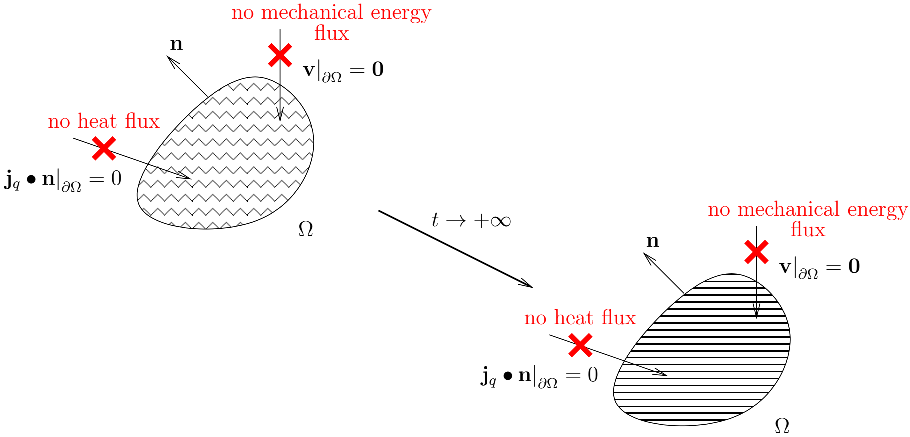
Thermodynamics of viscoelastic rate-type fluids and its implications for stability analysis

Vít Průša
prusv@karlin.mff.cuni.cz

Mathematical Institute, Faculty of Mathematics and Physics, Charles University, Czech Republic

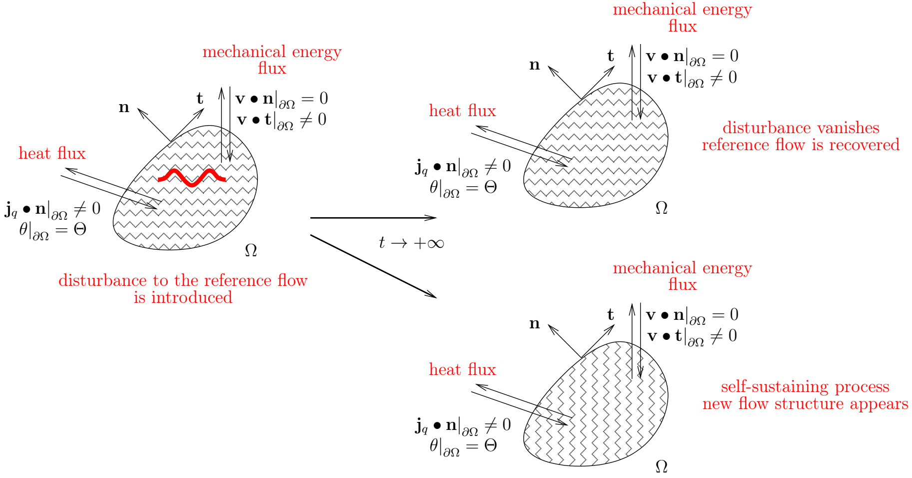
Workshop EXPRO 2020

Themodynamically isolated systems



Example: fluid in a closed vessel, no interaction with surroundings
Expected behaviour: unconditional asymptotic stability of the rest state

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

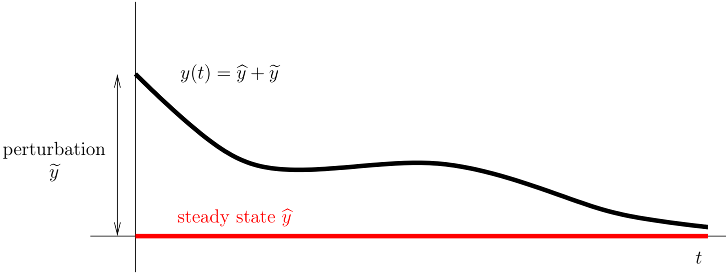
Key question

Can we show that such a behaviour is implied by the corresponding governing equations?

Is it possible to use some thermodynamical concepts?

Concept of stability – clarification

We have two solutions $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ starting from (slightly) different initial conditions. Is it true that $\boldsymbol{s}_1 - \boldsymbol{s}_2 \to 0$ as $t \to +\infty$?



Concept of stability – clarification

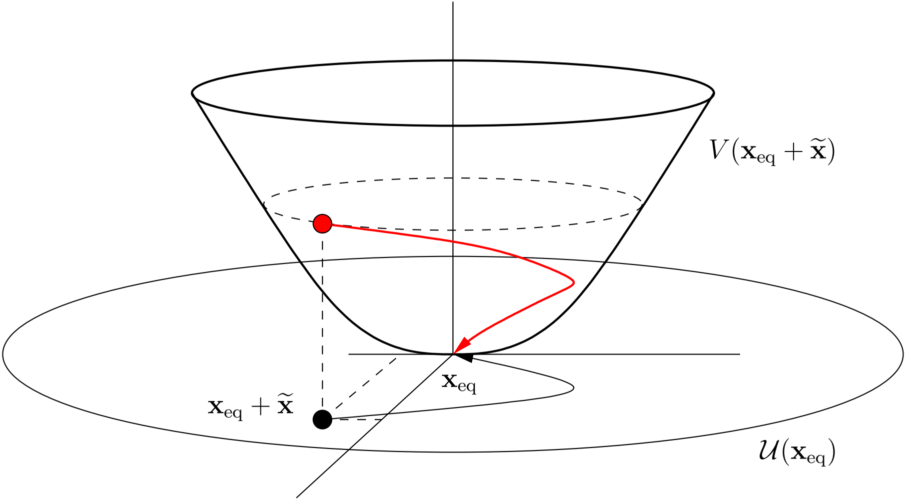
We are not interested in the question or “continuous dependence of thermodynamical processes upon initial state and supply terms”, in the sense of C. M. Dafermos. The second law of thermodynamics and stability. Arch. Ration. Mech. Anal., 70(2):167–179, 1979.

The typical result regarding “continuous dependence of thermodynamical processes upon initial state and supply terms” is just the following:

> *The Gronwall inequality thus gives an estimate*
>
> $$\int_\Omega \eta(u|v)\,\mathrm{d}x \leq \mathrm{e}^{C' t} \int_\Omega \eta(u_0|v_0)\,\mathrm{d}x,$$
>
> *where u_0 , v_0 are the initial data. This is the way uniqueness is proved for Lipschitz solutions, but also stability: if u_0 and v_0 are close to each other, then so are $u(t)$ and $v(t)$. Mind however that the distance between $u(t)$ and $v(t)$ may increase unboundedly as $t \rightarrow +\infty$. We speak of finite-time stability.*

D. Serre and A. F. Vasseur. About the relative entropy method for hyperbolic systems of conservation laws. In A panorama of mathematics: Pure and applied, volume 658 of Contemporary Mathematics, pages 237–248. American Mathematical Society, 2016

Stability – Lyapunov functional



nonlinear (finite amplitude) stability, basin of attraction

Micro-macro model for non-isothermal flows of dilute polymeric fluids

For ρ_{s}, θ_{s}, φ and $\boldsymbol{v}$ solve:

$$\frac{\mathrm{d}\rho_{\mathrm{s}}}{\mathrm{d}t} + \rho_{\mathrm{s}} \mathrm{div}_{\boldsymbol{x}} \boldsymbol{v} = 0$$

$$\rho_{\mathrm{s}} \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \mathrm{div}_{\boldsymbol{x}} \mathbb{T} + \rho_{\mathrm{s}} \boldsymbol{b}$$

$$\frac{\partial \varphi}{\partial t} + \mathrm{div}_{\boldsymbol{x}} \left(\boldsymbol{v}\varphi - \frac{k_{\mathrm{B}} \theta_{\mathrm{s}}}{2\zeta} \nabla_{\boldsymbol{x}} \varphi \right) + \mathrm{div}_{\boldsymbol{q}} \left((\nabla_{\boldsymbol{x}} \boldsymbol{v}) \boldsymbol{q} \varphi - \frac{2\boldsymbol{F}}{\zeta} \varphi - \frac{2k_{\mathrm{B}} \theta_{\mathrm{s}}}{\zeta} \nabla_{\boldsymbol{q}} \varphi \right) = 0$$

$$\begin{aligned} \rho_{\mathrm{s}} c_{\mathrm{V},\mathrm{s}} \frac{\mathrm{d}\theta_{\mathrm{s}}}{\mathrm{d}t} &= -\theta_{\mathrm{s}} \frac{\partial p_{\mathrm{th},\mathrm{s}}}{\partial \theta_{\mathrm{s}}} \mathrm{div}_{\boldsymbol{x}} \boldsymbol{v} + \mathrm{div}_{\boldsymbol{x}} \left(\kappa \nabla_{\boldsymbol{x}} \theta_{\mathrm{s}} \right) + \lambda \left(\mathrm{div}_{\boldsymbol{x}} \boldsymbol{v} \right)^2 + 2\nu \mathbb{D} : \mathbb{D} - 2k_{\mathrm{B}} \theta_{\mathrm{s}} n_{\mathrm{p}} \mathrm{div}_{\boldsymbol{x}} \boldsymbol{v} \\ &+ \left[\int_D \left(\nabla_{\boldsymbol{q}} \frac{\theta_{\mathrm{s}}}{\theta_{\mathrm{ref}}} U_\eta \right) \otimes \boldsymbol{q} \varphi \, \mathrm{d}\boldsymbol{q} \right] : \mathbb{D} + \frac{2}{\zeta} \int_D \left(\nabla_{\boldsymbol{q}} U_e \right) \bullet \nabla_{\boldsymbol{q}} \left(U_e + \frac{\theta_{\mathrm{s}}}{\theta_{\mathrm{ref}}} U_\eta \right) \mathrm{d}\boldsymbol{q} - \frac{2k_{\mathrm{B}} \theta_{\mathrm{s}}}{\zeta} \int_D \left[\Delta_{\boldsymbol{q}} U_e \right] \varphi \, \mathrm{d}\boldsymbol{q} \end{aligned}$$

Spring force $\boldsymbol{F}$ potentials U_e and U_η:

$$\boldsymbol{F} =_{\mathrm{def}} \nabla_{\boldsymbol{q}} \left[U_e \left(\frac{1}{2} \left| \frac{\boldsymbol{q}}{q_{\mathrm{ref}}} \right|^2 \right) + \frac{\theta_{\mathrm{s}}}{\theta_{\mathrm{ref}}} U_\eta \left(\frac{1}{2} \left| \frac{\boldsymbol{q}}{q_{\mathrm{ref}}} \right|^2 \right) \right]$$

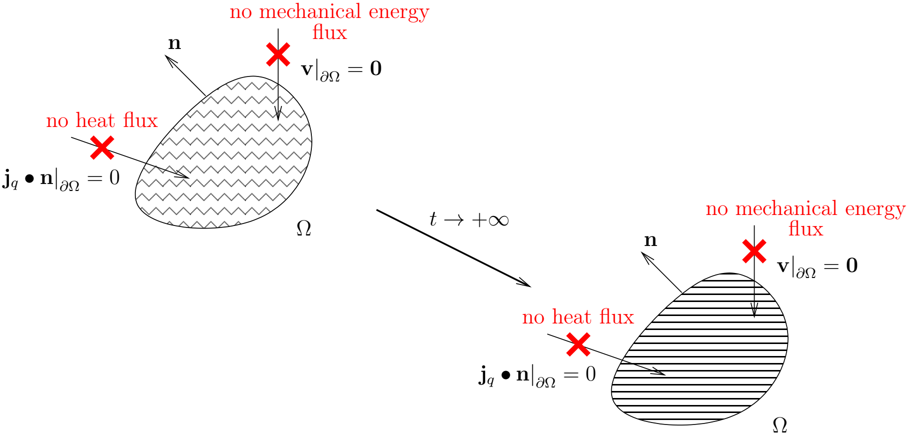
Cauchy stress tensor $\mathbb{T}$:

$$\mathbb{T} =_{\mathrm{def}} -p_{\mathrm{th},\mathrm{s}} \mathbb{I} + \lambda \left(\mathrm{div}_{\boldsymbol{x}} \boldsymbol{v} \right) \mathbb{I} + 2\nu \mathbb{D} - 2k_{\mathrm{B}} \theta_{\mathrm{s}} n_{\mathrm{p}} \mathbb{I} + \int_D \boldsymbol{F} \otimes \boldsymbol{q} \varphi \, \mathrm{d}\boldsymbol{q} \qquad p_{\mathrm{th},\mathrm{s}} =_{\mathrm{def}} \frac{c_{\mathrm{V},\mathrm{s}} \left(\gamma - 1 \right) \rho_{\mathrm{s}} \theta_{\mathrm{s}}}{1 - b\rho_{\mathrm{s}}} - p_\infty$$

M. Dostalík, J. Málek, V. Průša, and E. Süli. A simple construction of a thermodynamically consistent mathematical model for non-isothermal flows of dilute compressible polymeric fluids. Fluids, 5(3):133, 2020

Lyapunov functional – easier said than done

Themodynamically isolated systems



Example: fluid in a closed vessel, no interaction with surroundings
Expected behaviour: unconditional asymptotic stability of the rest state

Die Energie der Welt ist konstant; die Entropie der Welt strebt einem Maximum zu!

R. Clausius. Ueber verschiedene für die Anwendung bequeme Formen der Hauptgleichungen der mechanischen Wärmetheorie. Annalen der Physik und Chemie, 125(7):353–400, 1865

Pierre Duhem. Traité d'Énergetique ou Thermodynamique Générale. Paris, 1911; Bernard D. Coleman. On the stability of equilibrium states of general fluids. Arch. Ration. Mech. Anal., 36(1):1–32, 1970; Morton E. Gurtin. Thermodynamics and the energy criterion for stability. Arch. Ration. Mech. Anal., 52:93–103, 1973; Morton E. Gurtin. Thermodynamics and stability. Arch. Ration. Mech. Anal., 59(1):63–96, 1975

Lyapunov-type functional – isolated systems

Candidate for Lyapunov-type functional:

$$\mathcal{V}_{\mathrm{meq}} =_{\mathrm{def}} - \underbrace{S}_{\text{entropy}} + \lambda_1 \underbrace{\left(E_{\mathrm{tot}} - \widehat{E_{\mathrm{tot}}}\right)}_{\text{constant energy}} + \lambda_2 \underbrace{\int_{\Omega} \left(\rho_{\mathrm{s}} - \widehat{\rho_{\mathrm{s}}}\right) \, \mathrm{dv}}_{\text{constant mass}}$$
$$+ \lambda_3 \underbrace{\int_{\Omega} \left(n_{\mathrm{p}} - \widehat{n_{\mathrm{p}}}\right) \, \mathrm{dv}}_{\text{constant number of polymers}}$$

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

Functional $\mathcal{V}_{\mathrm{meq}}$ decreases along trajectories:

$$\frac{\mathrm{d}\mathcal{V}_{\mathrm{meq}}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \left\{ - \underbrace{S}_{\text{entropy}} + \lambda_1 \underbrace{\left(E_{\mathrm{tot}} - \widehat{E_{\mathrm{tot}}}\right)}_{\text{constant energy}} + \lambda_2 \underbrace{\int_{\Omega} \left(\rho_{\mathrm{s}} - \widehat{\rho_{\mathrm{s}}}\right) \, \mathrm{dv}}_{\text{constant mass}} + \lambda_3 \underbrace{\int_{\Omega} \left(n_{\mathrm{p}} - \widehat{n_{\mathrm{p}}}\right) \, \mathrm{dv}}_{\text{constant number of polymers}} \right\} = - \frac{\mathrm{d}S}{\mathrm{d}t}$$
$$= - \int_{\Omega} \xi \, \mathrm{dv} \leq 0$$

Micro-macro model for non-isothermal flows of dilute polymeric fluids

$$\boldsymbol{v} = \widehat{\boldsymbol{v}} + \widetilde{\boldsymbol{v}} \qquad \rho_{\mathrm{s}} = \widehat{\rho}_{\mathrm{s}} + \widetilde{\rho}_{\mathrm{s}} \qquad \theta_{\mathrm{s}} = \widehat{\theta}_{\mathrm{s}} + \widetilde{\theta}_{\mathrm{s}} \qquad \varphi = \widehat{\varphi} + \widetilde{\varphi}$$

$$\begin{aligned}
\mathcal{V}_{\mathrm{meq}} = \int_{\Omega} \frac{1}{2} \rho_{\mathrm{s}} \left|\boldsymbol{v}\right|^2 \,\mathrm{dv} + \int_{\Omega} \rho_{\mathrm{s}} c_{\mathrm{V,s}} \widehat{\theta}_{\mathrm{s}} \left[\frac{\theta_{\mathrm{s}}}{\widehat{\theta}_{\mathrm{s}}} - 1 - \ln \left(\frac{\theta_{\mathrm{s}}}{\widehat{\theta}_{\mathrm{s}}} \right) \right] \mathrm{dv} \\
+ \int_{\Omega} c_{\mathrm{V,s}} (\gamma - 1) \widehat{\theta}_{\mathrm{s}} \left[\rho_{\mathrm{s}} \ln \left(\frac{\rho_{\mathrm{s}}}{\widehat{\rho}_{\mathrm{s}}} \frac{1 - b\widehat{\rho}_{\mathrm{s}}}{1 - b\rho_{\mathrm{s}}} \right) - \frac{\rho_{\mathrm{s}} - \widehat{\rho}_{\mathrm{s}}}{1 - b\widehat{\rho}_{\mathrm{s}}} \right] \mathrm{dv} \\
+ k_{\mathrm{B}} \widehat{\theta}_{\mathrm{s}} \int_{\Omega} \left(\int_{D} M_{n_{\mathrm{p}}, \widehat{\theta}_{\mathrm{s}}} \left[\frac{\varphi}{M_{n_{\mathrm{p}}, \widehat{\theta}_{\mathrm{s}}}} \ln \left(\frac{\varphi}{M_{n_{\mathrm{p}}, \widehat{\theta}_{\mathrm{s}}}} \right) - \frac{\varphi}{M_{n_{\mathrm{p}}, \widehat{\theta}_{\mathrm{s}}}} + 1 \right] \mathrm{d}\boldsymbol{q} \right) \mathrm{dv} \\
+ k_{\mathrm{B}} \widehat{\theta}_{\mathrm{s}} \int_{\Omega} \widehat{n}_{\mathrm{p}} \left[\frac{n_{\mathrm{p}}}{\widehat{n}_{\mathrm{p}}} \ln \left(\frac{n_{\mathrm{p}}}{\widehat{n}_{\mathrm{p}}} \right) - \frac{n_{\mathrm{p}}}{\widehat{n}_{\mathrm{p}}} + 1 \right] \mathrm{dv}
\end{aligned}$$

M. Dostalík, J. Málek, V. Průša, and E. Süli. A simple construction of a thermodynamically consistent mathematical model for non-isothermal flows of dilute compressible polymeric fluids. Fluids, 5(3):133, 2020

Same calculation can be done whenever one knows the entropy production and the specific Helmholtz free energy.

Each material is (in a given class of processes) characterised by:

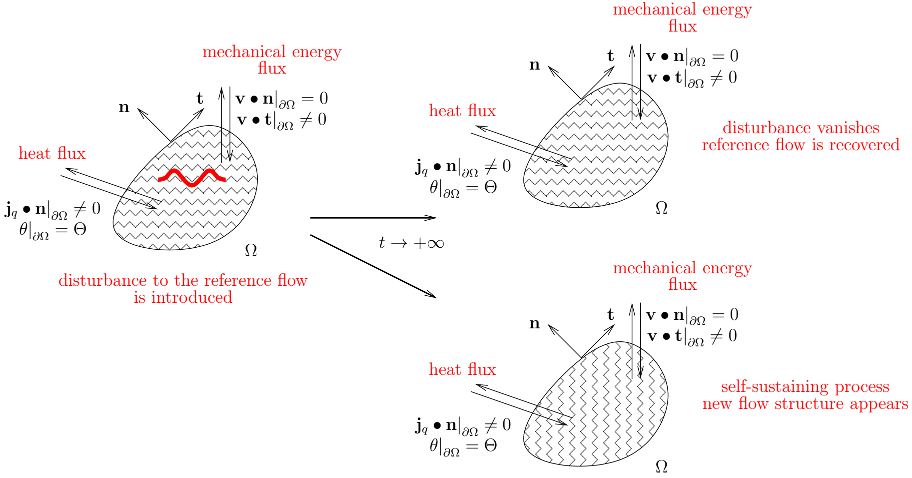
1. Energy storage ability. (Give a formula for the specific internal energy e or for the specific Helmholtz free energy ψ.)
2. Entropy production ability. (Give a formula for entropy production ξ.)

The constitutive relations between tensorial and vectorial quantities follow form the specification of the two scalar quantities.

K. R. Rajagopal and A. R. Srinivasa. On thermomechanical restrictions of continua. Proc. R. Soc. Lond., Ser. A, Math. Phys. Eng. Sci., 460(2042):631–651, 2004

J. Málek and V. Průša. Derivation of equations for continuum mechanics and thermodynamics of fluids. In Y. Giga and A. Novotný, editors, Handbook of Mathematical Analysis in Mechanics of Viscous Fluids, pages 3–72. Springer, 2018
M. Dostalík, V. Průša, and T. Skřivan. On diffusive variants of some classical viscoelastic rate-type models. AIP Conference Proceedings, 2107(1):020002, 2019

Thermodynamically open systems



mechanical energy flux

$\mathbf{n}$ $\mathbf{t}$

$\mathbf{v} \bullet \mathbf{n}|_{\partial\Omega} = 0$

$\mathbf{v} \bullet \mathbf{t}|_{\partial\Omega} \neq 0$

heat flux

$\mathbf{j}_q \bullet \mathbf{n}|_{\partial\Omega} \neq 0$

$\theta|_{\partial\Omega} = \Theta$

Ω

disturbance to the reference flow is introduced

$t \to +\infty$

mechanical energy flux

$\mathbf{n}$ $\mathbf{t}$

$\mathbf{v} \bullet \mathbf{n}|_{\partial\Omega} = 0$

$\mathbf{v} \bullet \mathbf{t}|_{\partial\Omega} \neq 0$

heat flux

$\mathbf{j}_q \bullet \mathbf{n}|_{\partial\Omega} \neq 0$

$\theta|_{\partial\Omega} = \Theta$

Ω

disturbance vanishes
reference flow is recovered

mechanical energy flux

$\mathbf{n}$ $\mathbf{t}$

$\mathbf{v} \bullet \mathbf{n}|_{\partial\Omega} = 0$

$\mathbf{v} \bullet \mathbf{t}|_{\partial\Omega} \neq 0$

heat flux

$\mathbf{j}_q \bullet \mathbf{n}|_{\partial\Omega} \neq 0$

$\theta|_{\partial\Omega} = \Theta$

Ω

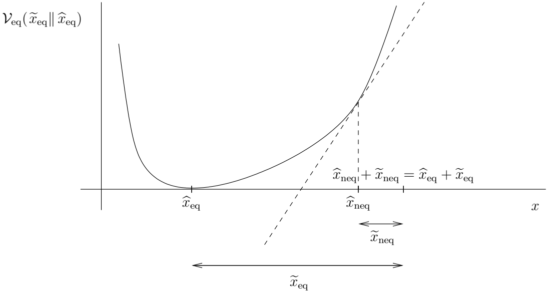
self-sustaining process
new flow structure appears

Entropy in nondecreasing function – NO
Energy is constant – NO

Fluxes through boundary

We have fluxes through the boundary. We have no control on fluxes.
Everything is lost. Really?

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. Entropy, 21(7), 2019

Lyapunov-type functional

Lyapunov-type functional for thermodynamically open systems:

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

$$\mathcal{S}_{\widehat{\theta}}(\,\widetilde{\boldsymbol{W}}\|\,\widehat{\boldsymbol{W}}) =_{\mathrm{def}} S_{\widehat{\theta}}\left(\widehat{\boldsymbol{W}}+\widetilde{\boldsymbol{W}}\right) - S_{\widehat{\theta}}\left(\widehat{\boldsymbol{W}}\right) - \mathrm{D}_{\boldsymbol{W}} S_{\widehat{\theta}}\left(\boldsymbol{W}\right)\Big|_{\boldsymbol{W}=\widehat{\boldsymbol{W}}}\left[\widetilde{\boldsymbol{W}}\right]$$

$$\mathcal{E}(\,\widetilde{\boldsymbol{W}}\|\,\widehat{\boldsymbol{W}}) =_{\mathrm{def}} E_{\mathrm{tot}}\left(\widehat{\boldsymbol{W}}+\widetilde{\boldsymbol{W}}\right) - E_{\mathrm{tot}}\left(\widehat{\boldsymbol{W}}\right) - \mathrm{D}_{\boldsymbol{W}} E_{\mathrm{tot}}\left(\boldsymbol{W}\right)\big|_{\boldsymbol{W}=\widehat{\boldsymbol{W}}}\left[\widetilde{\boldsymbol{W}}\right]$$

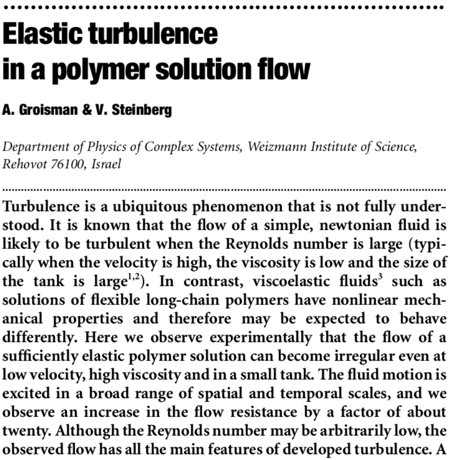
$$S_{\widehat{\theta}}\left(\boldsymbol{W}\right) =_{\mathrm{def}} \int_{\Omega} \rho\widehat{\theta}\eta(\boldsymbol{W})\,\mathrm{dv}$$

$$E_{\mathrm{tot}}\left(\boldsymbol{W}\right) =_{\mathrm{def}} \int_{\Omega} \rho e(\boldsymbol{W})\,\mathrm{dv}$$

Disclaimer

Let us assume that there exists a classical solution to the corresponding governing equations.

Elastic turbulence



Elastic turbulence in a polymer solution flow

A. Groisman & V. Steinberg

Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel

Turbulence is a ubiquitous phenomenon that is not fully understood. It is known that the flow of a simple, newtonian fluid is likely to be turbulent when the Reynolds number is large (typically when the velocity is high, the viscosity is low and the size of the tank is large[1,2]). In contrast, viscoelastic fluids[3] such as solutions of flexible long-chain polymers have nonlinear mechanical properties and therefore may be expected to behave differently. Here we observe experimentally that the flow of a sufficiently elastic polymer solution can become irregular even at low velocity, high viscosity and in a small tank. The fluid motion is excited in a broad range of spatial and temporal scales, and we observe an increase in the flow resistance by a factor of about twenty. Although the Reynolds number may be arbitrarily low, the observed flow has all the main features of developed turbulence. A

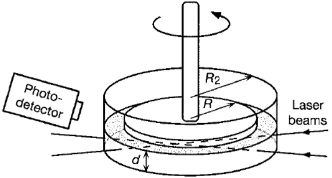


Figure 1 The experimental set-up. A stationary cylindrical cup with a plain bottom (the lower plate) is concentric with the rotating upper plate, which is attached to the shaft of a commercial rheometer. The radii of the upper and the lower plates are $R = 38$ mm and $R_2 = 43.6$ mm, respectively. The liquid is filled until a level d of 10 mm unless otherwise stated. The upper plate just touches the surface of the liquid. A special cover is used to minimize evaporation of the liquid. We used a solution of 65% saccharose and 1% NaCl in water, viscosity $\eta_s = 0.324$ Pa s, as a solvent for the polymer. We added polyacrylamide ($M_w = 18{,}000{,}000$; Polysciences) at a concentration of 80 p.p.m. by weight. The solution viscosity was $\eta = 0.424$ Pa s at $\dot{\gamma} = 1\,\mathrm{s}^{-1}$. The relaxation time, λ, estimated from the phase shift between the stress and the shear rate in oscillatory tests, was 3.4 s. The temperature is stabilized at 12 °C by circulating water under the steel lower plate. The walls of the cup are transparent which allows Doppler velocimeter measurements by collecting light scattered from the crossing point of two horizontal laser beams. In experiments where the flow has to be viewed from below, the lower plate is made from plexiglass and a mirror tilted by 45° is placed under the lower plate. The flow patterns are then captured by a CCD camera at the side and the temperature is stabilized by circulating air in a closed box.

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

Elastic turbulence

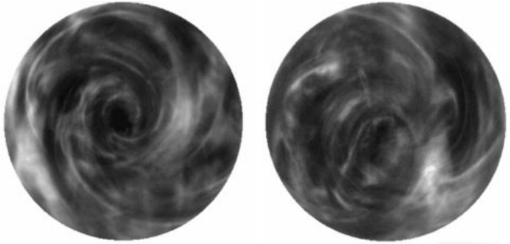


Figure 3 Two snapshots of the flow at Wi = 13, Re = 0.7. The flow under the black upper plate is visualized by seeding the fluid with light reflecting flakes (1% of the Kalliroscope liquid). The fluid is illuminated by ambient light. Although the pattern is quite irregular, structures that appear tend 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:

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

Cauchy stress tensor $\mathbb{T}$:

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

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

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

Specific Helmholtz free energy and entropy production

Specific Helmholtz free energy ψ:

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

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

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

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 $\left[\widetilde{\boldsymbol{v}}, \widetilde{\mathbb{B}_{\kappa_{p(t)}}}\right]$.

$$\boldsymbol{v} = \widehat{\boldsymbol{v}} + \widetilde{\boldsymbol{v}}$$

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

Lyapunov functional (energetic part only):

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

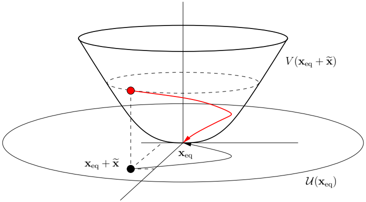
M. Dostalík, V. Průša, and K. Tůma. Finite amplitude stability of internal steady flows of the Giesekus viscoelastic rate-type fluid. Entropy, 21(12), 2019

Giesekus fluid – time derivative of Lyapunov functional

Time derivative of Lyapunov functional:

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

Distance



Bures–Wasserstein distance, symmetric positive definite matrices:

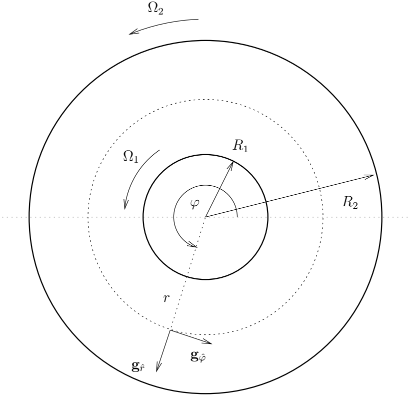
$$\mathrm{dist}_{\mathbb{P}(d),\,\mathrm{BW}}(\mathbb{A},\mathbb{B}) =_{\mathrm{def}} \left\{ \operatorname{Tr}\mathbb{A} + \operatorname{Tr}\mathbb{B} - 2\operatorname{Tr}\left[\left(\mathbb{A}^{\frac{1}{2}}\mathbb{B}\mathbb{A}^{\frac{1}{2}}\right)^{\frac{1}{2}}\right]\right\}^{\frac{1}{2}}$$

Another distance, symmetric positive definite matrices:

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

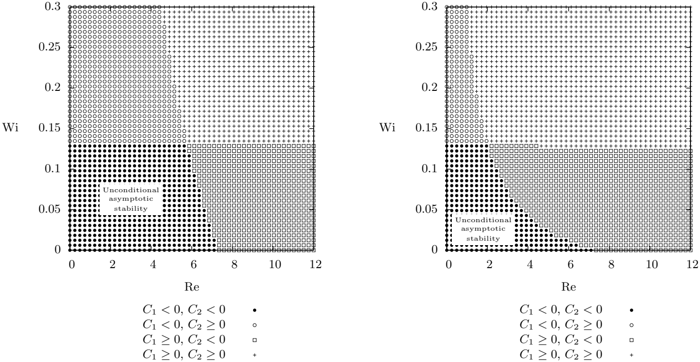
Rajendra Bhatia, Tanvi Jain, and Yongdo Lim. On the Bures–Wasserstein distance between positive definite matrices. Expo. Math., 37(2):165–191, 2019
Rajendra Bhatia. Positive definite matrices. Princeton University Press, Princeton, 2015

Taylor–Couette flow – problem setting



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

Taylor–Couette flow – stability bounds for Giesekus fluid

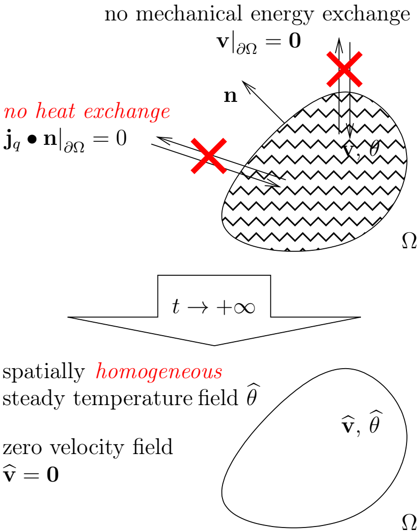


(a) Shear modulus $\Xi = 0.1$. (b) Shear modulus $\Xi = 1$.

Figure: Stability bounds for Taylor–Couette flow.

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

Isolated vessel



no mechanical energy exchange
$\mathbf{v}|_{\partial\Omega} = \mathbf{0}$

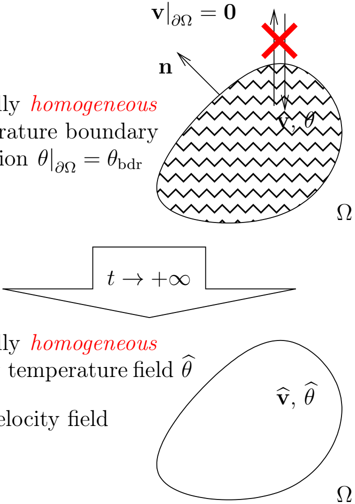
no heat exchange
$\mathbf{j}_q \bullet \mathbf{n}|_{\partial\Omega} = 0$

$t \to +\infty$

spatially *homogeneous*
steady temperature field $\widehat{\theta}$

zero velocity field
$\widehat{\mathbf{v}} = \mathbf{0}$

Thermal bath



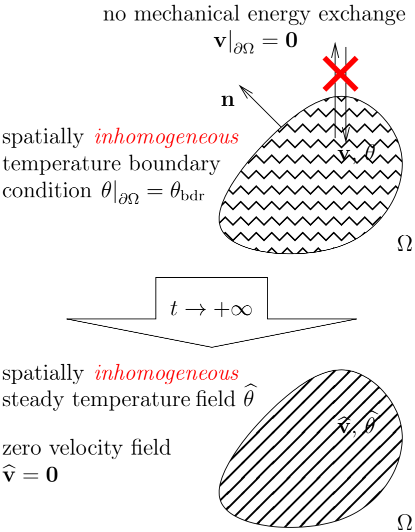
no mechanical energy exchange
$\mathbf{v}|_{\partial\Omega} = \mathbf{0}$

spatially *homogeneous*
temperature boundary
condition $\theta|_{\partial\Omega} = \theta_{\mathrm{bdr}}$

spatially *homogeneous*
steady temperature field $\widehat{\theta}$

zero velocity field
$\widehat{\mathbf{v}} = \mathbf{0}$

Spatially non-uniform wall temperature



no mechanical energy exchange
$\mathbf{v}|_{\partial\Omega} = \mathbf{0}$

spatially *inhomogeneous*
temperature boundary
condition $\theta|_{\partial\Omega} = \theta_{\mathrm{bdr}}$

$t \to +\infty$

spatially *inhomogeneous*
steady temperature field $\widehat{\theta}$

zero velocity field
$\widehat{\mathbf{v}} = \mathbf{0}$

Incompressible Navier–Stokes–Fourier fluid

Mechanical quantities:

$$\begin{aligned} \operatorname{div} \boldsymbol{v} &= 0 \\ \rho \frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} &= \operatorname{div} \mathbb{T} + \rho \boldsymbol{b} \end{aligned}$$

Cauchy stress tensor:

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

Temperature evolution equation:

$$\rho c_{\mathrm{V}} \frac{\mathrm{d}\theta}{\mathrm{d}t} = 2\nu\mathbb{D} : \mathbb{D} + \operatorname{div}\left(\kappa \nabla \theta\right)$$

Boundary conditions:

$$\begin{aligned} \boldsymbol{v}\big|_{\partial\Omega} &= \boldsymbol{0} \\ \theta\big|_{\partial\Omega} &= \theta_{\mathrm{bdr}} \end{aligned}$$

Expected result

Notation:

$$\boldsymbol{v} = \widehat{\boldsymbol{v}} + \widetilde{\boldsymbol{v}}$$

$$\theta = \widehat{\theta} + \widetilde{\theta}$$

Steady state:

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

$$\widehat{\theta} = \text{solution to steady heat equation}$$

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

$$0 = \operatorname{div}\left(\kappa \nabla \widehat{\theta}\right)$$

$$\left.\widehat{\theta}\right|_{\partial\Omega} = \theta_{\mathrm{bdr}}$$

Arbitrary perturbation should decay. If you are not able to explain this, you are doomed.

Decay of kinetic energy

Evolution equation for the velocity:

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

Evolution equation for the net kinetic energy:

$$\frac{\mathrm{d}}{\mathrm{d} t} \int_{\Omega} \frac{1}{2} \rho \left| \boldsymbol{v} \right|^2 \, \mathrm{dv} = - \int_{\Omega} 2 \mu \mathbb{D} : \mathbb{D} \, \mathrm{dv}$$

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

Main issues

Temperature evolution equation:

$$\rho c_{\mathrm{V}} \frac{\mathrm{d}\theta}{\mathrm{d}t} = 2\nu \mathbb{D} : \mathbb{D} + \operatorname{div}\left(\kappa \nabla \theta\right)$$

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 $\boldsymbol{v}$ is small, it is not necessarily true that $\mathbb{D}$ is small.

Dissipative heating:

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

Do not touch the dissipation. Use only its positivity!

Y. Kagei, M. Růžička, and G. Thäter. Natural convection with dissipative heating. Commun. Math. Phys., 214:287–313, 2000

Main issues

How to measure the distance form the steady state?

$$\rho c_{\mathrm{V,ref}} \frac{\mathrm{d}}{\mathrm{d}t} \int_{\Omega} \widetilde{\theta}^2 \,\mathrm{dv} = - \int_{\Omega} \kappa_{\mathrm{ref}} \nabla \widetilde{\theta} \bullet \nabla \widetilde{\theta} \,\mathrm{dv} + \int_{\Omega} 2\mu \widetilde{\mathbb{D}} : \widetilde{\mathbb{D}} \, \widetilde{\theta} \,\mathrm{dv} \\ + \int_{\Omega} \rho c_{\mathrm{V,ref}} \left(\widetilde{\boldsymbol{v}} \bullet \nabla \widehat{\theta} \right) \widetilde{\theta} \,\mathrm{dv}$$

Result

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

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

Lemma (Decay of integrable functions)

Let $y : [0, +\infty) \mapsto \mathbb{R}^+$ *be a continuous non-negative function such that*

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

where C_1 *is a constant. Moreover, let for all* $s, t \in [0, +\infty)$, $t > s$,

$$y(t) - y(s) \leq \int_{\tau=s}^{t} f(y(\tau)) \, \mathrm{d}\tau + \int_{\tau=s}^{t} h(\tau) \, \mathrm{d}\tau$$

hold, where f *is a nondecreasing function from* $\mathbb{R}^+$ *to* $\mathbb{R}^+$ *and* h *is a non-negative function such that* $\int_{\tau=0}^{+\infty} h(\tau) \, \mathrm{d}\tau \leq C_2$, *where* C_2 *is a constant. Then*

$$\lim_{t \to +\infty} y(t) = 0.$$

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

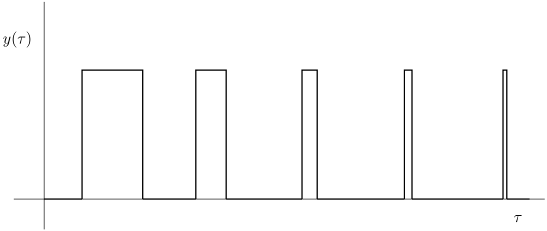
P. Krejčí and J. Sprekels. Weak stabilization of solutions to PDEs with hysteresis in thermovisco-elastoplasticity. In R. P. Agarwal, F. Neuman, and J. Vosmansky, editors, Proceedings of Equadiff 9, pages 81–96, Brno, 1998. Masaryk University

We know:

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

We want:

$$\lim_{t\to+\infty} y(t) = 0$$



We need:

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

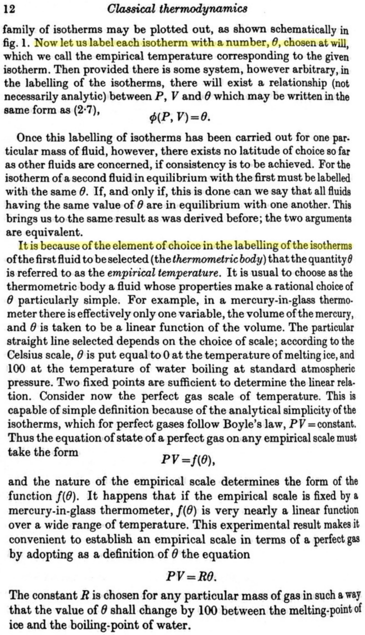
Candidate for Lyapunov functional

Convenient measure for the size of perturbation:

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

Time derivative:

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



12 *Classical thermodynamics*

family of isotherms may be plotted out, as shown schematically in fig. 1. Now let us label each isotherm with a number, θ, 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 isotherms, there will exist a relationship (not necessarily analytic) between P, V and θ which may be written in the same form as (2·7),

$$\phi(P, V) = \theta.$$

Once this labelling of isotherms has been carried out for one particular mass of fluid, however, there exists no latitude of choice so far as other fluids are concerned, if consistency is to be achieved. For the isotherm 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, $PV = \text{constant}$. 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. Elements of classical thermodynamics for advanced students of physics. Cambridge University Press, Cambridge, 1964

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

Choose a different temperature scale

Alternative temperature scale:

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

Corresponding candidate for Lyapunov functional:

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

Choose a different temperature scale – formal argument

Pointwise evolution equation, f is a given function:

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

$$
\eta_{\mathrm{diff}} =_{\mathrm{def}} c_{\mathrm{V,ref}} \ln\left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}}\right)
$$

Result – unconditional stability

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

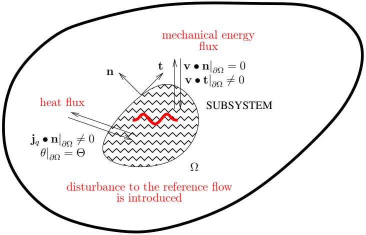
$$\int_\Omega \rho c_{\mathrm{V,ref}} \widehat{\theta} \left[\frac{1}{n} \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right)^n - \frac{1}{m} \left(1 + \frac{\widetilde{\theta}}{\widehat{\theta}} \right)^m + \frac{n-m}{mn} \right] \mathrm{dv} \xrightarrow{t \to +\infty} 0$$

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. Math. Comput. Simulat., 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. Contin. Mech. Thermodyn., 2020. In press

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.



Thank you for your attention.

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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:

- 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. Math. Comput. Simulat., 2020. In press
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