

**CDF: a theory of mathematical modeling for  
irreversible processes**

**Wen-An Yong**

TSINGHUA UNIVERSITY

**Duke Kunshan University, July 2020**

## OUTLINE

- Motivation
- Observation (Conservation-dissipation Principle)
- Conservation-dissipation Formalism (CDF)
- Generalized Hydrodynamics
- Model for Compressible Viscoelastic Fluids
- Maxwell Iteration
- Compatibility with the Navier-Stokes Equations
- Summary

# 1 Motivation

(Fluid Dynamics)

The motion of fluids (one-component) obeys conservation laws of mass, momentum and energy:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0, \\ \frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla \cdot \mathbf{P} &= 0, \\ \frac{\partial E}{\partial t} + \nabla \cdot (E \mathbf{v} + \mathbf{P} \mathbf{v} + \mathbf{q}) &= 0.\end{aligned}$$

Here  $\rho$  is the density,  $\mathbf{v}$  is the velocity,  $\mathbf{P}$  the pressure tensor,

$$E = \rho(u + |\mathbf{v}|^2/2),$$

$u$  the internal energy,  $\mathbf{q}$  represents the heat flux.

In 3D, we have 5 equations for 14 unknowns  $\rho, \mathbf{v}, u, \mathbf{P}$  (symmetric) and  $\mathbf{q}$ . This is a unclosed system of time-dependent first-order PDEs.

Conventionally, one writes

$$\mathbf{P} = pI + \tau.$$

with  $p = p(\rho, u)$  the hydrostatic pressure (the equation of state) and  $\tau$  a symmetric deviatoric pressure tensor.

Then the system of 5 PDEs was closed with the following **empirical laws**:

## 1.1 Newtonian fluids

Newton's law of viscosity:

$$\boldsymbol{\tau} = -\mu [(\nabla \mathbf{v}) + (\nabla \mathbf{v})^T - \frac{2}{3} \nabla \cdot \mathbf{v} I] - \lambda \nabla \cdot \mathbf{v} I (\equiv D[\mathbf{v}]),$$

Fourier's law of heat conduction:

$$\mathbf{q} = -\kappa \nabla T.$$

( $\kappa$ ,  $\mu$  and  $\lambda$  are the respective transport coefficients for heat conduction, shear viscosity, and bulk viscosity)

$\implies$  Compressible Navier-Stokes equations.

On the other hand, the empirical laws are not always valid.

## 1.2 Maxwell fluids

Maxwell's law of viscoelasticity (1867):

$$\boldsymbol{\tau} + \epsilon_1 \boldsymbol{\tau}_t = -\mu \left[ (\nabla \mathbf{v}) + (\nabla \mathbf{v})^T - \frac{2}{3} \nabla \cdot \mathbf{v} I \right] - \lambda \nabla \cdot \mathbf{v} I.$$

Cattaneo's law of heat conduction (1948):

$$\mathbf{q} + \epsilon_2 \mathbf{q}_t = -\kappa \nabla T.$$

Here  $\epsilon_1$  and  $\epsilon_2$  are two positive (small) parameters.

$\implies$  Time-dependent first-order PDEs!

Again, not always work well! There are many other constitutive equations in the literature. What to do next?

Mathematical modeling: to close the conservation laws, to discover new PDEs.

- Criteria: Conservation laws + Empirical laws.
- Are there any other (empirical) laws?
- Can we learn something from available “data” ?

## 2 Observation

(Conservation-dissipation Principle)

Many years ago, I studied first-order PDEs of the form:

$$U_t + \sum_{j=1}^d F_j(U)_{x_j} = Q(U). \quad (1)$$

Here  $t \geq 0, x = (x_1, x_2, \dots, x_d) \in \mathbb{R}^d$  ( $d = 1, 2, 3$ ),

$U = U(x, t) \in G$  (*open*)  $\subset \mathbb{R}^n$ ,

$Q(U), F_j(U) \in C^\infty(G, \mathbb{R}^n)$ .



Such PDE describe a large number of (all?) irreversible processes.

Important Examples:

non-Newtonian fluid flows, chemically reactive flows/combustion, dissipative relativistic fluid flows, kinetic theories (moment closure systems, discrete-velocity kinetic models), multi-phase flows, thermal non-equilibrium flows, radiation hydrodynamics, traffic flows, neuroscience (axonal transport), nonlinear optics, probability theory (the Master equation, also called Chapman-Kolmogorov equation), complex (reaction) networks ( $d=0$ ), geophysical flows, .....

Ref.: [1]. Ingo Müller, A history of thermodynamics, Springer, 2007.

[2]. D. Jou & J. Casas-Vazquez & G. Lebon, Extended irreversible thermodynamics, Springer, 1996.

**Example 1.** Multi-D Euler equations of gas dynamics with damping:

$$\begin{aligned}\rho_t + \operatorname{div}(\rho u) &= 0, \\ (\rho u)_t + \operatorname{div}(\rho u \otimes u) + \nabla p(\rho) &= -\rho u.\end{aligned}$$

Here  $\rho = \rho(x, t)$  stands for the density and  $u = u(x, t)$  is the velocity. This system is of the form (1) with  $U = (\rho, \rho u)^T$ .

**Example 2.** A 3-D quasilinear system for nonlinear optics:

$$\begin{aligned}\vec{D}_t - \nabla \times \vec{B} &= 0, \\ \vec{B}_t + \nabla \times \vec{E} &= 0, \\ \chi_t &= |\vec{E}|^2 - \chi\end{aligned}$$

with  $\vec{D} = (1 + \chi)\vec{E}$ .

**Example 3.** 1-D Euler equations of gas dynamics in vibrational non-equilibrium (in Lagrangian coordinates):

$$\begin{aligned}\nu_t - u_x &= 0, \\ u_t + p_x &= 0, \\ (e + q + \frac{u^2}{2})_t + (pu)_x &= 0, \\ q_t &= Q(\nu, e) - q.\end{aligned}$$

I observed (2008): the systems of PDEs from different fields All possess the following property (called “**Conservation-dissipation Principle**”):

(i). There is a strictly convex smooth function  $\eta(U)$  such that

$\eta_{UU}(U)F_{jU}(U)$  is symmetric for all  $U \in G$  and all  $j$ .

(ii). There is a symmetric and nonpositive-definite matrix  $\mathcal{L}(U)$  such that for all  $U \in G$ ,

$$Q(U) = \mathcal{L}(U)(\eta_U(U))^T.$$

(iii). The kernel space of  $\mathcal{L}(U)$  is independent of  $U$ .

Remark 1. Property (i) is the Lax entropy condition for hyperbolic conservation laws, characterizes the existence of an entropy function for the physical process and is consistent to the fundamental postulates of classical thermodynamics (H. B. Callen, 1985).

Remark 2. Property (ii) is a **nonlinearization** of the celebrated Onsager reciprocal relation in modern non-equilibrium thermodynamics:

$$Q(U) = \mathcal{L}(U_e)(\eta_U(U))^T$$

with fixed  $U_e$  satisfying  $Q(U_e) = 0$ .

Here  $Q(U)$  acts as the thermodynamic flux, while the entropy variable  $\eta_U(U)$  stands for the thermodynamic force.

**In contrast:** “There are difficulties in choosing the thermodynamic fluxes and forces when applying the notion” (P. Perrot, A to Z of Thermodynamics, Oxford Univ. Press, 1998, pp. 125–126).

Remark 3. Property (iii) describes the fact that the physical laws of conservation hold true no matter what state the system is in.

Remark 4. Balance laws relate irreversible processes (of scalar type) directly to the entropy change  $\eta_U$ :

$$U_t + \sum_j F_j(U)_{x_j} = \mathcal{L}(U)(\eta_U(U))^T$$

and incorporate the second law of thermodynamics!

Afterwards, I found that the Conservation-dissipation Principle is satisfied also by other first-order systems of PDEs from neuroscience, chemical engineering (multi-component diffusion) and so on.

A. Mielke (May 11, 2011): "Meanwhile I also found a few other sources, but none gives such a clear and general statement as yours."

## 3 Conservation-dissipation Formalism (CDF)

Guided by the Conservation-dissipation Principle (**nonlinear** Onsager relation), in 2015 we (Zhu & Hong & Yang & Y.) proposed a so-called CDF theory of non-equilibrium thermodynamics.

The underlying idea is simple! We observed that so many existing models all obey the principle. It is natural to respect the same principle when constructing new PDEs!



With fluid flows in mind, in CDF we assume that certain conservation laws are known *a priori*:

$$\partial_t u + \sum_{j=1}^3 \partial_{x_j} f_j = 0. \quad (2)$$

Here  $x = (x_1, x_2, x_3)$ ,  $u = u(t, x) \in \mathbb{R}^n$  represents conserved variables like  $u = (\rho, \rho\mathbf{v}, \rho E)$  in fluid dynamics, and  $f_j$  is the corresponding flux along the  $x_j$ -direction.

If each  $f_j$  is given in terms of the conserved variables, the system (2) becomes closed. In this case, the system is considered to be in local equilibrium and  $u$  is also referred to as equilibrium variables.

However, very often  $f_j$  depends on some extra variables in addition to the conserved ones. The extra variables characterize non-equilibrium features of the system under consideration and are called non-equilibrium or dissipative variables.

In CDF, we choose a dissipative variable  $v \in \mathbb{R}^r$  so that the flux  $f_j$  in (2) can be expressed as  $f_j = f_j(u, v)$  and seek evolution equations of the form

$$\partial_t v + \sum_{j=1}^3 \partial_{x_j} g_j(u, v) = q(u, v). \quad (3)$$

This is our constitutive equation to be determined, where  $g_j(u, v)$  is the corresponding flux and  $q = q(u, v)$  is the nonzero source, vanishing at equilibrium.

Together with the conservation laws (2), the dynamics of the non-equilibrium process is then governed by a system of first-order PDEs in the compact form

$$\partial_t U + \sum_{j=1}^3 \partial_{x_j} F_j(U) = Q(U), \quad (4)$$

where

$$U = \begin{pmatrix} u \\ v \end{pmatrix}, \quad F_j(U) = \begin{pmatrix} f_j(U) \\ g_j(U) \end{pmatrix}, \quad Q(U) = \begin{pmatrix} 0 \\ q(U) \end{pmatrix}.$$

For balance laws (4), the aforesaid conservation-dissipation principle consists of the following two conditions.

- (i). There is a strictly convex smooth function  $\eta = \eta(U)$ , called entropy (density), such that the matrix product  $\eta_{UU}F_{jU}(U)$  is symmetric for each  $j$  and for all  $U = (u, v)$  under consideration.
- (ii). There is a negative definite matrix  $M = M(U)$ , called dissipation matrix, such that the non-zero source can be written as  $q(U) = M(U)\eta_v(U)$ .

Remark 5. An Entropy-production Inequality (or called **a refined formulation of the 2nd law of thermodynamics**) follows from the conservation-dissipation principle.

It is direct to see that the entropy production

$$\begin{aligned}\sigma &\equiv \eta_U(U) \cdot Q(U) = \eta_v(U) \cdot M(U)\eta_v(U) \\ &\leq -\lambda(U)|\eta_v(U)|^2 \leq -\frac{\lambda(U)}{|M(U)|^2}|M(U)\eta_v(U)|^2 = -\frac{\lambda(U)}{|M(U)|^2}|Q(U)|^2,\end{aligned}$$

where  $\lambda(U)$  is the smallest eigenvalue of the positive-definite matrix  $-[M(U) + M^T(U)]/2$ .

Freedoms of CDF: convex entropy function  $\eta = \eta(U)$  and  
negative-definite matrix  $M = M(U)$ !

Having  $\eta = \eta(U)$ , we compute the change rate  $\eta(U)_t$  of entropy, use the balance laws (4) to identify entropy flux  $J(U)$  and entropy production  $\sigma(U)$ , and obtain

$$\eta(U)_t + \nabla \cdot J(U) = \sigma(U).$$

Finally, choose the  $g_j(u, v)$ 's so that

$$\sigma(U) \leq 0.$$

## 4 Generalized Hydrodynamics

To see how CDF works, we return to the equations for fluid flows:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0, \\ \frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) + \nabla \cdot \mathbf{P} &= 0, \\ \frac{\partial E}{\partial t} + \nabla \cdot (E \mathbf{v} + \mathbf{P} \mathbf{v} + \mathbf{q}) &= 0.\end{aligned}$$

Here  $\rho$  is the density,  $\mathbf{v}$  is the velocity,  $E = \rho(u + |\mathbf{v}|^2/2)$  with  $u$  the internal energy,  $\mathbf{q}$  represents the heat flux, and  $\mathbf{P}$  the pressure tensor

$$\mathbf{P} = pI + \tau.$$

with  $p = p(\rho, u)$  the hydrostatic pressure (the equation of state) and  $\tau$  a symmetric deviatoric pressure tensor.

**(P1)**. Specify a smooth strictly convex function (called the non-equilibrium specific entropy)  $s = s(\nu, u, \mathbf{z})$  satisfying  $s_u > 0$ .

Since the extra unknown variables are  $\mathbf{q}$  and  $\tau$ , the non-equilibrium variable  $\mathbf{z}$  is chosen to be of the same size of the unknown fluxes, i.e.,  $\mathbf{z} = (\mathbf{w}, \mathbf{c}) \in \mathbb{R}^d \times \mathbb{M}_s^d$  ( $d = 1, 2, 3$ ).

Define

$$\theta^{-1} = s_u, \quad \pi = \theta s_\nu, \quad \zeta = s_{\mathbf{z}}, \quad \tau = \mathbf{P} - \pi I.$$

In other words, the generalized Gibbs relation is

$$ds = \theta^{-1}(du + \pi d\nu) + \zeta \cdot d\mathbf{z}.$$



In order to be compatible with the classical theory, we introduce

$\theta$ : non-equilibrium temperature,

$\pi$ : non-equilibrium pressure.

$\zeta$ : the entropic variable and related to the dissipative fluxes which vanish at equilibrium

$\tau$ : non-equilibrium stress tensor.

We calculate

$$\begin{aligned}
 & \partial_t(\rho s) + \nabla \cdot (\rho s \mathbf{v}) \\
 = & \quad -\nabla \cdot (\theta^{-1} \mathbf{q}) + \underline{s_{\mathbf{w}} \cdot [\partial_t(\rho \mathbf{w}) + \nabla \cdot (\mathbf{v} \otimes \rho \mathbf{w})] + \mathbf{q} \cdot \nabla \theta^{-1}} \\
 & \quad + \underline{s_{\mathbf{c}}^T : [\partial_t(\rho \mathbf{c}) + \nabla \cdot (\mathbf{v} \otimes \rho \mathbf{c})] - \theta^{-1} \tau^T : \nabla \mathbf{v}} \\
 \equiv & \quad -\nabla \cdot \mathbf{J} + \sigma.
 \end{aligned}$$

Here  $\mathbf{J} = \theta^{-1} \mathbf{q}$  as the entropy flux and the rest as the entropy production  $\sigma$ . A nature choice of the unknowns is

$$\mathbf{q} = s_{\mathbf{w}}, \quad \tau = \theta s_{\mathbf{c}}$$

and then the entropy production becomes

$$\sigma = \mathbf{q} \cdot A + \theta^{-1} \tau^T : B$$

with

$$A = \partial_t(\rho \mathbf{w}) + \nabla \cdot (\mathbf{v} \otimes \rho \mathbf{w}) + \nabla \theta^{-1},$$

$$B = \partial_t(\rho \mathbf{c}) + \nabla \cdot (\mathbf{v} \otimes \rho \mathbf{c}) - \nabla \mathbf{v}.$$

This suggests the following **constitutive equations**

$$\begin{pmatrix} A \\ B \end{pmatrix} = \mathbf{M} \cdot \begin{pmatrix} \mathbf{q} \\ \theta^{-1} \boldsymbol{\tau} \end{pmatrix}$$

or

$$\begin{pmatrix} \partial_t(\rho \mathbf{w}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{w}) + \nabla \theta^{-1} \\ \partial_t(\rho \mathbf{c}) + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{c}) - \frac{1}{2}(\nabla \mathbf{v} + \nabla \mathbf{v}^T) \end{pmatrix} = \mathbf{M} \cdot \begin{pmatrix} \mathbf{q} \\ \theta^{-1} \boldsymbol{\tau} \end{pmatrix}$$

with  $\mathbf{M} = \mathbf{M}(\nu, u, \mathbf{z})$  **negative definite** (P2). Consequently, the entropy production rate is

$$\sigma = s_{\mathbf{z}} \cdot \mathbf{M} s_{\mathbf{z}}.$$

It is always negative as long as  $s_{\mathbf{z}}$  is not zero. The system reaches to equilibrium when  $s_{\mathbf{z}}$  is zero. In this context, the derivative of the entropy with respect to the non-equilibrium variables is regarded as the entropic force which drives the system to equilibrium.

A typical choice of the generalized entropy function  $s$  and dissipation matrix  $\mathbf{M}$ . They are

$$s = s(\nu, u, \mathbf{w}, \mathbf{c}) = -s^{eq}(\nu, u) + \frac{1}{2\alpha_1(\nu, u)} |\mathbf{w}|^2 + \frac{1}{2\alpha_2(\nu, u)} |\mathbf{c}|^2$$

and

$$\mathbf{M} \cdot \begin{pmatrix} \mathbf{q} \\ \theta^{-1}\tau \end{pmatrix} = \begin{pmatrix} \frac{\mathbf{q}}{\lambda\theta^2} \\ \frac{1}{2\xi} \left( \tau - \frac{1}{d} \text{tr}(\tau) I \right) + \frac{1}{d\kappa} \text{tr}(\tau) I \end{pmatrix}.$$

Here  $\alpha_1$  and  $\alpha_2$  are positive functions such that  $s(\nu, u, \mathbf{w}, \mathbf{c})$  satisfies the convexity and monotonicity in (P1). The simplest choice is that both  $\alpha_1$  and  $\alpha_2$  are constant.

With such a choice of the entropy function and dissipation matrix, we generalize Maxwell's law for viscoelastic fluids. They give a reasonable description of non-isothermal compressible viscoelastic fluid flows.

## 5 Model for compressible viscoelastic fluids (Y. 2014)

For isothermal flows, we have conservation laws of mass and momentum:

$$\partial_t \rho + \nabla \cdot (\rho v) = 0,$$

$$\partial_t(\rho v) + \nabla \cdot (\rho v \otimes v + pI + \tau) = 0.$$

Here  $\rho$  is the density of the fluid,  $\otimes$  denotes the tensorial product,  $p = p(\rho)$  is the hydrostatic pressure, and  $\tau$  is a tensor of order two.

On physical grounds, assume  $\tau$  is symmetric and decompose

$$\tau = \tilde{\tau}_1 + \tilde{\tau}_2 I$$

with  $\tilde{\tau}_1$  traceless and  $\tilde{\tau}_2$  scalar.

Denote by

$\tau_1$  a symmetric and traceless tensor of order two,

$\tau_2$  a scalar,

$\mathbf{Id}$  the unit tensor.

In CDF, take

$$\eta = \eta(\rho, \rho v, \tau_1, \tau_2) = 4\rho \int_1^\rho \frac{p(y)}{y^2} dy + 2\rho |v|^2 + |\tau_1|^2 + 2\tau_2^2,$$

which is strictly convex w. r. t.  $U = (\rho, \rho v, \tau_1, \tau_2)^T$ .



Compute

$$\begin{aligned}
 \eta_t &= \eta_\rho \rho_t + \eta_{\rho v} (\rho v)_t + \eta_{\tau_1} : \tau_{1t} + \eta_{\tau_2} \tau_{2t} \\
 &= -\nabla \cdot (\dots) + \eta_{\tau_1} : \tau_{1t} + \eta_{\tau_2} \tau_{2t} + 4\tau : \nabla v \\
 &= -\nabla \cdot (\dots) + \eta_{\tau_1} : \tau_{1t} + \eta_{\tau_2} \tau_{2t} + 4\tilde{\tau}_1 : \nabla v + 4\tilde{\tau}_2 \nabla \cdot v \\
 &= -\nabla \cdot (\dots) + \eta_{\tau_2} \tau_{2t} + 4\tilde{\tau}_2 \nabla \cdot v \\
 &\quad + \eta_{\tau_1} : \tau_{1t} + 2\tilde{\tau}_1 : [\nabla v + (\nabla v)^T - \frac{2}{3} \nabla \cdot v] .
 \end{aligned}$$

Take

$$\tilde{\tau}_1 = \frac{\eta_{\tau_1}}{2\epsilon_1} = \frac{\tau_1}{\epsilon_1}, \quad \tilde{\tau}_2 = \frac{\eta_{\tau_2}}{4\epsilon_2} = \frac{\tau_2}{\epsilon_2}$$

with  $\epsilon_1, \epsilon_2$  two positive numbers.

Then

$$\begin{aligned} \eta_t &= -\nabla \cdot (\dots) + \eta_{\tau_2} \left[ \tau_{2t} + \frac{\nabla \cdot v}{\epsilon_2} \right] \\ &\quad + \eta_{\tau_1} : \left[ \tau_{1t} + \frac{1}{\epsilon_1} \left( \nabla v + \nabla v^T - \frac{2}{3} \nabla \cdot v \right) \right]. \end{aligned}$$

In CDF, take

$$M = M(U) = -\text{diag} \left( \frac{\mathbf{Id}}{2\nu\epsilon_1^2}, \frac{1}{4\kappa\epsilon_2^2} \right)$$

with  $\nu, \kappa$  two positive numbers. We obtain

$$\partial_t \rho + \nabla \cdot (\rho v) = 0,$$

$$\partial_t(\rho v) + \nabla \cdot (\rho v \otimes v + pI) + \frac{1}{\epsilon_1} \nabla \cdot \tau_1 + \frac{1}{\epsilon_2} \nabla \tau_2 = 0,$$

$$\partial_t \tau_1 + \frac{1}{\epsilon_1} \left[ \nabla v + (\nabla v)^T - \frac{2}{3} \nabla \cdot v I \right] = -\frac{\tau_1}{\nu\epsilon_1^2},$$

$$\partial_t \tau_2 + \frac{1}{\epsilon_2} \nabla \cdot v = -\frac{\tau_2}{\kappa\epsilon_2^2}.$$

In 2015, D. Chakraborty & J. E. Sader (PoF) showed that this model can lead to the following classical results:

- Newton's law of viscosity, at low frequency (Y. 2014)
- Hooke's law of elasticity, at high frequency
- Landau-Lifshitz' formula for the difference between thermodynamic and mechanical pressures
- Landau-Lifshitz' formula for the speed of sound in slow compressible processes

Consequently, they claimed:

**unique correct** model for compressible viscoelastic fluid flows.

” Abstract: ..... In this article, we review and critically assess the **available** constitutive equations for compressible viscoelastic flows in their linear limits—such models are required for analysis of the above-mentioned measurements. We show that previous models, with the **exception of a very recent proposal**, do not reproduce the required response at high frequency. We explain the physical origin of this recent model and show that it recovers **all required features** of a linear viscoelastic flow. This constitutive equation thus provides a rigorous foundation for the analysis of vibrating nanostructures in simple liquids. The utility of this model is demonstrated by solving .....

J. E. Sader (2019): in good agreement with experiments.

B. Wu & Y. Gan & E. Carrera & W. Q. Chen (J. Fluid Mech. 2019):  
solving its linearization.

## 6 Maxwell iteration

To show the compatibility, we introduce the following transformation

$$U = \begin{pmatrix} u \\ v \end{pmatrix} \longrightarrow W \equiv \begin{pmatrix} u \\ z \end{pmatrix} = \begin{pmatrix} u \\ \eta_v(u, v) \end{pmatrix}. \quad (5)$$

for balance laws (4).

Thanks to the strict concavity of  $\eta(U)$ , the algebraic equation  $z = \eta_v(u, v)$  can be globally and uniquely solved to obtain  $v = v(u, z)$ .

Namely, this transformation is globally invertible.

Under this transformation, the system (4) for smooth solutions can be rewritten as

$$W_t + \sum_{j=1}^d (D_U W) F_j(U) x_j = \frac{1}{\varepsilon} \begin{pmatrix} 0 \\ \eta_{vv}(U) M(U) z \end{pmatrix} \quad (6)$$

with  $D_U W = \begin{bmatrix} I_n & 0 \\ \eta_{vu}(U) & \eta_{vv}(U) \end{bmatrix}$  and  $I_k$  the unit matrix of order  $k$ .

Transformation (5) preserves the original conservation laws in (4):

$$u_t + \sum_{j=1}^d f_j(u, z) x_j = 0. \quad (7)$$

Here and below, the simplified notation  $f_j(u, z)$  has been used to replace  $f_j(u, v(u, z))$ .



The  $z$ -equation in (6) can be rewritten as

$$z = \varepsilon M(U)^{-1} \eta_{vv}(U)^{-1} \left[ z_t + \eta_{vu}(U) \sum_j f_j(u, z)_{x_j} + \eta_{vv}(U) \sum_j g_j(u, z)_{x_j} \right].$$

This indicates that  $z = O(\varepsilon)$ . Iterating the last equation yields

$$z = \varepsilon \bar{M}(u)^{-1} \bar{\eta}_{vv}(u)^{-1} \sum_j \left[ \bar{\eta}_{vu}(u) f_{ju}(u, 0) + \bar{\eta}_{vv}(u) g_{ju}(u, 0) \right] u_{x_j} + O(\varepsilon^2),$$

where  $\bar{M}(u) = M(u, v(u, 0))$  giving the meaning of the bar.

Moreover,  $f_j(u, z)$  in (7) can be expanded into

$$f_j(u, z) = f_j(u, 0) + f_{jz}(u, 0)z + O(\varepsilon^2).$$

Substituting the two truncations above into (7), we arrive at the following second-order PDEs

$$u_t + \sum_{j=1}^3 f_j(u, 0)_{x_j} = \varepsilon \sum_{j,k=1}^3 (B^{jk}(u) u_{x_k})_{x_j} \quad (8)$$

with

$$B^{jk}(u) = -f_{jz}(u, 0) \bar{M}(u)^{-1} \bar{\eta}_{vv}(u)^{-1} [\bar{\eta}_{vu}(u) f_{ku}(u, 0) + \bar{\eta}_{vv}(u) g_{ku}(u, 0)].$$

This procedure in deriving (8) from (6) is called *Maxwell iteration* and gives the exactly same result as the Chapman-Enskog expansion does.

Denote by  $W_h^\varepsilon \equiv (u_h^\varepsilon, z_h^\varepsilon)$  and  $u_p^\varepsilon$  the solutions to systems (6) and (8), respectively. It was proved in (Y. 1999, JDE) for sufficiently smooth initial data that the expansion

$$u_h^\varepsilon - u_p^\varepsilon = O(\varepsilon^2)$$

holds in a certain Sobolev space.

This result indicates that the second-order PDEs (8) is a good approximation to the CDF-based first-order system (4) when the dissipative variables evolve much faster than the conserved ones.

Consequently, the Maxwell iteration makes up for the shortcoming of CDF that only first-order PDEs can be obtained.

It was shown in (Y. 2020, Phil.Trans.R.Soc.A **378**:20190177) that the derived second-order PDEs (8) preserve the gradient structure and strong dissipativeness of the CDF-based first-order ones.

Namely, the Maxwell iteration preserves both the Conservation-dissipation Principle and the Entropy-production Inequality (the refined formulation of the 2nd law of thermodynamics).

The gradient structure corresponds to nonlinear Onsager reciprocal relations for scalar processes (described with the first-order PDEs) and for vectorial or tensorial processes (described with the second-order PDEs).

## 7 Compatibility

For simplicity, we only consider the isothermal model for compressible viscoelastic fluids (Sec. 4)

$$\partial_t \rho + \nabla \cdot (\rho v) = 0,$$

$$\partial_t(\rho v) + \nabla \cdot (\rho v \otimes v + pI) + \frac{1}{\epsilon_1} \nabla \cdot \tau_1 + \frac{1}{\epsilon_2} \nabla \tau_2 = 0,$$

$$\partial_t \tau_1 + \frac{1}{\epsilon_1} \left[ \nabla v + (\nabla v)^T - \frac{2}{3} \nabla \cdot v I \right] = -\frac{\tau_1}{\nu \epsilon_1^2},$$

$$\partial_t \tau_2 + \frac{1}{\epsilon_2} \nabla \cdot v = -\frac{\tau_2}{\kappa \epsilon_2^2}.$$

Rewrite the last two lines and iterate them once

$$\begin{aligned}\tau_1 &= -\epsilon_1 \nu \left[ \nabla v + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \right] - \epsilon_1^2 \nu \tau_{1t} \\ &= -\epsilon_1 \nu \left[ \nabla v + (\nabla v)^T - \frac{2}{3} \nabla \cdot v \right] + \epsilon_1^3 O(1),\end{aligned}$$

$$\begin{aligned}\tau_2 &= -\epsilon_2 \kappa \nabla \cdot v - \epsilon_2^2 \kappa \tau_{2t} \\ &= -\epsilon_2 \kappa \nabla \cdot v + \epsilon_2^3 O(1).\end{aligned}$$

Substituting the truncations into the first two lines (conservation laws) yields the classical Navier-Stokes equations.

The above formal process can be justified and the result can be stated as follows.

**Theorem 7.1** *Suppose the density  $\rho$  and velocity  $\mathbf{v}$  are continuous and bounded in  $(x, t) \in \Omega \times [0, t_*]$  with  $t_* < \infty$ , and satisfy*

*$\inf_{x,t} \rho(x, t) > 0$  and*

$$\rho, \mathbf{v} \in C([0, t_*], H^{s+3}) \cap C^1([0, t_*], H^{s+1}(\Omega))$$

*with integer  $s \geq [d/2] + 2$ . Then there exist positive numbers  $\epsilon_0 = \epsilon_0(t_*)$  and  $K = K(t_*)$  such that for  $\epsilon \leq \epsilon_0$  the compressible viscoelastic model, with initial data in  $H^s(\Omega)$  satisfying*

*$\|(\rho^\epsilon, \rho^\epsilon \mathbf{v}^\epsilon)|_{t=0} - (\rho, \rho \mathbf{v})|_{t=0}\|_s = O(\epsilon^2)$ , has a unique classical solution satisfying*

$$(\rho^\epsilon, \rho^\epsilon \mathbf{v}^\epsilon, \tau_1^\epsilon, \tau_2^\epsilon) \in C([0, t_*], H^s(\Omega))$$

*and*

$$\sup_{t \in [0, t_*]} \|(\rho^\epsilon, \rho^\epsilon \mathbf{v}^\epsilon) - (\rho, \rho \mathbf{v})\|_s \leq K(t_*) \epsilon^2.$$

## 6. Summary

- It was observed that many many existing and well-validated PDE models from different fields all obey the Conservation-dissipation Principle—a **nonlinearization** of the Onsager reciprocal relation. Thanks to this, it is natural to respect the same principle when constructing new models.
- With the simple idea above, we developed a so-called Conservation-dissipation Formalism (CDF) of non-equilibrium thermodynamics and proposed a novel generalized hydrodynamics for non-isothermal compressible viscoelastic fluid flows.



- Within the CDF, a new model for isothermal compressible viscoelastic fluid flows was proposed. It was shown to be the unique correct model for viscoelastic fluid flows.
- The CDF has two freedoms (or called details): the strictly convex function  $\eta$  and the dissipation-matrix  $\mathbf{M}$ . The freedoms are problem-dependent and can be fixed with machine learning. PDEs thus discovered automatically possess “good” properties:

robustness or well-posedness, irreversibility, long-time tendency to equilibrium, compatibility with classical theories

**(4 fundamental requirements)!**

Ref.: W.-A. Yong (2020), *Phil.Trans.R.Soc.A* **378**:20190177.  
<http://dx.doi.org/10.1098/rsta.2019.0177>

**THANK You for Your Attention!**