Continuum vs. kinetic theory: the role of entropy flux

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Motivation: describing dissipative fluids

- Kinetic theory: mostly for rarefied gases, dense matter(?), closure problem(?), large system of PDEs, stability(?)
- **Second law**: stability, consistent constitutive equations
- Causality: hyperbolic or parabolic?
- Relativistic models $\rightarrow$ hyperbolic equations: finite but can be higher than c; parabolic eq.: preserves infinite speed
  In local equilibrium:
  Eckart theory, unstable due to heat conduction
  Out of local equilibrium:
  Israel-Stewart (hyperbolic?, stability?) Müller-Ruggeri (divergence type, hyperbolic), etc...
- A simple benchmark: non-relativistic experiments!

Motivation for extensions of classical ideas

Experiments:

Heat conduction: ballistic and over-diffusive propagation
NaF and inhomogeneous samples
low and room temperature

Acoustics: rarefied gas, ballistic transport
monatomic and polyatomic gases
low and room temperature

Analogy:

(kinetic) modeling of rarefied gases, $\boxed{\text{phonon vs particles}}$

Theory?

Goal:
SIMPLE
INDEPENDENT OF MICRO / MESO / MACRO STRUCTURE
EASY TO USE AND IMPLEMENT

$\rightarrow$ NON-EQUILIBRIUM THERMODYNAMICS WITH INTERNAL VARIABLES

See also: Berezovski - Ván: Internal Variables in Thermoelasticity (2017, Springer)

Generalizations of entropy density and entropy flux

Classical:

- entropy density: $s = s_e(e, \rho)$
- entropy current: $J^i = q^i / T$
- local equilibrium
- Navier-Stokes-Fourier system

Extended Thermodynamics:

- entropy density: $s(e, \rho, q^i) = s_e(e, \rho) - \frac{m_1}{2} q_i q^i$
- entropy current: $J^i = q^i / T$
- q^i: heat flux $\equiv$ vectorial internal variable
- a hope of $\boxed{\text{hyperbolic}}$ equations
- no coupling between q^i and P^{ij} with these assumptions

Generalizations of entropy density and entropy flux

Rational Extended Thermodynamics
derived from kinetic theory for dense gases:

$$\partial_t F + \partial_k F^k = 0, \text{ mass balance}$$
$$\partial_t F^i + \partial_k F^{ik} = 0, \text{ momentum balance}$$
$$\partial_t F^{ij} + \partial_k F^{ijk} = P^{ij},$$
$$\partial_t G^{ii} + \partial_k G^{iik} = 0, \text{ energy balance}$$
$$\partial_t G^{ppi} + \partial_k G^{ppik} = Q^{ppi}$$

Reason: energy is the trace of pressure

- doubled hierarchy
- reason: originally the energy balance is not independent
- $\boxed{\text{hyperbolic}}$ equations
- constraints for coefficients

Generalizations of entropy density and entropy flux

Non-equilibrium thermodynamics with $\boxed{\text{current multipliers}}$

- entropy density: $s(e,\rho,q^i,Q^{ij}) = s_e(e,\rho) - \frac{m_1}{2} q_i q^i - \frac{m_2}{2} Q_{ij} Q^{ij}$
- entropy current: $J^i = \boxed{b^i{}_j} q^j + \boxed{B^i{}_{jk}} Q^{jk}$

- q^i: heat flux $\equiv$ vectorial internal variable
- $Q^{jk} \equiv$ tensorial internal variable: pressure!
- $\boxed{b^i{}_j \text{ and } B^i{}_{jk}\text{: current multipliers}}$

  $\boxed{\rightarrow \text{coupling between } q^i \text{ and } P^{ij}}$ $\Rightarrow$ CONSEQUENCE:
- parabolic equations $\rightarrow$ simplified to hyperbolic ones

LET US SEE THE EXAMPLES!

Generalization of heat conduction

Rigid body $\rightarrow \rho = const.$

Entropy production: $\sigma_s = \dot{s} + \partial_i J^i \geq 0$ in 1 spatial dimension:

$$\left(b - \frac{1}{T}\right)\partial_x q + \left(\partial_x b - m_1 \partial_t q\right) q - \left(\partial_x B - m_2 \partial_t Q\right) Q + B \partial_x Q \geq 0$$

Linear relations between *thermodynamic fluxes* and *forces*, isotropy:

$$\begin{aligned}
m_1 \partial_t q - \partial_x b &= -l_1 q, \\
m_2 \partial_t Q - \partial_x B &= -k_1 Q + k_{12} \partial_x q, \\
b - \frac{1}{T} &= -k_{21} Q + k_2 \partial_x q, \\
B &= n \partial_x Q.
\end{aligned}$$

Generalization of heat conduction

Rigid body $\to \rho = const.$

Entropy production: $\sigma_s = \dot{s} + \partial_i J^i \geq 0$ in 1 spatial dimension:

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Linear relations between *thermodynamic fluxes* and *forces*:

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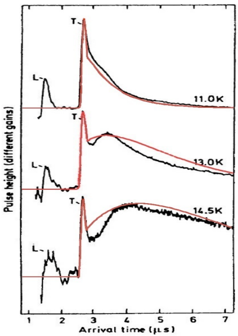
b - \frac{1}{T} &= -k_{21} Q + \cancel{k_2 \partial_x q}, \\
B &= \cancel{n \partial_x Q}.
\end{aligned}$$

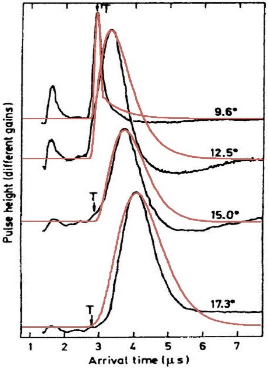
Compatibility with kinetic theory, hyperbolic eq.

$\Rightarrow$ SAME structure as 3 momentum eqs. of phonon hydro.

Ballistic-conductive system, tested on NaF experiments!

$$
\begin{aligned}
\rho c \partial_t T + \partial_x q &= 0, \\
\tau_q \partial_t q + q + \lambda \partial_x T + \kappa \partial_x Q &= 0, \\
\tau_Q \partial_t Q + Q + \kappa \partial_x q &= 0.
\end{aligned}
$$





Generalization of fluid dynamics: Meixner's theory

- Balances: mass, energy, momentum $\rightarrow$
  $\dot{\rho} + \rho\partial_i v^i = 0,$
  $\rho\dot{e} + \partial_i q^i = -P^{ij}\partial_i v_j,$
  $\rho\dot{v}^i + \partial_j P^{ij} = 0,$
  and $P^{ij} = \Pi^{ij} + p\delta^{ij}$ (static (p) és dynamic (Π^{ij}) pressure).
- entropy density: $s(e, \rho, Q^{ij}) = s_{eq}(e, \rho) - \frac{m_1}{2} Q_{ij} Q^{ij},$
- entropy current: $J^i = q^i/T$, classical! $\rightarrow$
- NO coupling!

Constitutive equations: generalized Navier-Stokes

$$q + \lambda\partial_x T = 0,$$
$$\tau_\Pi \dot{\Pi} + \Pi + \nu\partial_x v + \phi\partial_x \dot{v} = 0.$$

Q^{ij}: pressure!

Heat conduction? Coupling?

Generalization of fluid dynamics: RET

Rational Extended Thermodynamics
Arima et al. (2014)

$$\partial_t F + \partial_k F^k = 0, \text{ mass balance}$$
$$\partial_t F^i + \partial_k F^{ik} = 0, \text{ momentum balance}$$
$$\partial_t F^{ij} + \partial_k F^{ijk} = P^{ij},$$
$$\partial_t G^{ii} + \partial_k G^{iik} = 0, \text{ energy balance}$$
$$\partial_t G^{ppi} + \partial_k G^{ppik} = Q^{ppi}$$

Constitutive equations (1D), linearized, coupled!

$$\tau_q \dot{q} + q + \lambda \partial_x T + a T_0 \partial_x \Pi = 0,$$
$$\tau_\Pi \dot{\Pi} + \Pi + \nu \partial_x v + \frac{\nu}{1 + c_v^*} \partial_x q = 0.$$

Generalization of fluid dynamics: NET + IV

Non-equilibrium thermodynamics with internal variables

Balances +

- entropy density:
  $s(e, \rho, q^i, Q^{ij}) = s_e(e, \rho) - \frac{m_1}{2} q^i \cdot q^i - \frac{m_2}{2} Q_{ij} Q^{ij}$
- entropy current: $J^i = \boxed{b^i{}_j} q^j + \boxed{B^i{}_{jk}} Q^{jk} \to$ coupling!

Constitutive equations (1D), linearized, coupled!

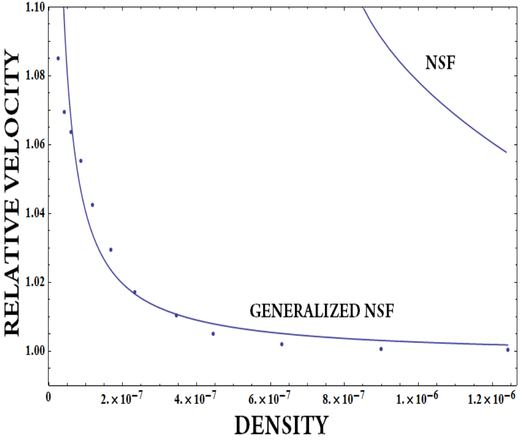
$$\tau_q \dot{q} + q + \lambda \partial_x T + \varepsilon \partial_x \Pi = 0,$$
$$\tau_\Pi \dot{\Pi} + \Pi + \nu \partial_x v + \eta \partial_x q = 0.$$

Q^{ij}: pressure = Meixner's theory!

"Ballistic generalization": **thermodynamic equivalence** between phonon and real gases!

Generalization of fluid dynamics: NET + IV

Preliminary test: acoustic damping in rarefied gases



Thank you for your kind attention!

"Death match" of different descriptions I.

Phonon hydrodynamics (RET) vs NET+IV

At least N=30 momentum eqs. vs 3 eqs.

No. of fitted parameters: 2 relaxation time vs. 2+1 parameters

Solved on semi-infinite region vs real domain

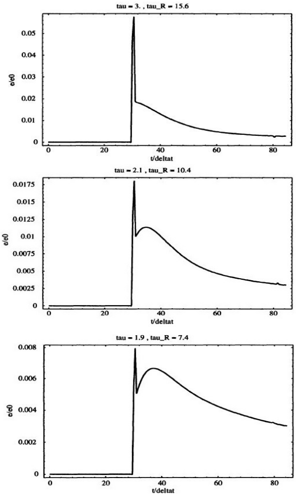
Relative amplitudes: false vs true

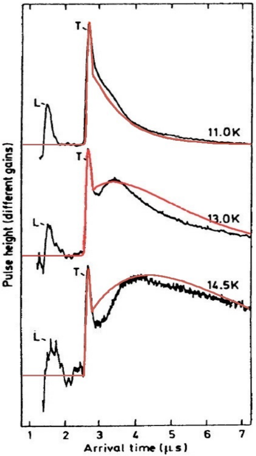
Summary: RET results are more like model testing than fitting;

Wrong: heat pulse length, sample size, thermal conductivity

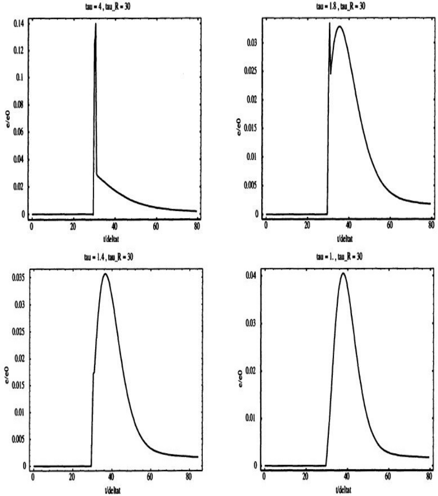
Is the RET model appropriate? Can not be decided.

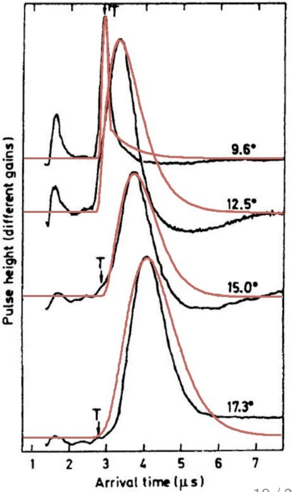
"Death match" of different descriptions II.





"Death match" of different descriptions III.





"Death match" of different descriptions IV.

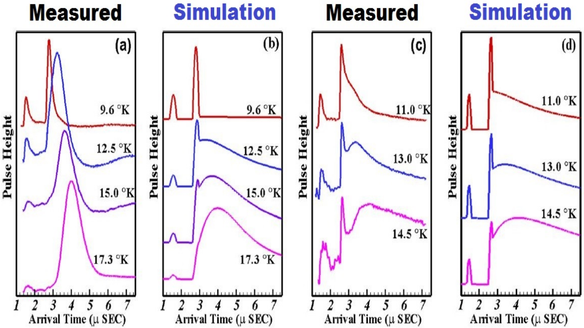
Hybrid phonon gas model of Y. Ma vs NET+IV

Longitudinal signal: artificial extension vs simplified model

Fitted parameters: 2 relaxation time vs 2+1

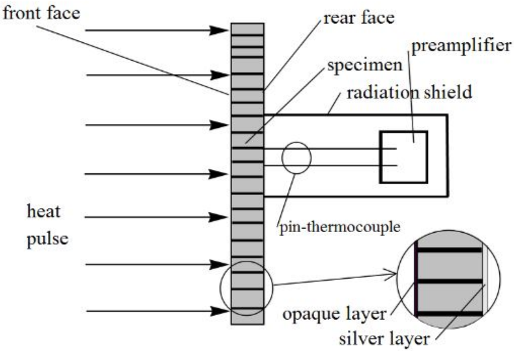
Boundary conditions: no information vs effective cooling

Wrong thermal conductivity, no information about the others.



What about on room temperature?

Role of material heterogeneities?! Let's see the experiments!

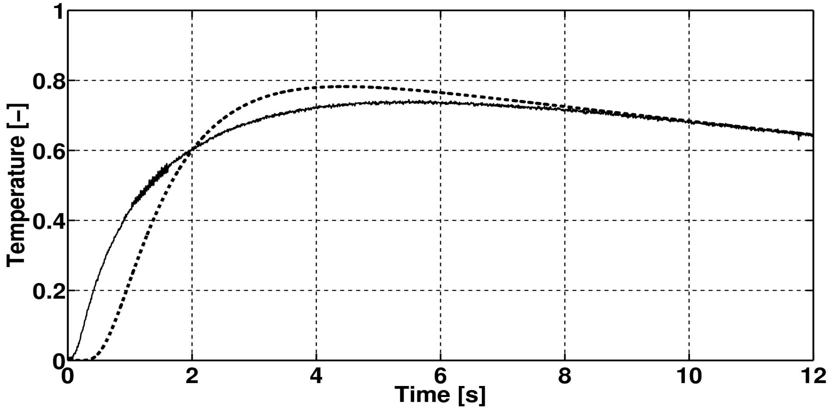


Arrangement of the measurement, DEE BME

Over-diffusive phenomenon I.

Measurement at room temperature, metal foam sample

$\tau_q \partial_{tt} T + \partial_t T = a \partial_{xx} T + \kappa^2 \partial_{txx} T$, Fourier equation



Over-diffusive phenomenon II.

Measurement at room temperature, metal foam sample

$\tau_q \partial_{tt} T + \partial_t T = a \partial_{xx} T + \kappa^2 \partial_{txx} T$, Guyer-Krumhansl equation,

$\kappa^2/\tau_q > a$!! Enhanced diffusion?!