of thermodynamics
- physical interpretation of the constants λ_1 , λ_2 , η_1 , η_2
- specification of the initial conditions (second order time derivative)
- correct choice of objective derivatives
- extension to compressible viscoelastic fluids
- extension to include thermal effects

Questions concerning PDE analysis

- weak solution primar concept of solution in continuum physics
- weak solution basic object for several powerful numerical methods
 - a priori estimates basis for long-time and large data existence theory
 - a priori estimates determine function spaces that are sufficient for making the weak formulation of PDEs meaningful and where solution should be look for
 - a priori estimates a tool to construct Lyapunov functional and distance measures to study qualitative behavior
- viscoelasticity bridge between viscous and elastic materials

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Thermodynamic approach

Building blocks

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

suffices to determine the constitutive equations for the Cauchy stress and other fluxes



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)



K. R. Rajagopal, A. R. Srinivasa: On thermomechanical restrictions to continua, *Proc. R. Soc. Lond. A* Vol. 460, 631–651 (2004)

- Extension of Leray's program developed for the Navier-Stokes equations to models of non-Newtonian fluid mechanics
- A close interconnection between continuum thermodynamics and PDE analysis can be fruitful

- 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 International Publishing, Cham, pp.3-72 (2018)

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- J. Málek, K. R. Rajagopal, K. Tůma: Derivation of the variants of the Burgers model using a thermodynamic approach and appealing to the concept of evolving natural configurations, *Fluids* **3** (2018) 69, 18 pages.

J. Hron, V. Miloš, V. Průša, O. Souček, K. Tůma: On thermodynamics of viscoelastic rate type fluids with temperature dependent material coefficients, Int. J. Non-Linear Mech. 95 (2017) 193–208.



M. Bulíček, J. Málek, V. Průša, E. Süli: PDE analysis of a class of thermodynamically compatible viscoelastic rate-type fluids with stress diffusion, *Contemporary mathematics*, Vol. 710, Am. Math. Soc., Providence, RI pp. 25–51 (2018)



M. Bulíček, E. Feireisl, J. Málek: On the analysis of a class of thermodynamically compatible viscoelastic fluids with stress diffusion, to appear in *Nonlinearity*, arXiv: 1810.00271 (2018)

Section 7

Methodology applied to compressible materials

Governing equations

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

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

Helmholtz free energy

Restriction to isothermal processes

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

If $\mathbf{j}_\eta = rac{\mathbf{j}_e}{ heta}$, then

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

General thermodynamic framework

Constitutive equation for the Helmholtz free energy ψ :

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

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 :

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

leads to

$$J_{\alpha} = \gamma_{\alpha} A_{\alpha} \qquad \gamma_{\alpha} > 0$$
Compressible Navier-Stokes fluids

$$\begin{split} & \psi = \psi_0(\varrho) & p_{\rm th}(\varrho) := \varrho^2 \psi_0'(\varrho) \\ & \xi = \mathbb{T} : \mathbb{D} - \varrho \frac{d\psi}{dt} \implies \qquad & \xi = \mathbb{T}_{\delta} : \mathbb{D}_{\delta} + (m + p_{\rm th}) \operatorname{div} \mathbf{v} \\ \hline & \xi = 2\nu \mathbb{D}_{\delta} : \mathbb{D}_{\delta} + \lambda |\operatorname{div} \mathbf{v}|^2 \\ \hline & \mathbb{T} = m\mathbb{I} + \mathbb{T}_{\delta} = -p_{\rm th}\mathbb{I} + 2\nu \mathbb{D}_{\delta} + \lambda \operatorname{div} \mathbf{v} \mathbb{I} & \text{Compressible NS} \\ & \bullet \mathbb{T}_{\delta} = \mathbb{O} \quad m + p_{\rm th} = 0 \\ & \overline{\mathbb{T} = -p_{\rm th}\mathbb{I}} & \text{Compressible Euler} \\ & \bullet \mathbb{T}_{\delta} = \mathbb{O} \quad m + p_{\rm th} = \lambda \operatorname{div} \mathbf{v} \end{split}$$

 $\left|\mathbb{T}=-p_{\mathrm{th}}\mathbb{I}+\lambda\operatorname{div}\mathbf{v}\mathbb{I}
ight|$ no dissipation due to shearing

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

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

•
$$\mathbb{T}_{\delta} = 2\nu \mathbb{D}_{\delta}$$

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

Incompressible Navier-Stokes

•
$$\mathbb{T}_{\delta} = \mathbb{O}$$

 $\mathbb{T} = m\mathbb{I}$

Incompressible Euler

Elastic and Kelvin-Voigt solids

 $\left|\psi = \frac{\mu}{2\rho}(\operatorname{tr}\mathbb{B} - 3 - \ln\det\mathbb{B})\right|$ $\mathbb{B} := \mathbb{F}\mathbb{F}^{\mathrm{T}}$ Since $\frac{d\mathbb{F}}{dt} = \mathbb{LF}$, we get $\frac{d\mathbb{B}}{dt} = \mathbb{L}\mathbb{B} + \mathbb{B}\mathbb{L}^{\mathrm{T}} \iff \overset{\nabla}{\mathbb{B}} = \mathbb{O} \quad \text{and} \quad \frac{d}{dt} \operatorname{tr} \mathbb{B} = 2\mathbb{B} : \mathbb{D}$ $\xi = \mathbb{T} : \mathbb{D} - \varrho \frac{d\psi}{dt}$ with $\xi \ge 0$ Hence $\xi = (\mathbb{T} - \mu \mathbb{B}) : \mathbb{D} = (\mathbb{T}_{\delta} - \mu \mathbb{B}_{\delta}) : \mathbb{D}$ with $\xi > 0$ $\xi = 0 \qquad \Longrightarrow \qquad |\mathbb{T} = m\mathbb{I} + \mu\mathbb{B}_{\delta} = -p\mathbb{I} + \mu\mathbb{B}$ Incompressible neo-Hokeean solid $\xi = 2\nu \mathbb{D} : \mathbb{D} | \implies | \mathbb{T} = -p\mathbb{I} + \mu \mathbb{B} + 2\nu \mathbb{D}$ 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 $\mathbb G$



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

Kinematics



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

7

 $\begin{array}{ll} \bullet \ \mathbb{F}, \ \mathbb{G}, \ \mathbb{F}_{\kappa_{p(t)}} & \mathbb{B}_{\kappa_{p(t)}} := \mathbb{F}_{\kappa_{p(t)}} \mathbb{F}_{\kappa_{p(t)}}^{\mathrm{T}} & \mathbb{C}_{\kappa_{p}(t)} := \mathbb{F}_{\kappa_{p(t)}}^{\mathrm{T}} \mathbb{F}_{\kappa_{p(t)}} \\ \bullet & \frac{d\mathbb{F}}{dt} = \mathbb{L}\mathbb{F} \implies \mathbb{L} = \frac{d\mathbb{F}}{dt} \mathbb{F}^{-1} & \mathbb{D}, \ \mathbb{W} \\ \bullet & \mathbb{L}_{\kappa_{p(t)}} := \frac{d\mathbb{G}}{dt} \mathbb{G}^{-1} & \mathbb{D}_{\kappa_{p(t)}}, \ \mathbb{W}_{\kappa_{p(t)}} \end{array}$

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

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

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

Compressible and Incompressible responses/Maxwell & Oldroyd-B

Natural configuration provides more variants for imposing compressibility



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

lead to Maxwell and Oldroyd-B fluid

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 International Publishing, Cham, pp.3-72 (2018)

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

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

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

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

Equivalent to a standard Burgers model

$$\mathbb{T} = -p\mathbb{I} + 2\mu\mathbb{D} + \mathbb{S}$$
$$\mathbb{S}^{\vee\vee} + \left(\frac{1}{\tau_1} + \frac{1}{\tau_2}\right)\mathbb{S} + \frac{1}{\tau_1\tau_2}\mathbb{S} = 2\left(\frac{G_1}{\tau_2} + \frac{G_2}{\tau_1}\right)\mathbb{D} + 2(G_1 + G_2)\mathbb{D}^{\vee}$$

Energy estimates and specification of ψ and ξ

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

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

• Reduced thermodynamical identity

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

 \bullet Specification of the constitutive equations of ψ and ξ

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

• Updated energy equality

$$\|\mathbf{v}(t)\|_{2}^{2} + \|\tilde{\psi}(\dots)(t)\|_{1} + 2\int_{0}^{t}\int_{\Omega}\tilde{\xi}(\dots) = \|\mathbf{v}_{0}\|_{2}^{2} + \|\tilde{\psi}_{0}(\dots)\|_{1}$$

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Thank you for your attention.