Thermodynamics of viscoelastic rate-type fluids and its implications for stability analysis

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8th ECM

Thermodynamically open systems



Example: any system with external forcing (Rayleigh-Bénard convection, Taylor-Couette flow) Expected behaviour: conditional asymptotic stability of the non-equilibrium steady state until some critical forcing is reached (Rayleigh number, Taylor number)

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Concept of stability

We have two solutions s_1 and s_2 starting from (slightly) different initial conditions:

- Is it true that $s_1 s_2$ stay close to each other?
- Is it true that $s_1 s_2 \rightarrow 0$ as $t \rightarrow +\infty$?



Key question

Is it possible to use some thermodynamical concepts – especially for open systems?

Introduction

Lyapunov-type functional, ISOLATED SYSTEMS:



constant number of polymers

Identification of Lagrange multiplier (homogeneous steady state): $\lambda_1 = \frac{1}{\widehat{\theta}}$

$$\frac{\mathrm{d}\mathcal{V}_{\mathrm{meq}}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \left\{ -\underbrace{S}_{\mathrm{entropy}} + \lambda_1 \underbrace{\left(\mathcal{E}_{\mathrm{tot}} - \widehat{\mathcal{E}_{\mathrm{tot}}} \right)}_{\mathrm{constant \ energy}} + \lambda_2 \underbrace{\int_{\Omega} \left(\rho_{\mathrm{s}} - \widehat{\rho_{\mathrm{s}}} \right) \, \mathrm{d}v}_{\mathrm{constant \ number \ of \ polymers}} \right\} = -\frac{\mathrm{d}S}{\mathrm{d}t} = -\int_{\Omega} \xi \, \mathrm{d}v \le 0$$

Pierre Duhem. Traité d'Énergetique ou Thermodynamique Générale. Paris, 1911

Bernard D. Coleman and James M. Greenberg. Thermodynamics and the stability of fluid motion. <u>Arch. Ration. Mech. Anal.</u>, 25(5):321–341, 1967

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Stability analysis

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Spatially inhomogeneous steady state

Isolated system (Lyapunov-type functional):

$$\mathcal{V}_{\mathrm{meq}} =_{\mathrm{def}} - \underbrace{S}_{\mathrm{entropy}} + \frac{1}{\widehat{\theta}} \underbrace{\left(\mathcal{E}_{\mathrm{tot}} - \widehat{\mathcal{E}_{\mathrm{tot}}} \right)}_{\mathrm{constant \ energy}} + \cdots$$

Spatially inhomogenous steady state:

 $\widehat{\theta} = \widehat{\theta}(\boldsymbol{x})$

We do not have a natural Lyapunov-type functional as well. Everything is lost. Really?

Issues

Lyapunov-type functional – heuristics



Affine correction.

$$\mathcal{V}_{\mathrm{neq}}(\widetilde{x}_{\mathrm{neq}} \| \, \widehat{x}_{\mathrm{neq}}) =_{\mathrm{def}} \mathcal{V}_{\mathrm{eq}}(\widehat{x}_{\mathrm{neq}} + \widetilde{x}_{\mathrm{neq}}) - \mathcal{V}_{\mathrm{eq}}(\widehat{x}_{\mathrm{neq}}) - \left. \frac{\mathrm{d}\mathcal{V}_{\mathrm{eq}}}{\mathrm{d}x} \right|_{x = \widehat{x}_{\mathrm{neq}}} \widetilde{x}_{\mathrm{neq}}$$

J. L. Ericksen. A thermo-kinetic view of elastic stability theory. Int. J. Solids Struct., 2(4):573–580, 1966 M. Bulíček, J. Málek, and V. Průša. Thermodynamics and stability of non-equilibrium steady states in open systems. <u>Entropy</u>, 21(7), 2019

Lyapunov-type functional

Lyapunov-type functional for thermodynamically OPEN SYSTEMS:

$$\mathcal{V}_{\mathrm{neq}}\left(\left.\widetilde{\boldsymbol{W}}\right\|\left.\widehat{\boldsymbol{W}}\right) =_{\mathrm{def}} - \left\{\mathcal{S}_{\widehat{\boldsymbol{\theta}}}(\left.\widetilde{\boldsymbol{W}}\right\|\left.\widehat{\boldsymbol{W}}\right) - \mathcal{E}(\left.\widetilde{\boldsymbol{W}}\right\|\left.\widehat{\boldsymbol{W}}\right)\right\}$$

This is not the second variation, $\delta^2 S!$ The functional is not "quadratic" in state variables. Other "Lagrange multipliers" should be added if necessary.

$$\begin{split} \mathcal{S}_{\widehat{\theta}}(\widetilde{\boldsymbol{W}} \left\| \left. \widehat{\boldsymbol{W}} \right) =_{\mathrm{def}} \mathcal{S}_{\widehat{\theta}}\left(\widehat{\boldsymbol{W}} + \widetilde{\boldsymbol{W}} \right) - \mathcal{S}_{\widehat{\theta}}\left(\widehat{\boldsymbol{W}} \right) - \mathrm{D}_{\boldsymbol{W}} \mathcal{S}_{\widehat{\theta}}\left(\boldsymbol{W} \right) \Big|_{\boldsymbol{W} = \widehat{\boldsymbol{W}}} \left[\widetilde{\boldsymbol{W}} \right] \\ \mathcal{E}(\left. \widetilde{\boldsymbol{W}} \right\| \left. \widehat{\boldsymbol{W}} \right) =_{\mathrm{def}} \mathcal{E}_{\mathrm{tot}}\left(\widehat{\boldsymbol{W}} + \widetilde{\boldsymbol{W}} \right) - \mathcal{E}_{\mathrm{tot}}\left(\widehat{\boldsymbol{W}} \right) - \mathrm{D}_{\boldsymbol{W}} \mathcal{E}_{\mathrm{tot}}\left(\boldsymbol{W} \right) \Big|_{\boldsymbol{W} = \widehat{\boldsymbol{W}}} \left[\widetilde{\boldsymbol{W}} \right] \\ \mathcal{S}_{\widehat{\theta}}\left(\boldsymbol{W} \right) =_{\mathrm{def}} \int_{\Omega} \rho \widehat{\theta} \eta(\boldsymbol{W}) \, \mathrm{dv} \\ \mathcal{E}_{\mathrm{tot}}\left(\boldsymbol{W} \right) =_{\mathrm{def}} \int_{\Omega} \frac{1}{2} \rho \left| \boldsymbol{v} \right|^{2} + \rho \boldsymbol{e}(\boldsymbol{W}) \, \mathrm{dv} \end{split}$$

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Fluxes through the boundary

Time derivative:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{V}_{\mathrm{neq}}\left(\left.\widetilde{\boldsymbol{W}}\right\|\left.\widehat{\boldsymbol{W}}\right)\right| \leq 0$$

In our Lyapunov-type functional:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\rho\widehat{\theta}\eta\left(\boldsymbol{W}\right)-\rho\boldsymbol{e}\left(\boldsymbol{W}\right)\right)$$

Fluxes through the boundary (Dirichlet data for temperature):

Isolated vessel



Thermal bath



Spatially non-uniform wall temperature



Incompressible Navier-Stokes-Fourier fluid

Mechanical quantities:

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

 $ho rac{\mathrm{d} oldsymbol{v}}{\mathrm{d} t} = \operatorname{div} \mathbb{T}$

Cauchy stress tensor:

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

Temperature:

$$\rho c_{\rm V} \frac{\mathrm{d}\theta}{\mathrm{d}t} = \underbrace{2\nu\mathbb{D}:\mathbb{D}}_{\zeta_{\rm mech}, \text{ dissipative heating}} + \operatorname{div}(\kappa\nabla\theta)$$

Boundary conditions:

$$oldsymbol{v}|_{\partial\Omega} = oldsymbol{0} \qquad heta|_{\partial\Omega} = oldsymbol{ heta}_{
m bdr}$$

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Incompressible Oldroyd-B fluid

Mechanical quantities:

$$\begin{split} \operatorname{div} \mathbf{v} &= 0\\ \rho \frac{\mathrm{d} \mathbf{v}}{\mathrm{d} t} &= \operatorname{div} \mathbb{T}\\ \nu_1 \overline{\mathbb{B}_{\kappa_{p(t)}}} + \mu \left(\mathbb{B}_{\kappa_{p(t)}} - \mathbb{I} \right) &= \mathbb{O} \end{split}$$

Cauchy stress tensor:

$$\mathbb{T} = -p\mathbb{I} + 2\nu\mathbb{D} + \mu\Big(\mathbb{B}_{\kappa_{p(t)}}\Big)_{\delta}$$

Temperature:

$$\rho c_{\mathrm{V}} \frac{\mathrm{d}\theta}{\mathrm{d}t} = \underbrace{2\nu \mathbb{D} : \mathbb{D} + \frac{\mu^2}{2\nu_1} \left(\mathrm{Tr} \, \mathbb{B}_{\kappa_{p(t)}} + \mathrm{Tr} \left(\mathbb{B}_{\kappa_{p(t)}}^{-1} \right) - 6 \right)}_{\zeta_{\mathrm{mech}}, \text{ dissipative heating}} + \operatorname{div} \left(\kappa \nabla \theta \right)$$

Boundary conditions:

$$oldsymbol{
u}|_{\partial\Omega} = oldsymbol{0} \qquad eta|_{\partial\Omega} = oldsymbol{ heta}_{
m bdr}$$

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Expected result

Notation:

Steady state:

$$\widehat{\mathbf{v}} = \mathbf{0}$$

 $\widehat{\mathbf{ heta}} =$ solution to steady heat equation

Steady state temperature $\hat{\theta}$ solves:

$$0 = \operatorname{div}\left(\kappa \nabla \widehat{\theta}\right)$$
$$\widehat{\theta}\Big|_{\partial \Omega} = \theta_{\mathrm{bdr}}$$

Arbitrary perturbation $\tilde{\mathbf{v}}$, $\tilde{\theta}$ should decay! No "close to equilibrium", "we can neglect" excuses, only "classical solution exists".

Decay of kinetic energy

Evolution equation for the velocity:

$$\rho \frac{\mathrm{d} \boldsymbol{v}}{\mathrm{d} t} = \mathsf{div} \left(-\boldsymbol{\rho} \mathbb{I} + 2\boldsymbol{\nu} \mathbb{D} \right)$$

Evolution equation for the net kinetic energy:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega} \frac{1}{2} \rho \, |\mathbf{v}|^2 \, \mathrm{d}v = -\int_{\Omega} 2\nu \mathbb{D} : \mathbb{D} \, \mathrm{d}v$$

James Serrin. On the stability of viscous fluid motions. Arch. Ration. Mech. Anal., 3:1-13, 1959

Main issues

Temperature:

$$\rho c_{\mathrm{V}} \frac{\mathrm{d}\theta}{\mathrm{d}t} = \underbrace{2\nu \mathbb{D}:\mathbb{D}}_{\zeta_{\mathrm{mech}}, \text{ dissipative heating}} + \mathsf{div} \left(\kappa \nabla \theta\right)$$

Problem:

- We do not know when and where is the kinetic energy dissipated.
- We do not know what are the fluxes through the boundary.
- If \mathbf{v} is small, it is not necessarily true that \mathbb{D} is small.

Dissipative heating:

$$\int_{t=0}^{+\infty} \left(\int_{\Omega} \zeta_{\mathrm{mech}} \, \mathrm{dv} \right) \mathrm{d}t = \int_{t=0}^{+\infty} \left(\int_{\Omega} 2\nu \mathbb{D} : \mathbb{D} \, \mathrm{dv} \right) \mathrm{d}t < +\infty$$

Do not touch the dissipative heating. Use only its positivity!

Main issues

How to measure the distance form the steady state?

$$\begin{split} \rho c_{\mathrm{V,ref}} \frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega} \widetilde{\theta}^2 \, \mathrm{d}\mathbf{v} &= -\int_{\Omega} \kappa_{\mathrm{ref}} \nabla \widetilde{\theta} \bullet \nabla \widetilde{\theta} \, \mathrm{d}\mathbf{v} + \int_{\Omega} \underbrace{2\nu \widetilde{\mathbb{D}} : \widetilde{\mathbb{D}}}_{\zeta_{\mathrm{mech}}, \text{ dissipative heating}} \\ &+ \int_{\Omega} \rho c_{\mathrm{V,ref}} \left(\widetilde{\mathbf{v}} \bullet \nabla \widehat{\theta} \right) \widetilde{\theta} \, \mathrm{d}\mathbf{v} \end{split}$$

Key tool – decay of integrable functions

We know:

$$\int_{\tau=0}^{+\infty} y(\tau) \,\mathrm{d}\tau \leq C_1$$

We want:



We need:

$$\frac{\mathrm{d}y}{\mathrm{d}t} \le f(y) + h$$

Songmu Zheng. Nonlinear evolution equations, volume 133 of Chapman & Hall/CRC Monographs and Surveys in Pure and Applied Mathematics. Chapman & Hall/CRC, Boca Raton, FL, 2004

P. Krejčí and J. Sprekels. Weak stabilization of solutions to PDEs with hysteresis in thermovisco-elastoplasticity. In R. P. Agarwal, F. Neuman, and J. Vosmansky, editors, Proceedings of Equadiff 9, pages 81–96, Brno, 1998. Masaryk University

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Candidate for Lyapunov functional

Convenient measure for the size of perturbation:

$$\mathcal{V}_{\mathrm{meq}}\left(\left.\widetilde{\boldsymbol{W}}\right\|\left.\widehat{\boldsymbol{W}}\right) =_{\mathrm{def}} \int_{\Omega} \rho \boldsymbol{c}_{\mathrm{V,ref}} \widehat{\theta} \left[\frac{\widetilde{\theta}}{\overline{\theta}} - \ln\left(1 + \frac{\widetilde{\theta}}{\overline{\theta}}\right)\right] \,\mathrm{dv} + \int_{\Omega} \frac{1}{2} \rho \left|\widetilde{\boldsymbol{v}}\right|^{2} \,\mathrm{dv}$$

Time derivative:

$$\begin{split} \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{V}_{\mathrm{meq}} \left(\left. \widetilde{\boldsymbol{W}} \right\| \left. \widehat{\boldsymbol{W}} \right) &= -\int_{\Omega} \kappa_{\mathrm{ref}} \widehat{\theta} \nabla \ln \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right) \bullet \nabla \ln \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right) \, \mathrm{dv} \\ &- \int_{\Omega} \frac{2\nu \widetilde{\mathbb{D}} : \widetilde{\mathbb{D}}}{1 + \frac{\widetilde{\theta}}{\widehat{\theta}}} \, \mathrm{dv} + \int_{\Omega} \rho c_{\mathrm{V,ref}} \left(\nabla \widehat{\theta} \bullet \widetilde{\boldsymbol{v}} \right) \ln \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right) \, \mathrm{dv} \end{split}$$

We are "almost done", $x \in (-1, x_{crit})$:

$$- \left[\ln (1+x) \right]^2 \le - \left[x - \ln (1+x) \right]$$

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12 Classical thermodynamics

family of isotherms may be plotted out, as shown schematically in fig. 1. Now let us hole each isotherm with a number, θ_c chosen at will, which we call the empirical temperature corresponding to the given isotherm. Then provided there is some system, however arbitrary, in the labelling of the isotherma, there will exist a relationship (not necessarily analytic) between P, V and θ which may be written in the same form as (2^n) , $\theta_c(P, V) = \theta$.

Once this labelling of isotherms has been carried out for one particular mass of fluid, however, there exists no latitude of choices of a as other fluids are concerned, if consistency is to be achieved. For the sisotherm of a second fluid in equilibrium with the first must be labelled with the same θ . If, and only if, this is done can we say that all fluids having the same value of θ are in equilibrium with one another. This brings us to the same result as was derived before; the two arguments are equivalent.

It is because of the element of choice in the labelling of the isotherms of the first fluid to be selected (the thermometric body) that the quantity θ is referred to as the empirical temperature. It is usual to choose as the thermometric body a fluid whose properties make a rational choice of θ particularly simple. For example, in a mercury-in-glass thermometer there is effectively only one variable, the volume of the mercury, and θ is taken to be a linear function of the volume. The particular straight line selected depends on the choice of scale; according to the Celsius scale, θ is put equal to 0 at the temperature of melting ice, and 100 at the temperature of water boiling at standard atmospheric pressure. Two fixed points are sufficient to determine the linear relation. Consider now the perfect gas scale of temperature. This is capable of simple definition because of the analytical simplicity of the isotherms, which for perfect gases follow Boyle's law, PV = constant. Thus the equation of state of a perfect gas on any empirical scale must take the form $PV = f(\theta),$

and the nature of the empirical scale determines the form of the function $f(\theta)$. It happens that if the empirical scale is fixed by a mercury-in-glass thermometer, $f(\theta)$ is very nearly a linear function over a wide range of temperature. This experimental result makes it convenient to establish an empirical scale in terms of a perfect gas by adopting as a definition of θ the equation

 $PV = R\theta$.

The constant R is chosen for any particular mass of gas in such a way that the value of θ shall change by 100 between the melting-point of ice and the boiling-point of water.

A. B. Pippard. <u>Elements of classical thermodynamics for</u> <u>advanced students of physics</u>. Cambridge University Press, Cambridge, 1964

R. L. Fosdick and K. R. Rajagopal. On the existence of a manifold for temperature. <u>Arch. Ration. Mech. Anal.</u>, 81(4):317–332, 1983

Choose a different temperature scale

Alternative temperature scale:

$$\frac{\vartheta}{\vartheta_{\rm ref}} =_{\rm def} \left(\frac{\theta}{\theta_{\rm ref}}\right)^{1-m}$$

Corresponding candidate for Lyapunov functional:

$$\begin{split} \mathcal{V}_{\mathrm{meq}}^{\vartheta,\,m}\left(\left.\widetilde{\boldsymbol{W}}\right\|\left.\widetilde{\boldsymbol{W}}\right) =_{\mathrm{def}} \int_{\Omega} \rho c_{\mathrm{V,ref}} \widehat{\theta} \left[\frac{\widetilde{\theta}}{\overline{\theta}} - \frac{1}{m}\left(\left(1 + \frac{\widetilde{\theta}}{\overline{\theta}}\right)^{m} - 1\right)\right] \,\mathrm{dv} \\ &+ \int_{\Omega} \frac{1}{2} \rho \,|\widetilde{\boldsymbol{v}}|^{2} \,\,\mathrm{dv} \end{split}$$

Choose a different temperature scale – formal argument

Pointwise evolution equation, f is a given function:

$$\begin{split} \rho \frac{\mathrm{d}\widetilde{\mathbf{v}}}{\mathrm{d}t} \left[c_{\mathrm{V,ref}} \widehat{\theta} f\left(\mathrm{e}^{\frac{\eta_{\mathrm{diff}}}{c_{\mathrm{V,ref}}}}\right) \right] &= \mathrm{div} \left[\kappa_{\mathrm{ref}} \nabla \left(\widehat{\theta} f\left(\mathrm{e}^{\frac{\eta_{\mathrm{diff}}}{c_{\mathrm{V,ref}}}}\right) \right) \right] \\ &- \kappa_{\mathrm{ref}} \widehat{\theta} f'' \left(\mathrm{e}^{\frac{\eta_{\mathrm{diff}}}{c_{\mathrm{V,ref}}}}\right) \nabla \mathrm{e}^{\frac{\eta_{\mathrm{diff}}}{c_{\mathrm{V,ref}}}} \bullet \nabla \mathrm{e}^{\frac{\eta_{\mathrm{diff}}}{c_{\mathrm{V,ref}}}} \\ &+ f' \left(\mathrm{e}^{\frac{\eta_{\mathrm{diff}}}{c_{\mathrm{V,ref}}}}\right) \zeta_{\mathrm{mech}} \left(\widehat{\mathbf{W}} + \widetilde{\mathbf{W}} \right) \\ &+ \rho c_{\mathrm{V,ref}} \left[f \left(\mathrm{e}^{\frac{\eta_{\mathrm{diff}}}{c_{\mathrm{V,ref}}}}\right) - f' \left(\mathrm{e}^{\frac{\eta_{\mathrm{diff}}}{c_{\mathrm{V,ref}}}}\right) \mathrm{e}^{\frac{\eta_{\mathrm{diff}}}{c_{\mathrm{V,ref}}}} \right] \widetilde{\mathbf{v}} \bullet \nabla \widehat{\theta} \\ &\eta_{\mathrm{diff}} =_{\mathrm{def}} c_{\mathrm{V,ref}} \ln \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right) \end{split}$$

Result – unconditional stability

Steady state $\widehat{\theta}$, perturbation $\widetilde{\theta}$, $m, n \in (0, 1)$, $n > m > \frac{n}{2}$:

$$\int_{\Omega} \rho c_{\mathrm{V,ref}} \widehat{\theta} \left[\frac{1}{n} \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right)^n - \frac{1}{m} \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right)^m + \frac{n-m}{mn} \right] \, \mathrm{dv} \xrightarrow{t \to +\infty} 0$$

Corollary:

$$\forall p \in [1, +\infty) \colon \left| \int_{\Omega} \rho c_{\mathrm{V, ref}} \widehat{\theta} \left| \ln \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right) \right|^p \, \mathrm{dv} \xrightarrow{t \to +\infty} 0$$

Not based on a Lyapunov-type technique! Neat thermodynamics based trick: We are exploiting ambiguity in the choice of temperature scale.

M. Dostalík, V. Průša, and J. Stein. Unconditional finite amplitude stability of a viscoelastic fluid in a mechanically isolated vessel with spatially non-uniform wall temperature. <u>Math. Comput. Simulat.</u>, 2020. In press
M. Dostalík, V. Průša, and K. R. Rajagopal. Unconditional finite amplitude stability of a fluid in a mechanically isolated vessel with spatially non-uniform wall temperature. <u>Contin. Mech. Thermodyn.</u>, 33:515-543, 2021

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Elastic turbulence



Figure 3 Two snapshots of the flow at Wi = 13, Re = 0.7. The flow under the black upper plate is visualized by seeding the fluid with light reflecting flakes (1% of the Kalliroscope liquid). The fluid is illuminated by ambient light. Although the pattern is quite irregular, structures that appear tend to have spiral-like forms. The dark spot in the middle corresponds to the centre of a big persistent thoroidal vortex that has dimensions of the whole set-up.

A. Groisman and V. Steinberg. Elastic turbulence in a polymer solution flow. Nature, 405(6782):53-55, 2000

Stability of flows of Giesekus fluid

Mechanical variables:

$$\begin{split} \operatorname{div} \boldsymbol{\nu} &= 0\\ \rho \frac{\mathrm{d}\boldsymbol{\nu}}{\mathrm{d}t} &= \operatorname{div} \mathbb{I}\\ \overline{\mathbb{B}}_{\kappa_{p(t)}}^{\underline{\vee}} &= -\frac{1}{\mathrm{Wi}} \left[\alpha \mathbb{B}_{\kappa_{p(t)}}^{2} + (1 - 2\alpha) \mathbb{B}_{\kappa_{p(t)}} - (1 - \alpha) \mathbb{I} \right] \end{split}$$

Cauchy stress tensor \mathbb{T} :

$$\mathbb{T} = m\mathbb{I} + \frac{2}{\mathrm{Re}}\mathbb{D}_{\delta} + \Xi \Big(\mathbb{B}_{\kappa_{p(t)}}\Big)_{\delta}$$

Upper convected derivative, $\mathbb{L} = \nabla \mathbf{v}$:

$$\bar{\mathbb{A}} =_{\mathrm{def}} \frac{\mathrm{d}\mathbb{A}}{\mathrm{d}t} - \mathbb{L}\mathbb{A} - \mathbb{A}\mathbb{L}^\top \qquad \frac{\mathrm{d}\mathbb{A}}{\mathrm{d}t} =_{\mathrm{def}} \frac{\partial\mathbb{A}}{\partial t} + (\mathbf{v} \bullet \nabla)\mathbb{A}$$

Specific Helmholtz free energy and entropy production

Specific Helmholtz free energy $\psi:$

$$\psi =_{\text{def}} - c_{\text{V}}\theta \left(\ln \left(\frac{\theta}{\theta_{\text{ref}}} \right) - 1 \right) + \frac{\mu}{2\rho} \left(\text{Tr } \mathbb{B}_{\kappa_{p(t)}} - 3 - \ln \det \mathbb{B}_{\kappa_{p(t)}} \right)$$

Entropy production $\xi = \frac{\zeta}{\theta}$:

$$\begin{split} \zeta =_{\mathrm{def}} 2\nu \mathbb{D} : \mathbb{D} \\ &+ \frac{\mu^2}{2\nu_1} \operatorname{Tr} \left[\alpha \mathbb{B}^2_{\kappa_{p(t)}} + (1 - 3\alpha) \mathbb{B}_{\kappa_{p(t)}} + (1 - \alpha) \mathbb{B}^{-1}_{\kappa_{p(t)}} + (3\alpha - 2) \mathbb{I} \right] \\ &+ \kappa \frac{|\nabla \theta|^2}{\theta} \end{split}$$

Giesekus fluid – Lyapunov functional

Pair $\left[\widehat{\boldsymbol{v}}, \widehat{\mathbb{B}_{\kappa_{p(t)}}}\right]$ is a steady solution to the governing equations, we want to show that perturbation vanishes $\left[\widetilde{\boldsymbol{v}}, \widehat{\mathbb{B}_{\kappa_{p(t)}}}\right]$.

$$\mathbf{v} = \hat{\mathbf{v}} + \widetilde{\mathbf{v}}$$
$$\widehat{\mathbb{B}_{\kappa_{p(t)}}} = \widehat{\mathbb{B}_{\kappa_{p(t)}}} + \widetilde{\mathbb{B}_{\kappa_{p(t)}}}$$

Lyapunov functional (energetic part only):

$$\begin{split} \mathcal{V}\left(\left.\widetilde{\boldsymbol{W}}\right\|\left.\widehat{\boldsymbol{W}}\right) &=_{\mathrm{def}} \frac{1}{2} \int_{\Omega} \rho \left|\widetilde{\boldsymbol{v}}\right|^{2} \, \mathrm{dv} \\ &+ \frac{\Xi}{2} \int_{\Omega} \left[-\ln \det \left(\mathbb{I} + \widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1} \widetilde{\mathbb{B}_{\kappa_{p(t)}}}\right) + \mathrm{Tr}\left(\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1} \widetilde{\mathbb{B}_{\kappa_{p(t)}}}\right)\right] \, \mathrm{dv} \end{split}$$

M. Dostalík, V. Průša, and K. Tůma. Finite amplitude stability of internal steady flows of the Giesekus viscoelastic rate-type fluid. Entropy, 21(12), 2019

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Giesekus fluid - time derivative of Lyapunov functional

Time derivative of Lyapunov functional:

$$\frac{\mathrm{d}\mathcal{V}_{\mathrm{neq}}}{\mathrm{d}t}\left(\widetilde{\boldsymbol{W}}\right\|\widehat{\boldsymbol{W}}\right) = -\int_{\Omega} \frac{2}{\mathrm{Re}}\widetilde{\mathbb{D}}:\widetilde{\mathbb{D}}\,\mathrm{dv} - \int_{\Omega} \Xi \widetilde{\mathbb{B}_{\kappa_{p(t)}}}:\widetilde{\mathbb{D}}\,\mathrm{dv} \\ -\int_{\Omega} \widehat{\mathbb{D}}\widetilde{\boldsymbol{v}} \bullet \widetilde{\boldsymbol{v}}\,\mathrm{dv} \\ -\int_{\Omega} \frac{\Xi}{2}\operatorname{Tr}\left[\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}\widehat{\mathbb{B}_{\kappa_{p(t)}}}\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}(\widetilde{\boldsymbol{v}} \bullet \nabla)\widehat{\mathbb{B}_{\kappa_{p(t)}}}\right]\,\mathrm{dv} \\ +\int_{\Omega} \frac{\Xi}{2}\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}:\left(\widetilde{\mathbb{L}}\widehat{\mathbb{B}_{\kappa_{p(t)}}}+\widehat{\mathbb{B}_{\kappa_{p(t)}}}\widetilde{\mathbb{L}}^{\top}\right)\,\mathrm{dv} \\ -\int_{\Omega} \frac{\Xi}{2(1-\alpha)\mathrm{Wi}}\operatorname{Tr}\left[\left(\widehat{\mathbb{B}_{\kappa_{p(t)}}}+\widehat{\mathbb{B}_{\kappa_{p(t)}}}\right)^{-1}\left(\widehat{\mathbb{B}_{\kappa_{p(t)}}}\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}\right)\left(\widehat{\mathbb{B}_{\kappa_{p(t)}}}\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}\right)^{\top}\right] \\ -\int_{\Omega} \alpha \frac{\Xi}{2\mathrm{Wi}}\operatorname{Tr}\left[\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}\widehat{\mathbb{B}_{\kappa_{p(t)}}}^{-1}\right]\,\mathrm{dv}$$

Distance



Bures-Wasserstein distance, symmetric positive definite matrices:

$$\mathsf{dist}_{\mathbb{P}(d),\,\mathrm{BW}}\left(\mathbb{A},\mathbb{B}\right) =_{\mathrm{def}} \left\{\mathsf{Tr}\,\mathbb{A} + \mathsf{Tr}\,\mathbb{B} - 2\,\mathsf{Tr}\left[\left(\mathbb{A}^{\frac{1}{2}}\mathbb{B}\mathbb{A}^{\frac{1}{2}}\right)^{\frac{1}{2}}\right]\right\}^{\frac{1}{2}}$$

Another distance, symmetric positive definite matrices:

$$\mathsf{dist}_{\mathbb{P}(d),\,\delta_2}\left(\mathbb{A},\mathbb{B}
ight) =_{\mathrm{def}} \left| \mathsf{ln}\left(\mathbb{A}^{-rac{1}{2}}\mathbb{B}\mathbb{A}^{-rac{1}{2}}
ight)
ight|$$

Rajendra Bhatia, Tanvi Jain, and Yongdo Lim. On the Bures–Wasserstein distance between positive definite matrices. <u>Expo.</u> <u>Math.</u>, 37(2):165–191, 2019 Rajendra Bhatia. <u>Positive definite matrices</u>. Princeton University Press, Princeton, 2015

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Taylor-Couette flow - problem setting



Governing equations have a steady solution $[\hat{p}, \hat{v}, \widehat{\mathbb{B}_{\kappa_{p(t)}}}, \hat{\theta}]$. One (almost) has an analytical formula for the solution.

Taylor-Couette flow - stability bounds for Giesekus fluid



Figure: Stability bounds for Taylor-Couette flow.



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Conclusion

- Thermodynamic framework for stability analysis of open systems.
- Description of proximity of two different solutions.
- Tested for complex fluid models such as incompressible viscoelastic rate-type fluids.

Collaborators: Miroslav Bulíček, Mark Dostalík, K. R. Rajagopal, Josef Málek, Judith Stein

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Thermodynamics and stability of open systems:

 M. Bulíček, J. Málek, and V. Průša. Thermodynamics and stability of non-equilibrium steady states in open systems. Entropy, 21(7), 2019

Applications:

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