Mechanics with missing details

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Thermodynamics – human endeavor

History of nonequilibrium thermodynamics:

I. Mu¨ller, W. Weiss, Thermodynamics of irreversible processes: past and present, European Physical Journal H, 37, 139 (2012)

G. Lebon, D. Jou, Early history of extended irreversible thermodynamics (1953-1983),. An exploration beyond local equilibrium and classical transport theory, European Physical Journal H, 40, 205 (2015)

History of science in general:

Thomas Kuhn: The structure of scientific revolutions (1962)

Paradigm shift (can the creators of one paradigm switch to a new one?)

Anthropology:

Nonequilibrium-thermodynamics scientific community as a **tribe**

Tribal chiefs, ceremonies (regular meetings, potlatch, regular wars,…), ….

- By ignoring unimportant details (by making a pattern-recognition process) we (as well as all animals) are able to survive [note: not a coarse-graining, something possibly related to aesthetics]

- A large majority of time evolutions that we observe are time-irreversible (Aristotle : Physics - Martinas, K.; Ropolyi, L. Aristotelian and Modern Physics. International Studies in the Philosophy of Science 1987, 2, 1–9)
  thermodynamic time evolution

$$\frac{dx}{dt} = \Lambda \frac{dS(x)}{dx} \Rightarrow \frac{dS(x)}{dt} = \frac{dS}{dx}\frac{dx}{dt} = \Lambda \left(\frac{dS}{dx}\right)^2 > 0 \; provided \; \Lambda > 0$$

- Galileo, Newton - Time reversible (permanent) time evolution
  mechanic time evolution

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial E(x_1,x_2)}{\partial x_1} \\ \frac{\partial E(x_1,x_2)}{\partial x_2} \end{pmatrix} \Rightarrow \frac{dE(x_1,x_2)}{dt} = \frac{\partial E}{\partial x_1}\frac{\partial E}{\partial x_2} - \frac{\partial E}{\partial x_2}\frac{\partial E}{\partial x_1} = 0$$

question: mechanic time evolution combined with thermodynamic time evolution so that

$$\frac{dE(x)}{dt} = 0, \ and \ \frac{dS(x)}{dt} > 0 \qquad where\ state\ variables: \ x = (x_1, x_2, ..., x_n)$$

answer: one of the simplest examples

$$state\ variables: \ x = (p, q, e); \ E = e, \ assume \ \frac{\partial S(p,q,e)}{\partial e} > 0$$

$$\frac{d}{dt}\begin{pmatrix} p \\ q \\ e \end{pmatrix} = \begin{pmatrix} 0 & -1 & \frac{S_q}{S_e} \\ 1 & 0 & -\frac{S_p}{S_e} \\ -\frac{S_q}{S_e} & \frac{S_p}{S_e} & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} + \begin{pmatrix} [\Xi_{p^*}]_{p^*=S_p} \\ 0 \\ 0 \end{pmatrix}$$

$$e.g.\ \Xi(p^*) = \frac{1}{2}\Lambda(p^*)^2, \ i.e.\ \Xi_{p^*} = \frac{\partial \Xi}{\partial p^*} = \Lambda p^*, \ i.e.\ [\Xi_{p^*}]_{p^*=S_p} = \Lambda S_p;$$

$$\dot{x} = LE_x + [\chi \Xi_{x^*}]_{x^* = S_x}$$

GENERIC

e.g.

$x = f(\boldsymbol{r}, \boldsymbol{v});\ x = (\rho(\boldsymbol{r}), e(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r}));$

$x = f(\hat{x}, t)\ fluctuations; \ldots$

kinetic theory as both : (i) nonequilibrium thermodynamics itself and
(ii) a mesoscopic microscopic theory providing microscopic foundation of the classical (local equilibrium) nonequilibrium thermodynamics

History:

Alfred Clebsch (1859), Vladimir Arnold (1966) - mechanic time evolution-, Landau, Ginzburg (1950) Cahn, Hilliard (1958) - thermodynamic time evolution -, Dzyaloshinskii, Volovick (1980) - combined

AMS-IMS-SIAM Joint Summer Research Conference
in the Mathematical Sciences on Fluids and Plasmas:Geometry and Dynamics
- held at the University of Colorado, Boulder, July 17-23 1983), - proceedings in Contemp. Math. (1984)

(summer 1983, the first conference about EIT)

GENERIC (1997)

More recently: two monographs (one written by Antony Beris and Brian Edwards (1994) and the other by Hans Christian Oettinger (2005)) and one review article in Advances in Chemical Engineering written by M.G. (2010)

Three routes to GENERIC

1. Common structure of mesoscopic dynamical theories , started by A. Clebsch in 1859

   note: non-uniqueness, it depends on the pool of dynamical theories and on the focus (e.g. rational mechanics)

2. Agreement of theoretical predictions with results of experimental observations

   quantitative and qualitative observations - quantitative and qualitative theoretical predictions

3. Mesoscopic dynamics as a natural extension of thermodynamics toward time evolution

   dynamical MaxEnt Principle

GENERIC

$$\frac{dE}{dt} = 0$$
$$\frac{dS}{dt} \geq 0$$

$$\dot{x} = LE_x + \Lambda S_x$$

Equivalent reformulation of GENERIC

$$\Phi(x; \tfrac{1}{T}) = -S(x) + \tfrac{1}{T}E(x)$$

$$\dot{x} = TLE_x\Phi_x - \Lambda\Phi_x$$

energy conservation $\Rightarrow$ x stays on an energy shell during the total time evolution (T parametrizes the energy shell)

classification

potentials	requirements	*geometrical structures*	time evolution	geometry of the state space
$E(x),\ S(x)$ $\Phi(x;\frac{1}{T}) = -S(x) + \frac{1}{T}E(x)$	$\frac{dE}{dt} = 0$ $\frac{dS}{dt} \geq 0$	symplectic Riemannian	$\dot{x} = LE_x + \Lambda S_x$ $\dot{x} = TLE_x\Phi_x - \Lambda\Phi_x$	
$\Phi(x;\frac{1}{T}) = -S(x) + \frac{1}{T}E(x)$	$\frac{d\Phi}{dt} \leq 0$	symplectic Riemannian	$\dot{x} = L\Phi_x - \Lambda\Phi_x$	
$\mathcal{H}(x,\frac{1}{T});\ S(x)$	$\frac{dE}{dt} = 0$ $\frac{dS}{dt} \geq 0$	contact	$\dot{x} = \ldots$ $\dot{x}^* = \ldots$ $\dot{s} = \ldots$	Gibbs-Legendre Manifold (thermodynamics)

CLASSICAL EQUILIBRIUM THERMODYNAMICS

mechanical state variables: (V, N)
and mechanical energy E_{mec} (overall kinetic plus potential); "mechanical wall" separating the system from the environment (**work**)

thermodynamical state variables: E **internal energy**
the total energy $E + E_{mec}$, ""thermodynamical walls" separating the system from the environment (**heat**)

the influence of ignored details is expressed in *MaxEnt Principle*
entropy $S = S(V, N, E)$ (fundamental thermodynamic relation) reaches its maximum allowed by constraints

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thermodynamic potential $\Phi(E, N; E^*, N^*) = -S(E, N) + E^*E + N^*N$
$(E^* = \frac{1}{T}; N^* = -\frac{\mu}{T})$

MaxEnt: $\Phi_E = 0; \Phi_N = 0$ solution $(E_{eq}(E^*, N^*), N_{eq}(E^*, N^*))$, evaluate $\Phi(E, N)$ at $(E_{eq}, N_{eq}) \Rightarrow S^*(E^*, N^*) = [\Phi]_{(E_{eq}, N_{eq})}$
Legendre transformation $S(E, N) \rightarrow S^*(E^*, N^*)$

Robert Hermann (1984), *Contact geometry formulation of thermodynamics* argument:

Maxent is the basis of thermodynamics → MaxEnt is in fact a Legendre transformation → group of Legendre transformations is the fundamental group of thermodynamics → the space in which Legendre transformations appear as natural transformations is the space equipped with contact geometry (1-form specifying the contact geometry is preserved in Legendre transformations)

state variables: (E, N, E^*, N^*, ϕ);, 1-form: $d\phi - E^* dE - N^* dN$;

Gibbs-Legendre manifold (representing geometrically the fundamental thermodynamic relation):

$(E, N) \hookrightarrow (E, N, \Phi_E(E, N), \Phi_N(E, N).\Phi(E, N))$

MESOSCOPIC EQUILIBRIUM THERMODYNAMICS thermodynamic reduction

state variables: x
fundamental thermodynamic relation: $S = S(x), E = E(x), N = N(x)$
thermodynamic potential: $\Phi(x, E^*, N^*) = -S(x) + E^*E(x) + N^*N(x)$
thermodynamic reduction (Legendre transformation): $S^*(E^*, N^*) = [\Phi]_{x=x_{eq}(E^*,N^*)}$

example: (Boltzmann kinetic theory)
$x = f(\boldsymbol{r}, \boldsymbol{v}), \quad S(x) = -k_B \int d\boldsymbol{r} \int d\boldsymbol{v}(f \ln f - 1), \quad E(x) = \int d\boldsymbol{r} \int d\boldsymbol{v} f \frac{\boldsymbol{v}^2}{2m},$
$N(x) = \int d\boldsymbol{r} \int d\boldsymbol{v} f$

Ideal gas fundamental thermodynamic relation

SOLUTION OF GENERIC - GENERIC reduction

$$\frac{dE}{dt} = 0; \ \frac{dN}{dt} = 0, \ \ \frac{d\Phi}{dt} < 0 \Rightarrow x \to x_{eq} \text{ as } t \to \infty \Rightarrow$$

$$\text{thermodynamic reduction} \equiv \text{GENERIC reduction}$$

GENERIC addresses the passage between two levels of description.
usually it is the passage between a dynamical theory and equilibrium thermodynamics but it can also be a passage between a dynamical theory and another dynamical theory involving less details

Since the results of the GENERIC time evolution from t=0 to t=∞ is a Legendre transformation (thermodynamic reduction), we suggest that the GENERIC time evolution is a sequence of infinitesimal Legendre (contact-structure-preserving) transformations

MaxEnt → Dynamical MaxEnt

$$\begin{aligned} \dot{x} &= \Psi_{x^*} \\ \dot{x}^* &= -\Psi_x + x^* \Psi_\phi \\ \dot{\phi} &= -\Psi + < x^*, \Psi_{x^*} > \end{aligned} \qquad (1)$$

$\Psi(x, x^*, \phi)$ contact Hamiltonian

Problem: Find $\Psi(x, x^*, \phi)$ such that the Gibbs-Legendre manifold is an invariant manifold and the time evolution (1) evaluated on it becomes GENERIC

$$\Psi(x,x^*,e^*,n^*) = -\chi\mathcal{S}(x,x^*,e^*,n^*) + \frac{1}{e^*}\mathcal{H}(x,x^*,e^*,n^*)$$

where

$$\begin{aligned}
\mathcal{S}(x,x^*,e^*,n^*) &= \Xi(x,x^*,y^*) - [\Xi(x,x^*,e^*,n^*)]_{x^*=\Phi_x} \\
\mathcal{H}(x,x^*,e^*,n^*) &= < x^*, L\Phi_x >
\end{aligned}$$

and $\chi : \mathbb{M}^{(\mathbb{N})} \to \mathbb{R}^+$. It is a matter of direct verification to show that the contact-structure preserving dynamics with the contact Hamiltonian Ψ becomes on the Gibbs-Legendre manifold GENERIC.

Variational formulation

$$\mathcal{I} = \int dt[\Psi(x, x^*, y^*) - < x^*, \dot{x} >]$$

Observations:

(i) $[\mathcal{I}]_{GL-manifold}$ has the physical interpretation of the entropy generated during the time evolution.

(ii) The Euler-Lagrange equations $\delta\mathcal{I} = 0$ become on the GL-manifold equivalent to GENERIC.

Properties of solutions to GENERIC

quantitative (detailed) compare with quantitative experimental observations

qualitative compare with qualitative experimental observations

Examples of quantitative experimental observations: shear rate versus shear stress in complex fluids

Examples of qualitative experimental observations: compatibility with equilibrium thermodynamics
more generally,
compatibility with more macroscopic description

Qualitative properties of solutions to GENERIC

1. $t \to \infty$ GENERIC reduction

2. H. Grad (1965), C. Villani (2005) Boltzmann kinetic equation

only thermodynamic time evolution $t \to \infty$ approach to local equilibrium
only mechanic time evolution $f(r,v,0) \to f(r-vt/m,v,0)$ no approach
Combined mechanic and thermodynamic time evolution
$t \to \infty$ approach to total equilibrium

Conjecture: a very small nucleus of ignorance introduced on the microscopic level growths during the time evolution and the resulting irreversibility brings macroscopic systems to states of thermodynamic equilibrium

Complementary dynamics

EXTERNALLY UNFORCED SYSTEMS

$$\begin{array}{c} \text{micro} \\ \Big\downarrow \text{GENERIC reduction } S^{(micro\to eq)} \\ \text{eq} \end{array}$$

$[S^{(micro\to eq)}]_{x_\infty}$ is the classical-equilibrium-thermodynamics entropy; x_∞ is the state approached (as $t\to\infty$)in the GENERIC time evolution evolution

EXTERNALLY UNFORCED SYSTEMS

micro

↓ GENERIC reduction $S^{(micro \rightarrow eq)}$

eq

micro

↓ GENERIC reduction $S^{(micro \rightarrow n-Grad)}$

n-Grad

n-Grad

↓ GENERIC reduction $S^{(n-Grad \rightarrow hyd)}$

hyd

hyd

↓ GENERIC reduction $S^{(hyd \rightarrow eq)}$

eq

$a^{(j)}_{k_1,...,k_j}(\boldsymbol{r}) = \int d\boldsymbol{v} v_{k_1}...v_{k_j} f(\boldsymbol{r},\boldsymbol{v})$
$A = (a^{(1)},...,a^{(n)});\ \ B = (a^{(n+1)},......)$

$$\frac{\partial A}{\partial t} = [...]_{\mathcal{M}_{closure}} \tag{2}$$

How to get $\mathcal{M}_{closure}$?
Route 1: ***investigate solutions of the hierarchy 2***
Route 2: ***investigate solutions of the complementary hierarchy 3***

$$\frac{\partial B}{\partial t} = L^{(B)}\Phi_B - \Lambda\Phi_B \tag{3}$$

$\Phi(B;A^*) = \phi(B) - \int d\boldsymbol{r} b^{(n+1)}(A^*)a^{(n+1)}$

As $t \to \infty$, solutions to 3 approach solutions to $\Phi_B = 0$ that form the closure manifold $\mathcal{M}_{closure}$

moreover, we obtain

$$[\Phi]_{\mathcal{M}_{closure}} = \qquad S(A)$$

EXTERNALLY DRIVEN SYSTEMS

micro

$\downarrow$ GENERIC reduction $S^{(micro \to mes)}$

meso (externally driven)

$[S^{(micro \to meso)}]_{x_\infty}$ is the entropy of driven systems; x_∞ is the state approached (as $t \to \infty$)in the GENERIC time evolution evolution

Chapman-Enskog type reductions; new emerging entropies

$$
\begin{array}{ccc}
S_0 & \xrightarrow{\text{Ch-E}} & S_1 \\
\Big\downarrow \text{MaxEnt} & & \Big\downarrow \text{MaxEnt} \\
\mathcal{M}_0 & \xrightarrow[\text{Ch-E}]{} & \mathcal{M}_1
\end{array}
$$

The new emerging entropies are typically weakly nonlocal (Cahn-Hilliard type)

VARIATIONS ON GENERIC

natural, desirable, to be encouraged

classification

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Variations on $L E_x$

- Godunov (1972), Friedrichs, Lax (1971) local conservation laws (e.g. Grad's hierarchy) implying
- another local conservation law
- for entropy physical regularity → mathematical regularity
- (Euler fluid mechanics is both Hamiltonian and Godunov)

- example:
- slip in advection of an internal structure

Variations on $[\Xi_{x^*}]_{x^*=S_x}$

$$\Xi(x,0)=0,\ \forall x \in M$$
$$\Xi\ reaches\ its\ minimum\ at\ x^*=0$$
$$\Xi\ is\ a\ convex\ function\ in\ a\ neighborhood\ of\ x^*=0$$

We shall first consider a special case when Ξ is a quadratic function of x^*, i.e.

$$\Xi(x,x^*)=\frac{1}{2}<x^*,\Lambda(x)x^*>$$

Consequences of dissipation potential in chemical kinetics

Involving two reactions

$$\left(\frac{\partial X^{(1)}}{\partial J^{(2)}}\right)_{J^{(1)}}=\left(\frac{\partial X^{(2)}}{\partial J^{(1)}}\right)_{J^{(2)}}$$
$$\left(\frac{\partial J^{(1)}}{\partial X^{(2)}}\right)_{X^{(1)}}=\left(\frac{\partial J^{(2)}}{\partial X^{(1)}}\right)_{X^{(2)}}$$
$$\left(\frac{\partial J^{(1)}}{\partial J^{(2)}}\right)_{X^{(1)}}=-\left(\frac{\partial X^{(2)}}{\partial X^{(1)}}\right)_{J^{(2)}}$$
$$\left(\frac{\partial J^{(2)}}{\partial J^{(1)}}\right)_{X^{(2)}}=-\left(\frac{\partial X^{(1)}}{\partial X^{(2)}}\right)_{J^{(1)}}$$

M. Huetter

C. Beretta (later this afternoon)

A. Mielke (in the context of diffusion – 2013)

reminder:

(Grad-Villani) solutions of (and thus physics associated with) $\frac{dx}{dt} = [\Xi_{x^\star}]_{x^\star = S_x}$ are very different from solutions of (and the physics associated with) $\frac{dx}{dt} = LE_x + [\Xi_{x^\star}]_{x^\star = S_x}$

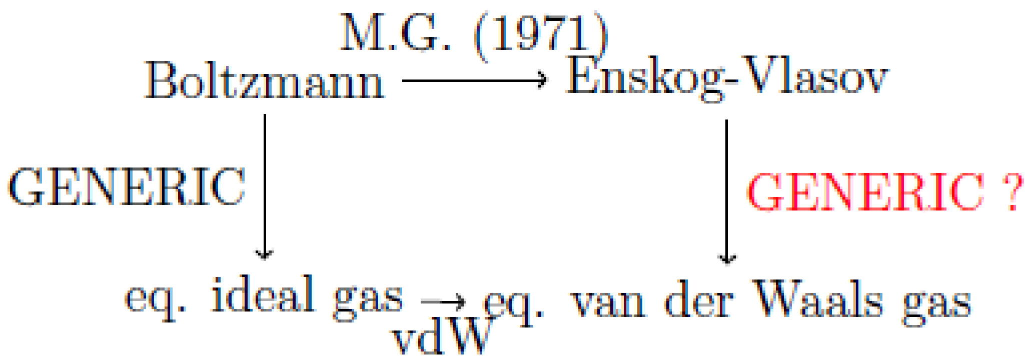
What is common to all of us   a bright future

Framework for modeling ; modules (1) state variables, (2) their kinematics (i.e. Poisson bracket), (3) thermodynamic forces, dissipation, (4) energy and entropy as functions of the chosen state variables
(e.g. !!! many new rheological models of complex fluids have been introduced in in this way)

Multiscale descriptions absolutely needed in nano and bio technologies
e.g biological systems – systems of membranes – heterogeneous systems
Dick Bedeaux, Hans Christian Oettinger, Leonard Sagis

Big data   artists are being employed; thermodynamics - aesthetics

Example of an open problem:



Enskog-Vlasov kinetic equation:

$\frac{\partial f(\boldsymbol{r},\boldsymbol{v})}{\partial t}$ = free flow term + Vlasov term + Enskog collision term

Enskog collision term = Boltzmann collision term with excluded volume $\Rightarrow$ the Enskog collision term becomes a sum of the Boltzmann dissipative (and time irreversible) term and a new term that is time reversible $\Rightarrow$ entropy is a sum of the Botzmann entropy and a new entropy corresponding to the excluded volume constraint. Problem: the standard Poisson bracket appearing in the Boltzmann kinetic theory $\rightarrow$ a new Poisson bracket taking into account the excluded volume constraint

A comment about derivations from “first principles”

1. What are the “first principles”
   (particle mechanics)
2. What is the (ideal) “derivation”
   step 1: get the phase portrait
   step 2: recognize a pattern in it (a pattern that represents a reduced – mesoscopic – experience)
3. What are the (real) derivations
   (various short cuts)