#### Derivation of Equations for Continuum Mechanics and Thermodynamics of Fluids

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May 20 2025

We discuss

J. Málek and V. Průša. "Derivation of Equations for Continuum Mechanics and Thermodynamics of Fluids". In: *Handbook of Mathematical Analysis in Mechanics of Viscous Fluids*. Ed. by Y. Giga and A. Novotný. Cham: Springer International Publishing, 2018, pp. 3–72. ISBN: 978-3-319-13344-7. DOI: 10.1007/978-3-319-13344-7\_1.

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The presentation is also influenced by

- I. Müller. Thermodynamics. Interaction of Mechanics and Mathematics Series. Pitman, 1985. ISBN: 9780273085775.
- K. R. Rajagopal and A. R. Srinivasa. "On thermomechanical restrictions of continua". In: Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences 460.2042 (2004), pp. 631–651. DOI: 10.1098/rspa.2002.1111.
- D. Bothe and W. Dreyer. "Continuum thermodynamics of chemically reacting fluid mixtures". In: Acta Mechanica 226.6 (2015), pp. 1757–1805. DOI: 10.1007/s00707-014-1275-1.

### All models in continuum mechanics start from

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Universal relations that hold for any continuous medium.

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#### So we must close our model with

### Constitutive relations

Relations specific to a given material within a certain range of conditions describing its response to stimuli.

# Boundary conditions

Relations describing the mechanical and thermodynamic interaction between our system of interest and the rest of the universe.

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Derive the balance laws of continuum mechanics.

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# Objective 2

Explain how all constitutive relations can be derived from knowledge of two scalar functions:

the internal energy and the entropy production.

This is tantamount to the proposition that material behaviour is fully characterised by the way it stores energy and produces entropy.

# Section 1

Balance laws

Our primary goal is the determination of

 $\begin{array}{ll} {\rm density} & \rho \\ {\rm velocity} & \vec{v} \\ {\rm temperature} & \theta \end{array}$ 

for all particles in a fluid and for all times.

### Balance of mass states

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \nabla \cdot v = 0,$$

 $\frac{\mathrm{d}\phi}{\mathrm{d}t}\coloneqq \frac{\partial\phi}{\partial t} + (\vec{v}\cdot\nabla)\phi$ 

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$$\frac{\mathrm{d}\phi}{\mathrm{d}t} \coloneqq \frac{\partial\phi}{\partial t} + (\vec{v}\cdot\nabla)\phi$$

is the material derivative.

No constitutive relations are required for this equation.

Balance of (linear) momentum states

$$\rho \frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = \nabla \cdot \mathbb{T} + \rho \vec{b},$$

where  $\mathbb{T}$  is the Cauchy stress tensor and b the (specified) body force density.

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The stress  $\mathbb{T}$  is a key concept in continuum mechanics: it characterises forces on a volume V(t) of the body due to the resistance of the material surrounding V(t).

We need our first constitutive relation, expressing

$$\mathbb{T} = \mathbb{T}(\rho, \vec{v}, \theta) \text{ or } \mathbb{G}(\mathbb{T}, \rho, \vec{v}, \theta) = 0.$$

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This is a deep fact. The stress tensor takes in normals and returns forces. Why does the non-polar nature of the fluid mean that there is a dual relationship between forces and normals?

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We can therefore expect analogues of key ideas like internal energy and entropy to arise.

By manipulating the balance of total energy, we derive a balance equation for internal energy:

$$\rho \frac{\mathrm{d}e}{\mathrm{d}t} = \mathbb{T} : \mathbb{D}(\vec{v}) - \nabla \cdot \vec{j}_q$$

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- e specific internal energy
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The heat flux quantifies nonmechanical energy exchange (transferred heat) between a volume V(t) and its surroundings.

We need constitutive relations for e and  $\vec{j}_q.$  For a simple ideal gas,

$$e = c_V \theta$$

where  $c_V > 0$  is the (constant) latent heat at constant volume.

# Section 2

Constitutive relations

Experience with viscous fluids shows that the constitutive relations have the general forms

$$\begin{split} \mathbb{T} &= \mathbb{T}(\rho, \vec{v}, \theta) \text{ or } \mathbb{G}(\mathbb{T}, \rho, \vec{v}, \theta) = 0, \\ e &= e(\rho, \vec{v}, \theta) \text{ or } \mathbb{E}(e, \rho, \vec{v}, \theta) = 0, \\ \vec{j}_q &= \vec{j}_q(\rho, \vec{v}, \theta) \text{ or } \mathbb{J}(\vec{j}_q, \rho, \vec{v}, \theta) = 0. \end{split}$$

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For this reason thermodynamicists are making every effort to get to know these functions better. They attempt to restrict the generality of these functions ... The main tools of constitutive theory for restricting the constitutive functions are universal physical principles which have been abstracted from long experience with bodies of arbitrary material. The most important ones among such principles are the **principle of material frame indifference**, the **entropy principle** and **thermodynamic stability**.

## Subsection 1

Entropy

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These will both be consequences of the *entropy principle*.

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For many fluids, the entropy flux is given by

$$\vec{\Phi} = \frac{\vec{j}_q}{\theta}$$

which we adopt henceforth. This also tells you the boundary conditions.

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Taking the material derivative of this yields

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Defining the temperature and pressure as

$$\theta \coloneqq \frac{\partial e}{\partial \eta}, \quad p \coloneqq \rho^2 \frac{\partial e}{\partial \rho}$$

isolates an expression for the material derivative of entropy:

$$\frac{\mathrm{d}\eta}{\mathrm{d}t} = \theta^{-1} \left[ \frac{\mathrm{d}e}{\mathrm{d}t} - \frac{p}{\rho^2} \frac{\mathrm{d}\rho}{\mathrm{d}t} \right]$$

Substituting the balance laws for density and energy, and algebraic manipulation, finally yields

$$\theta \xi \coloneqq \operatorname{dev}(\mathbb{T}) : \operatorname{dev}(\mathbb{D}(\vec{v})) + (m+p)\nabla \cdot \vec{v} - \vec{j}_q \cdot (\nabla \theta/\theta),$$

for fluids, where

$$\operatorname{dev} \mathbb{S} \coloneqq \mathbb{S} - (1/d) \operatorname{tr}(\mathbb{S})I$$
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Let us now state a more refined version of the second law:

### Second law of thermodynamics (summarised from Bothe & Dreyer)

The entropy production  $\xi$  is a sum of binary products, each an independent mechanism.

Each summand is the product of a quantity of *positive parity* and *negative parity*.

Each summand individually must be nonnegative for all thermodynamic processes.

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For example, nonnegativity of the stress power implies that drag forces oppose motion.

### Subsection 2

Constitutive relations from entropy

$$\begin{aligned} \theta \xi &= \left[ \operatorname{dev}(\mathbb{T}), (m+p), \vec{j}_q \right] \cdot \left[ \operatorname{dev}(\mathbb{D}(\vec{v})), \nabla \cdot \vec{v}, -(\nabla \theta/\theta) \right] \\ &= \mathbf{J} \cdot \mathbf{A}. \end{aligned}$$

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We want to specify  $\mathbf{J} = \mathbf{\tilde{J}}(\mathbf{A})$ .

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Specify an expression for the entropy production  $\zeta(\mathbf{A})$  in terms of  $\mathbf{A}$ .

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Our example will be

$$\zeta(\mathbf{A}) \coloneqq 2\nu \operatorname{dev}(\mathbb{D}(\vec{v})) : \operatorname{dev}(\mathbb{D}(\vec{v})) + \tilde{\lambda}(\nabla \cdot \vec{v})^2 + \kappa \frac{|\nabla \theta|^2}{\theta},$$

where  $\nu, \tilde{\lambda}, \kappa$  are positive functions of state variables.

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In other words, specify the constitutive relations by solving

$$\begin{array}{ll} \underset{\mathbf{A}}{\text{maximise}} & \zeta(\mathbf{A}) \\ \text{subject to} & \zeta(\mathbf{A}) - \tilde{\mathbf{J}}(\mathbf{A}) \cdot \mathbf{A} = 0. \end{array}$$

For our running example, we have

$$\begin{array}{ll} \underset{\mathbf{A}}{\operatorname{maximise}} & 2\nu \operatorname{dev}(\mathbb{D}(\vec{v})) : \operatorname{dev}(\mathbb{D}(\vec{v})) + \tilde{\lambda}(\nabla \cdot \vec{v})^2 + \kappa \frac{|\nabla \theta|^2}{\theta} \\ \\ \text{subject to} & 2\nu \operatorname{dev}(\mathbb{D}(\vec{v})) : \operatorname{dev}(\mathbb{D}(\vec{v})) + \tilde{\lambda}(\nabla \cdot \vec{v})^2 + \kappa \frac{|\nabla \theta|^2}{\theta} = \tilde{\mathbf{J}}(\mathbf{A}) \cdot [\operatorname{dev}(\mathbb{D}(\vec{v})), \nabla \cdot \vec{v}, (\nabla \theta/\theta)] \\ \end{array}$$

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In this case of quadratic  $\zeta(\mathbf{A})$ , there is only one choice  $\mathbf{\tilde{J}}(\mathbf{A})$  that satisfies the constraint:

$$\begin{split} \operatorname{dev}(\mathbb{T}) &= 2\nu \operatorname{dev}(\mathbb{D}(\vec{v})), \\ m + p &= \tilde{\lambda} \nabla \cdot \vec{v}, \\ \vec{j}_q &= -\kappa \nabla \theta. \end{split}$$

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These are the constitutive relations for the classical Navier-Stokes-Fourier fluid.

You can get other classical models with different  $\zeta$ :

Euler 
$$\zeta = 0$$
  
Euler–Fourier  $\zeta = \kappa \frac{|\nabla \theta|^2}{\theta}$ 

and every possible combination of activating different entropy dissipation mechanisms.

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Incompressible and isothermal models arise by demanding that  $\nabla \cdot \vec{v} = 0$  or  $\nabla \theta = 0$  respectively. These demands can be combined with different  $\zeta$  to arrive at different models.

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Various papers of Rajagopal, Málek and coworkers show how you can get

#### More examples

neo-Hookean and Kelvin–Voigt solids; Maxwell, Oldroyd-B and Giesekus viscoelastic fluids; Korteweg fluids; power-law fluids, Bingham fluids, . . .