Extended Thermodynamics and Moment Methods: Successes and Challenges

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The Topic as Questions

- **which physical quantities do we need to describe a system?**
- **what are the equations for these variables?**
- **what features of description do we need/want/wish for?**

Answers depend on

- **desired resolution**
- **degree of non-equilibrium in the system**

Restriction: we only talk about ideal gases

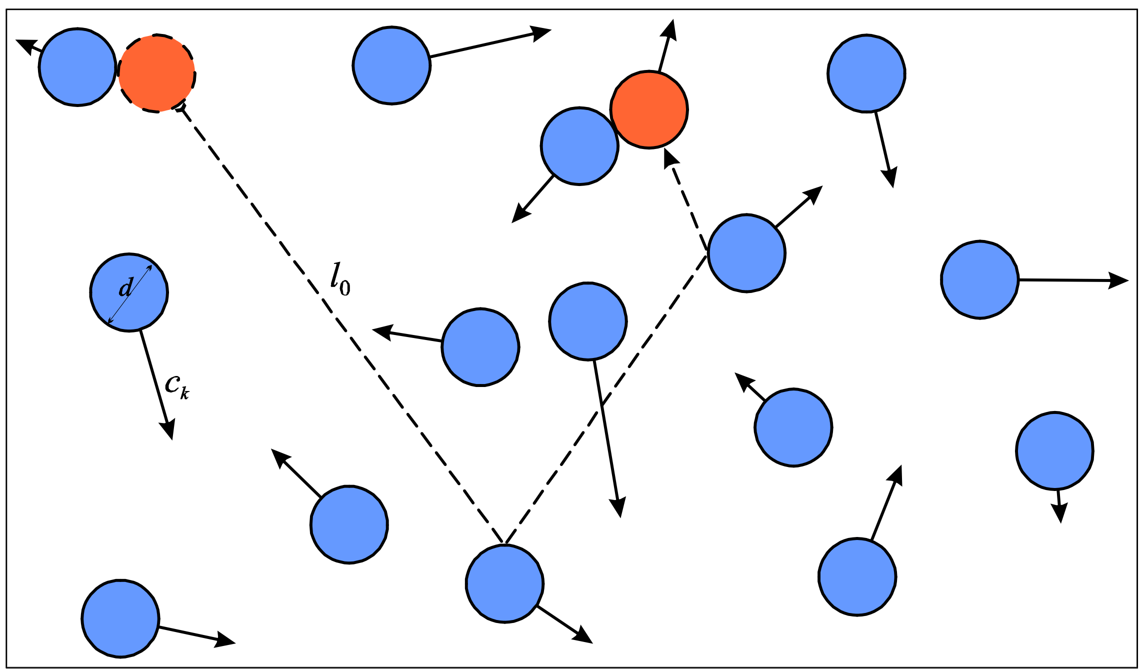
Let's look at a gas

mean free path d - particle diameter, n - number density

$$l_0 = \frac{1}{\sqrt{2}\pi d^2 n}$$

Knudsen number

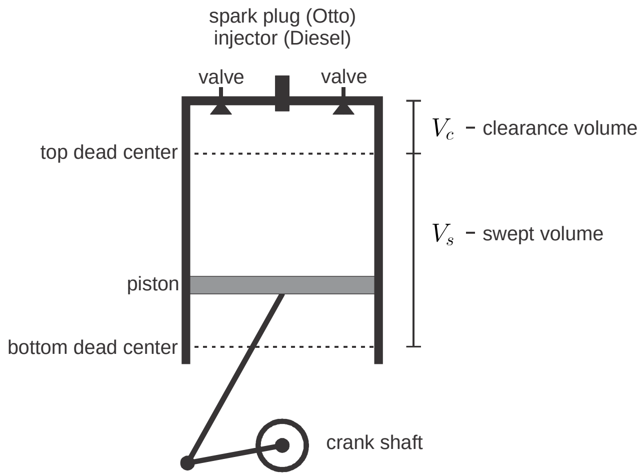
$$\mathrm{Kn} = \frac{\text{mean free path}}{\text{relevant process length}} = \frac{l_0}{L}$$



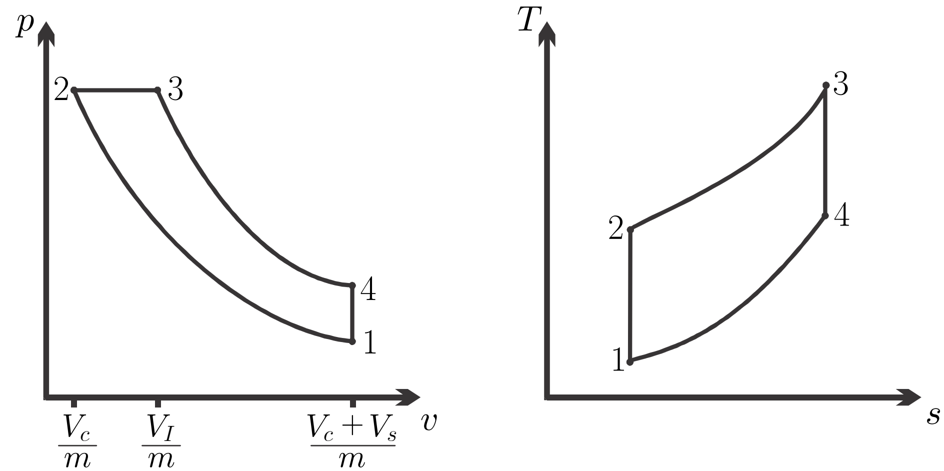
micro: **for** $p = 1$ bar $\Rightarrow l_0 \simeq 0.1\,\mu$m, **vacuum:** **for** $p = 1$ Pa $\Rightarrow l_0 \simeq 1\,\mathrm{cm}$

$\Rightarrow$ **up to 10^{23} particles in interaction**

Classical Thermodynamics



internal combustion engine



Diesel cycle

temperature, volume, mass $T \quad , \quad V \quad , \quad m$

equations of state $(\rho = m/V)$ $p\,(\rho, T) \quad , \quad u\,(\rho, T) \quad , \quad s\,(\rho, T)$

pressure, int. energy, entropy

1st and 2nd law $\frac{d\,(mu)}{dt} = \dot{Q} - p\frac{dV}{dt} \quad , \quad \frac{d\,(ms)}{dt} = \frac{\dot{Q}}{T} + \dot{S}_{gen}$

10^{23} particles described by a handful of properties/equations!

Dominated by global collective behavior (independent of details of interaction)

Classical Hydrodynamics

spatial/temporal resolution: density, velocity, temperature in a continuum cell at x_k, t

$$\rho\left(x_k, t\right) \quad , \quad v_i\left(x_k, t\right) \quad , \quad T\left(x_k, t\right)$$

equilibrium eqs. of state hold locally

$$p\left(T, \rho\right) \quad , \quad u\left(T, \rho\right) \quad , \quad s\left(T, \rho\right)$$

Conservation laws

mass $$\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} = 0$$

momentum $$\rho\frac{Dv_i}{Dt} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = G_i$$

energy $$\frac{3}{2}\rho\frac{Du}{Dt} + \frac{\partial q_k}{\partial x_k} = -\left(p\delta_{ik} + \sigma_{ik}\right)\frac{\partial v_i}{\partial x_k}$$

stress and heat flux as constitutive eqs: Navier-Stokes, Fourier

$$\sigma_{ik} = -2\mu\frac{\partial v_{\langle i}}{\partial x_{k\rangle}} \quad , \quad q_i = -\kappa\frac{\partial \theta}{\partial x_i}$$

dominated by local collective behavior at x_k and vicinity dx_k

viscosity, heat conductiovity μ, κ depend on molecular interaction

How do we know?

- **Experience!!**

- **Macroscopic model development from reasonable assumptions**
  - Equilibrium Thermodynamics
  - Non-equilibrium Thermodynamics
  - Extended Thermodynamics

- **Approximation or coarse graining of microscopic models**
  - **Mechanics:** location x_i and velocity c_i for 10^{23} particles
  - **Kinetic theory:** Boltzmann equation for velocity distribution $f\left(x_i, t, c_i\right)$

best macroscopic models based on:

experience, reasonable assumptions, microscopic model

Microscopic Model: Boltzmann equation (mon-atomic gas)

particle location x_i, velocity c_i

velocity distribution

$$f(x_k, t, c_k)\, d\mathbf{c} d\mathbf{x} \;=\; \#\text{ of particles in } d\mathbf{c} d\mathbf{x} \text{ at } t$$

Boltzmann equation change of f due to transport, particle-particle collisions

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = \mathcal{S}(f, f) = \int \int_0^{2\pi} \int_0^{\pi/2} \left(f' f^{1\prime} - f f^1 \right) \, g\, \sigma_{coll} \sin\Theta \, d\Theta \, d\varepsilon \, d\mathbf{c}^1$$

macroscopic quantities are moments of f (peculiar velocity $C_i = c_i - v_i$)

mass density	$\rho = m \int f \, d\mathbf{c}$
momentum density	$\rho v_i = m \int c_i f \, d\mathbf{c}$
energy density	$\rho u = \frac{3}{2}\rho\theta = \frac{m}{2} \int C^2 f \, d\mathbf{c}$
pressure tensor	$p_{ij} = p\delta_{ij} + \sigma_{ij} = m \int C_i C_j f d\mathbf{c}$
heat flux vector	$q_i = \frac{m}{2} \int C^2 C_i f d\mathbf{c}$

If we know $f(x_k, t, c_k)$ we know everything we want to know (and far more)!

Boltzmann equation and moments (mon-atomic gas)

define velocity moments/fluxes/productions of f: base functions $\varphi_A(c_i)$

$$u_A = \int \varphi_A(c_i)\, f d\mathbf{c} \quad , \quad F_{Ak} = \int \varphi_A(c_i)\, c_k f d\mathbf{c} \quad , \quad P_A = \int \varphi_A(c_i)\, \mathcal{S}(f,f)\, d\mathbf{c}$$

moment equations: have balance law form

$$\frac{\partial u_A}{\partial t} + \frac{\partial F_{Ak}}{\partial x_k} = P_A \quad , \quad A = 1, \cdots, N$$

includes conservation laws for mass, momentum, energy

entropy and 2nd law (H-theorem): special choice $\varphi = -k \ln \frac{f}{y}$

$$\frac{\partial \eta}{\partial t} + \frac{\partial \phi_k}{\partial x_k} = \Sigma \geq 0$$

$$\eta = -k \int f \ln \frac{f}{y} d\mathbf{c} \quad , \quad \phi_k = -k \int c_k f \ln \frac{f}{y} d\mathbf{c} \quad , \quad \Sigma = -\int \ln \frac{f}{y} \mathcal{S}(f,f)\, d\mathbf{c} \geq 0$$

Boltzmann equation has thermodynamic structure!

Generalization: entropy as number of microstates $H = k \ln \Omega$

note: $\Sigma \geq 0$ due to special form of collision term $\mathcal{S}(f,f)$, no details

Boltzmann Equation and Equilibrium Thermodynamics

Knudsen number as smallness parameter

$$\mathrm{Kn} = \frac{\text{mean free path } l_0}{\text{macroscopic length scale } L}$$

scaled Boltzmann equation

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = \frac{1}{\mathrm{Kn}} \mathcal{S}\left(f, f\right)$$

$\mathrm{Kn} \longrightarrow 0$: **equilibrium condition** (infinitely many collisions)

$$\mathcal{S}\left(f_{|E}, f_{|E}\right) = 0$$

equilibrium distribution is the Maxwellian: ideal gas: $p = \rho\theta,\ \ \theta = RT,\ \ C_i = c_i - v_i$

$$f_{|E} = \frac{\rho}{m} \sqrt{\frac{1}{2\pi\theta}}^{3} \exp\left[-\frac{C^2}{2\theta}\right]$$

equilibrium described through a handful of (local) properties: ρ, θ, v_i

note: for Maxwellian $\sigma_{ij} = m \int C_i C_j f_{|E} d\mathbf{c} = 0$, $\quad q_i = \frac{m}{2} \int C^2 C_i f_{|E} d\mathbf{c} = 0 \quad \Rightarrow$ Euler

Boltzmann Equation and Hydrodynamics

Chapman-Enskog expansion: Knudsen number as smallness parameter

$$f \simeq f_{|E} + \mathrm{Kn}\, f^{(1)} + \mathrm{Kn}^2\, f^{(2)} + \cdots$$

$\mathcal{O}\left(\mathrm{Kn}^1\right)$ **approximation to Boltzmann** with variables ρ, v_i, θ

$$f_{CE}\left(\rho, v_i, T; \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \frac{\partial \theta}{\partial x_i}; \sigma_{coll}\right) = f_{|E}\left[1 + \sum_{r=0}^{n_b} a_r S_{\frac{5}{2}}^{(r)} \xi_{\langle i}\xi_{j\rangle} \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + \sum_{r=1}^{n_a} b_r S_{\frac{3}{2}}^{(r)} \xi_i \sqrt{\frac{2}{\theta}} \frac{\partial \theta}{\partial x_i}\right]$$

$\xi_i = C_i/\sqrt{\theta}$, coefficients a_r, b_r depend on collision cross section σ_{coll}; Sonine polynomials $S_{k+\frac{1}{2}}^{(r)}\left(\xi^2\right)$

constitutive equations for σ_{ij}, q_i : Navier-Stokes-Fourier

$$\sigma_{ij} = m \int C_i C_j f_{CE} d\mathbf{c} = -2\,\mu\left(T\right) \frac{\partial v_{\langle i}}{\partial x_{k\rangle}}$$

$$q_i = \frac{m}{2} \int C^2 C_i f_{CE} d\mathbf{c} = -\kappa\left(T\right) \frac{\partial \theta}{\partial x_i}$$

CE expansion provides explicit link between viscosity $\mu\left(T\right)$, heat conductivity $\kappa\left(T\right)$ and microscopic interaction σ_{coll}

Boltzmann Equation and Hydrodynamics (cont'd)

CE expansion

$$f_{CE} = f_{|E} + \mathrm{Kn}\, f^{(1)} + \mathrm{Kn}^2\, f^{(2)} + \cdots$$

thermal and caloric eqs of state for monatomic gas

$$p = \rho\theta \quad , \quad u = \frac{3}{2}\theta = \frac{3}{2}\frac{p}{\rho}$$

entropy to first order in Kn is equilibrium entropy $(\eta = \rho s)$

$$\eta = -k \int f_{CE} \ln \frac{f_{CE}}{y} d\mathbf{c} = \rho \ln \frac{\theta^{3/2}}{\rho} + \mathcal{O}\left(\mathrm{Kn}^2\right)$$

entropy flux to first order in Kn is Clausius entropy flux

$$\phi_k = -k \int c_k f_{CE} \ln \frac{f_{CE}}{y} d\mathbf{c} = \eta v_i + \frac{q_i}{T} + \mathcal{O}\left(\mathrm{Kn}^2\right)$$

$\Longrightarrow$

for the ideal gas all elements of equilibrium thermodynamics and hydrodynamics follow from kinetic theory to orders $\mathcal{O}\left(\mathrm{Kn}^0\right)$ and $\mathcal{O}\left(\mathrm{Kn}^1\right)$!

CE expansion identifies collective behavior when Kn is sufficiently small!

Now we can ask:

How can we describe systems far from equilibrium where Equilibrium Thermodynamics or Hydrodynamics are not valid anymore?

Our aim:

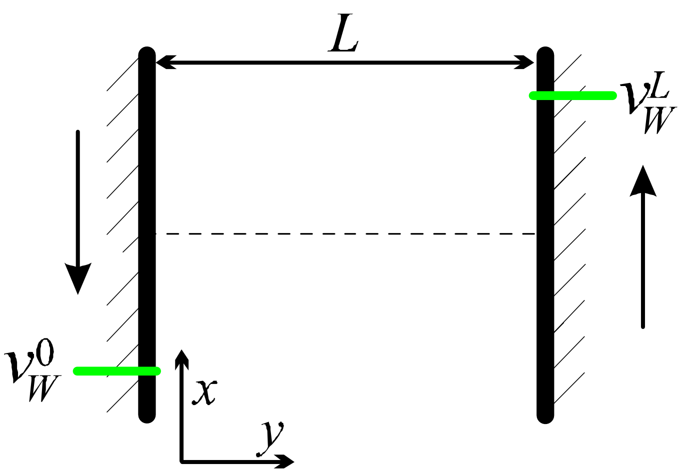
Systematic macroscopic description at arbitrary orders $O\left(\mathrm{Kn}^{\lambda}\right)$

Knudsen number and transport processes

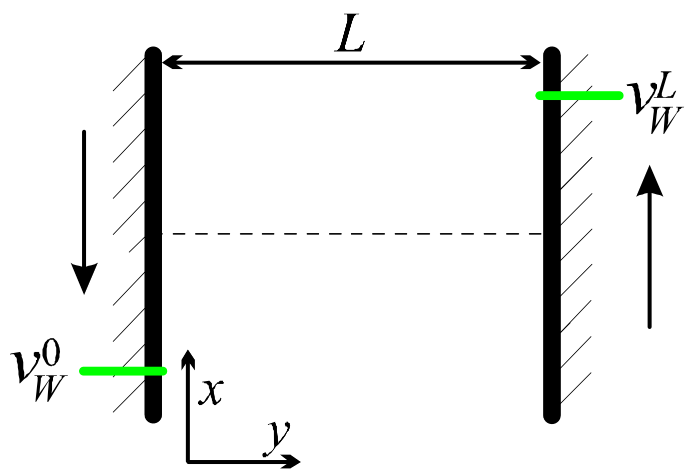
Knudsen number:

$$\mathrm{Kn} = \frac{l_0}{L}$$

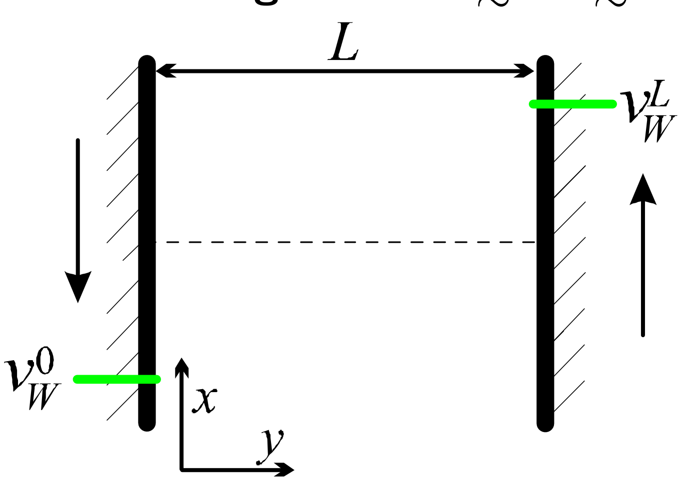
Navier-Stokes-Fourier: $\mathrm{Kn} \ll 1$



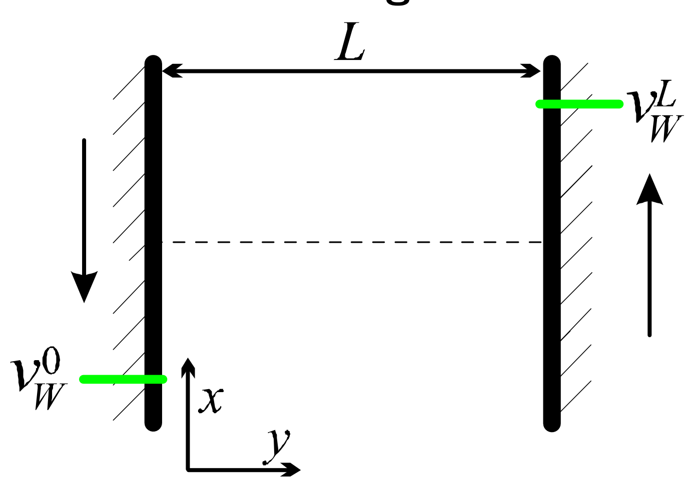
slip flow: $\mathrm{Kn} \lesssim 0.05$



transition regime: $0.05 \lesssim \mathrm{Kn} \lesssim 10$



free molecular flight: $\mathrm{Kn} \to \infty$



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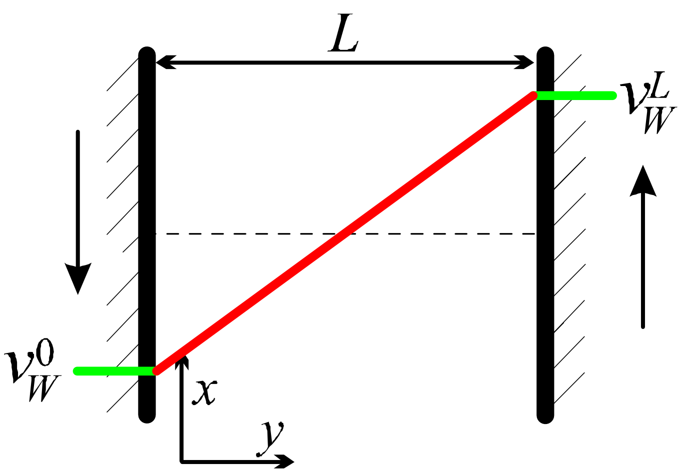

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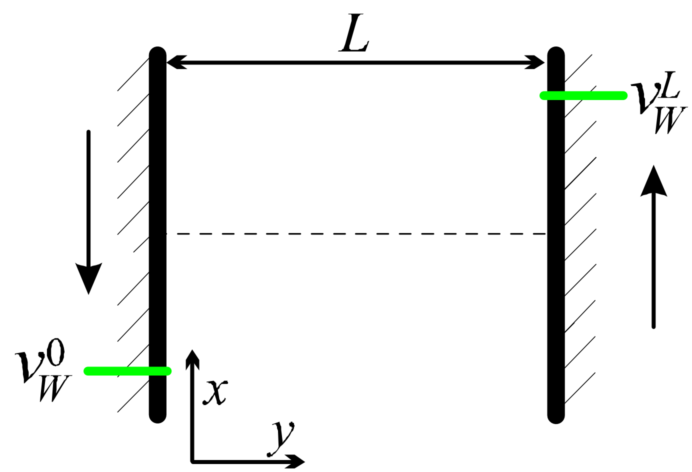

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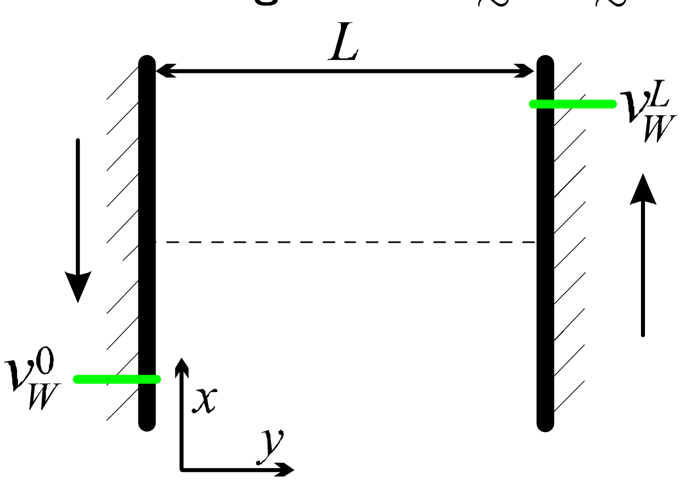

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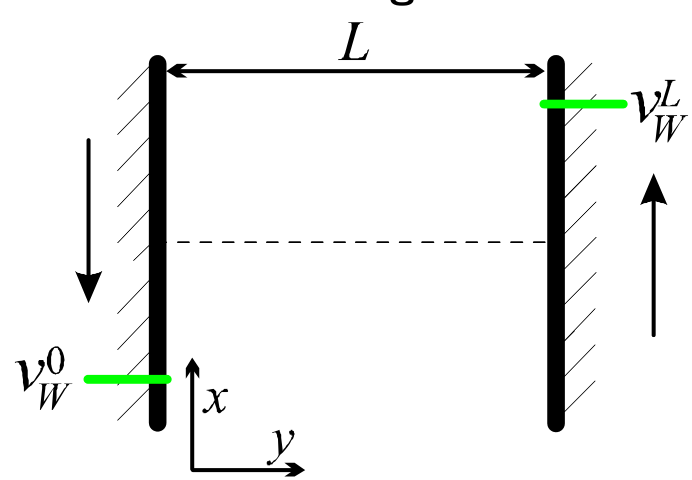

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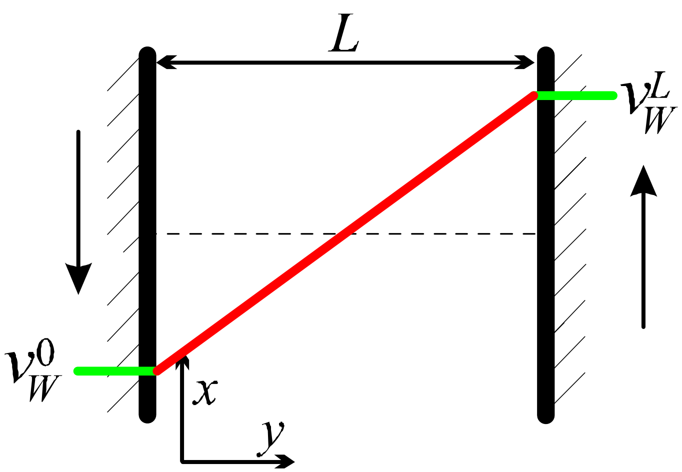

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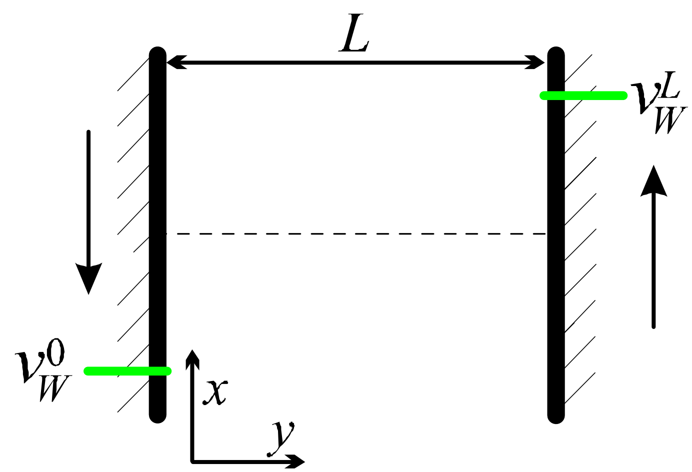

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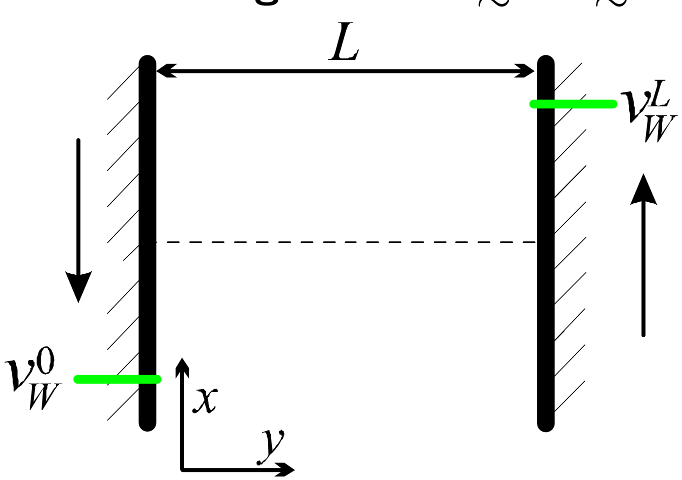

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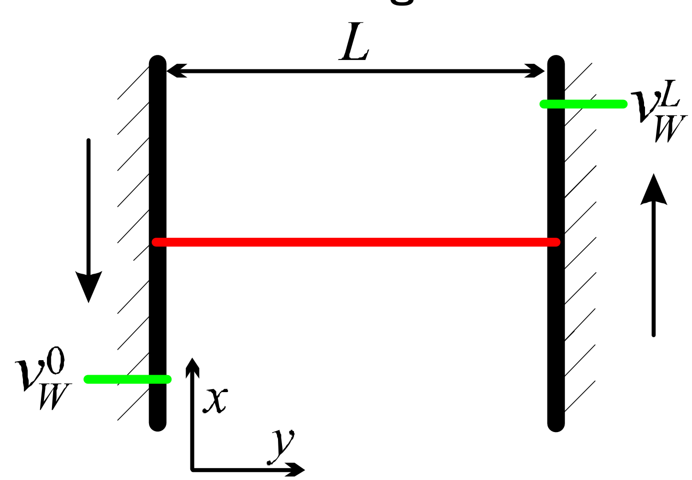

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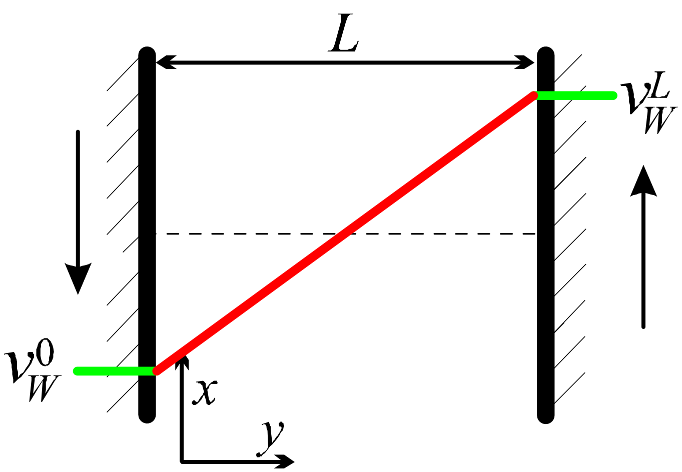

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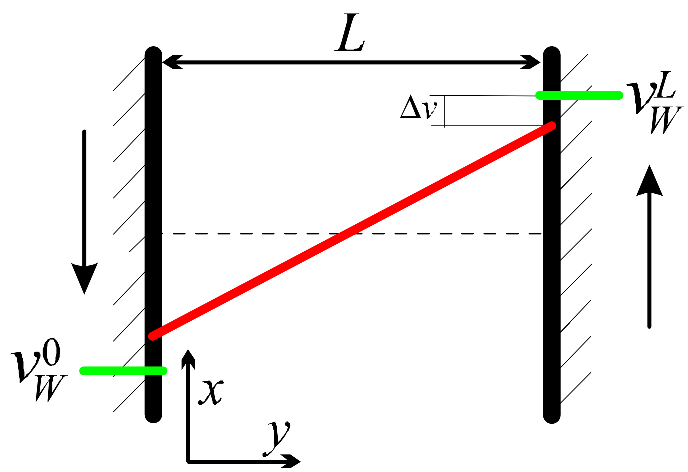

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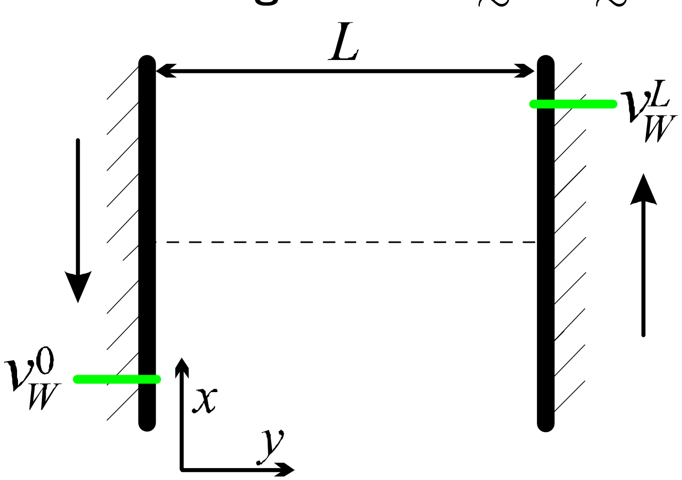

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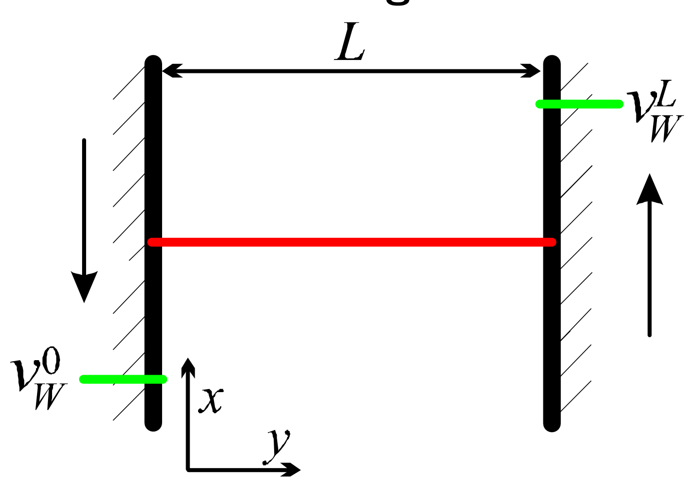

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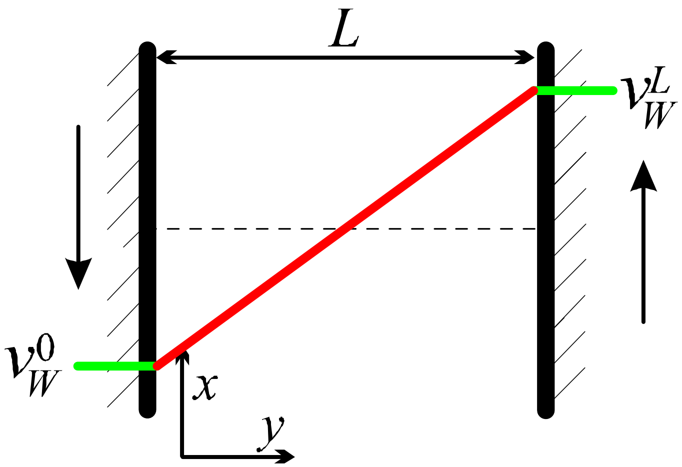

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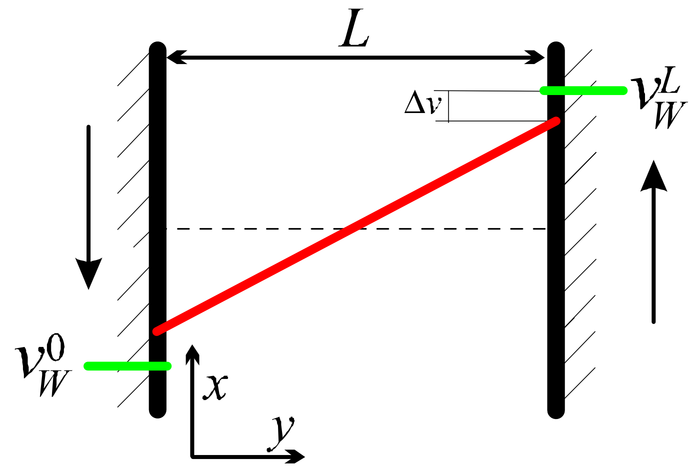

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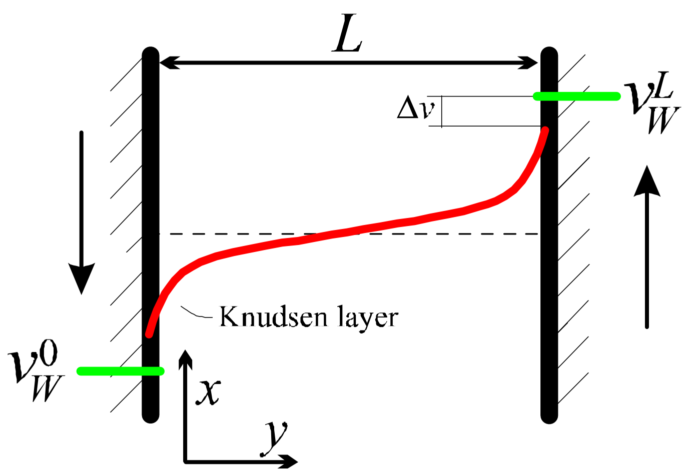

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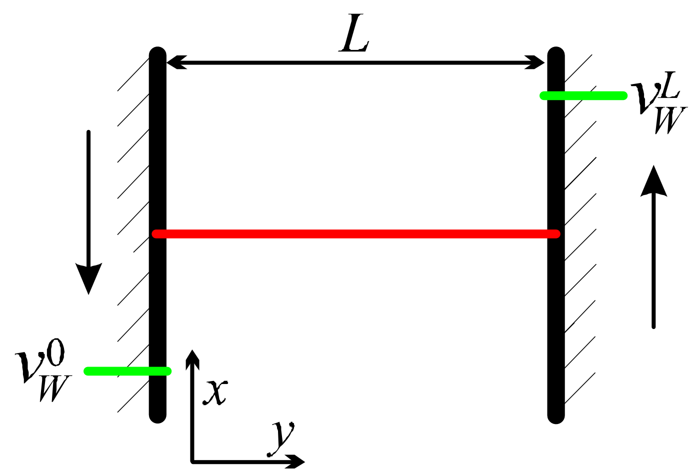
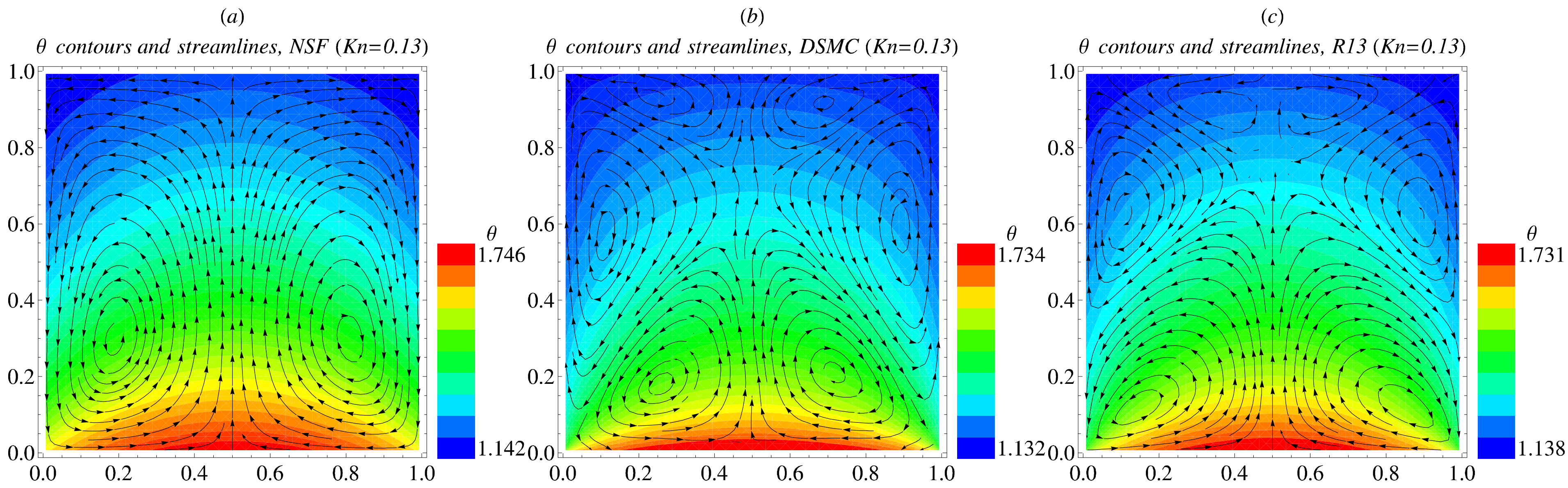


Example **(failure of hydrodynamics):**

2D Bottom heated plate, $\mathrm{Kn} = 0.13$

temperature contures and velocity streamlines



[Rana et al., Cont. Mech. Thermodyn. **27**, 2015]

Middle: DSMC solution of Boltzmann equation, exact, but takes days

Left: Classical Hydrodynamics (jump/slip NSF): minutes, but misses flow details

Right: Extended Thermodynamics (R13 eqs): minutes, has all details (approx)!!

Microscopic vs Macroscopic Description

Microscopic:

Particles as individuals, or groups of individuals

e.g., location x_i and momentum c_i at time t for *each* particle

$\Longrightarrow$ large number of variables

$\Longrightarrow$ tremendous effort of (numerical) calculation

$\Longrightarrow$ complete knowledge (too much!!)

Macroscopic:

Collective properties of particles

e.g., density ρ, velocity v_i, temperature T, stress σ_{ij}, heat flux q_i, etc., all at (x_k, t)

$\Longrightarrow$ small number of variables

$\Longrightarrow$ fast calculations possible

$\Longrightarrow$ explicit equations allow deeper insight into flow interactions

$\Longrightarrow$ limited knowledge (but *all we need*!!)

The Task:

Identify the relevant macroscopic properties/variables and their equations

We need good methods and good principles to guide us

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Let's look at Chapman-Enskog to higher order

CE expansion to 2nd order: Burnett equations

First order CE expansion worked well, so what about 2nd (or higher) orders?

$$\sigma_{ij} = \sigma_{ij}^{(1)} + \sigma_{ij}^{(2)} \quad , \quad q_i = q_i^{(1)} + q_i^{(2)}$$

$$\sigma_{ij}^{(1)} = -2\mu S_{ij} \text{ and } q_i^{(1)} = -\kappa \frac{\partial \theta}{\partial x_i} \qquad \text{with} \qquad \mu = \mu_0 \left(\frac{\theta}{\theta_0}\right)^{\omega} \quad , \quad \kappa = \frac{5}{2}\frac{\mu}{\mathrm{Pr}} \quad , \quad S_{ij} = \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$$

$$\sigma_{ij}^{(2)} = \frac{\mu^2}{p}\left[\varpi_1 \frac{\partial v_k}{\partial x_k} S_{ij} - \varpi_2 \left(\frac{\partial}{\partial x_{\langle i}}\left(\frac{1}{\rho}\frac{\partial p}{\partial x_{j\rangle}}\right) + \frac{\partial v_k}{\partial x_{\langle i}}\frac{\partial v_{j\rangle}}{\partial x_k} + 2\frac{\partial v_k}{\partial x_{\langle i}} S_{j\rangle k}\right) + \varpi_3 \frac{\partial^2 \theta}{\partial x_{\langle i}\partial x_{j\rangle}} + \varpi_4 \frac{\partial \theta}{\partial x_{\langle i}}\frac{\partial \ln p}{\partial x_{j\rangle}} + \varpi_5 \frac{1}{\theta}\frac{\partial \theta}{\partial x_{\langle i}}\frac{\partial \theta}{\partial x_{j\rangle}} + \varpi_6 S_{k\langle i} S_{j\rangle k}\right]$$

$$q_i^{(2)} = \frac{\mu^2}{\rho}\left[\theta_1 \frac{\partial v_k}{\partial x_k}\frac{\partial \ln \theta}{\partial x_i} - \theta_2\left(\frac{2}{3}\frac{\partial^2 v_k}{\partial x_k \partial x_i} + \frac{2}{3}\frac{\partial v_k}{\partial x_k}\frac{\partial \ln \theta}{\partial x_i} + 2\frac{\partial v_k}{\partial x_i}\frac{\partial \ln \theta}{\partial x_k}\right) + \theta_3 S_{ik}\frac{\partial \ln p}{\partial x_k} + \theta_4 \frac{\partial S_{ik}}{\partial x_k} + 3\theta_5 S_{ik}\frac{\partial \ln \theta}{\partial x_k}\right]$$

Burnett coefficients for power potentials [Reinecke & Kremer]

γ	ω	ϖ_1	ϖ_2	ϖ_3	ϖ_4	ϖ_5	ϖ_6	θ_1	θ_2	θ_3	θ_4	θ_5
ES-BGK		$\frac{4}{3}\left(\frac{7}{2}-\omega\right)$	2	$\frac{2}{\mathrm{Pr}}$	0	$\frac{2\omega}{\mathrm{Pr}}$	8	$\frac{5}{3}\frac{1}{\mathrm{Pr}^2}\left(\frac{7}{2}-\omega\right)$	$\frac{5}{2}\frac{1}{\mathrm{Pr}^2}$	$-\frac{2}{\mathrm{Pr}}$	$\frac{2}{\mathrm{Pr}}$	$\frac{7}{3}\frac{1}{\mathrm{Pr}}\left(1+\frac{1}{\mathrm{Pr}}+\frac{2\omega}{7}\right)$
5	1	3.333	2	3	0	3	8	9.375	5.625	-3	3	9.75
	ES	3.333	2	3	0	3	8	9.375	5.625	-3	3	9.75
7	0.833	3.561	2.003	2.793	0.217	1.942	7.781	10.038	5.647	-3.010	2.793	9.113
7.66	0.8	3.600	2.004	2.761	0.254	1.784	7.748	10.160	5.656	-3.014	2.761	9.019
9	0.75	3.679	2.007	2.695	0.328	1.466	7.681	10.402	5.674	-3.023	2.695	8.829
17	0.625	3.863	2.016	2.553	0.500	0.814	7.543	10.995	5.736	-3.053	2.553	8.442
∞	0.5	4.056	2.028	2.418	0.681	0.219	7.424	11.644	5.822	-3.09	2.418	8.286
	ES	4	2	3	0	1.5	8	11.25	5.625	-3	3	9.25

Burnett terms describe actual physics, such as thermal stresses, flow driven by heat flux

note: actual flow pattern results form interplay of bulk and boundary effects

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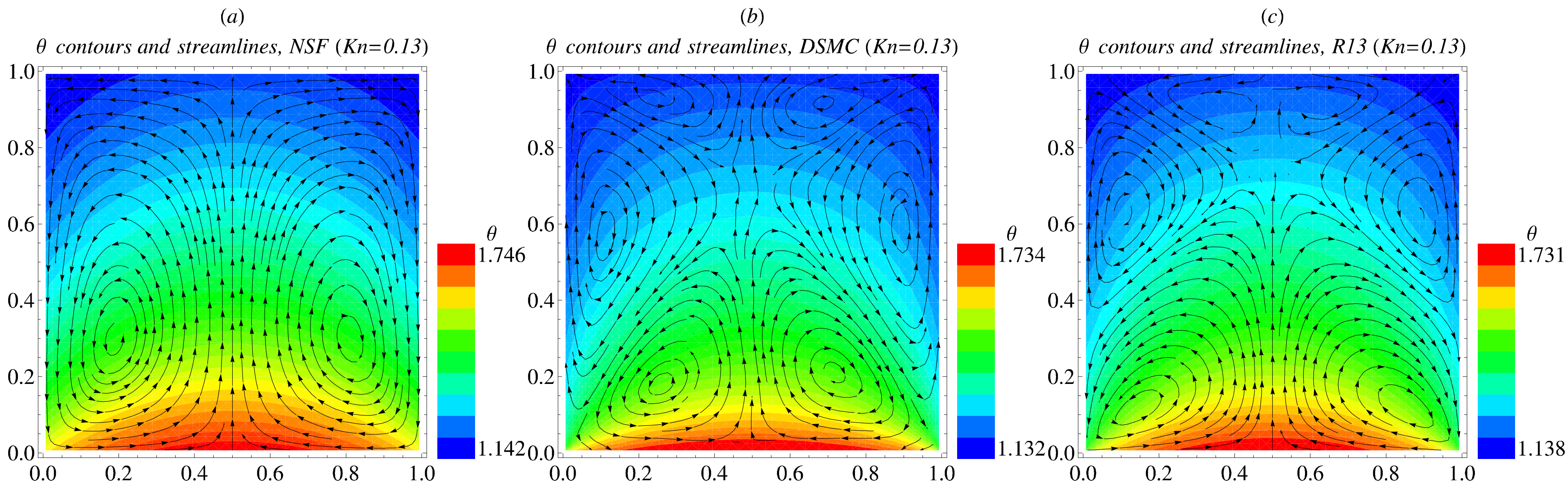

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Stability in time: Burnett/super-Burnett are unstable

disturbance in space: k real, $\Omega = \Omega_r(k) + i\Omega_i(k)$ complex

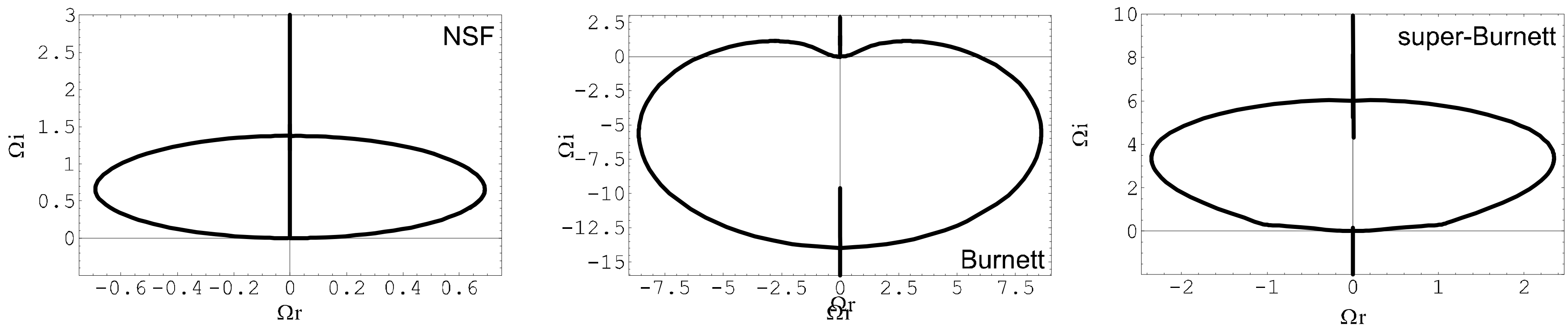
$$u_A = \tilde{u}_A \exp\left[i\left(\Omega t - kx\right)\right] = \tilde{u}_A \exp\left[-\alpha t\right] \exp\left[ik\left(v_{ph}t - x\right)\right]$$

phase velocity and damping:

$$v_{ph} = \frac{\Omega_r(k)}{k} \quad \text{and} \quad \alpha = \Omega_i(k)$$

stability:

$$\Omega_i(k) = \alpha \geq 0$$



CE expansion leads to instabilities!

The Task:

Identify the relevant macroscopic properties/variables and their equations

We need good methods and good principles to guide us

Let's look at phenomenological methods

The Task of Finding Continuum Approximations

conservation laws for mass, momentum, energy

5 equations for $\rho\,(x_k,t)$, $v_i\,(x_k,t)$, $\theta\,(x_k,t) = RT\,(x_k,t)$ [id. gas, $p = \rho\theta$, $e = \frac{3}{2}\rho\theta$]

$$\frac{D\rho}{Dt}+\rho\frac{\partial v_k}{\partial x_k}=0\ ,\quad \rho\frac{Dv_i}{Dt}+\frac{\partial\rho\theta}{\partial x_i}+\left[\frac{\partial\sigma_{ik}}{\partial x_k}\right]=0\ ,\quad \frac{3}{2}\rho\frac{D\theta}{Dt}+\rho\theta\frac{\partial v_k}{\partial x_k}+\left[\frac{\partial q_k}{\partial x_k}+\sigma_{kl}\frac{\partial v_k}{\partial x_l}\right]=0$$

closure problem: find equations for stress deviator σ_{ij}, heat flux q_i, etc

- **Linear Irreversible Thermodynamics:**
  few variables, some *non-local* constituitive relations

- **Extended Thermodynamics:**
  additional variables and balance law(s), only *local* constitutive relations

- **Moment methods:** based on kinetic theory
  additional variables and balance law(s) with *local* or *non-local* constit. relations

Pure Heat Transfer: Linear Irreversible Thermodynamics

1st law: conservation of energy e, therm. eq of state $e = e(T)$

$$\frac{\partial e}{\partial t} + \frac{\partial q_i}{\partial x_i} = 0$$

local thermodynamic equilibrium: Gibbs eq. $T d\eta = de$

construct entropy balance:

$$\frac{\partial \eta}{\partial t} \overset{\text{Gibbs}}{=} \frac{1}{T}\frac{\partial e}{\partial t} \overset{\text{1st law}}{=} -\frac{1}{T}\frac{\partial q_i}{\partial x_i} = -\frac{\partial \frac{q_i}{T}}{\partial x_i} + q_i \frac{\partial \frac{1}{T}}{\partial x_i} = -\frac{\partial \phi_i}{\partial x_i} + \Sigma$$

entropy flux and production

$$\phi_i = \frac{q_i}{T} \quad , \quad \Sigma = q_i \frac{\partial \frac{1}{T}}{\partial x_i} \overset{!!}{\geq} 0$$

constitutive eq. for q_i ensures $\sigma \geq 0$ $\implies$ **Fourier's law**, $\kappa(T) > 0$

$$q_i = \hat{\kappa} \frac{\partial \frac{1}{T}}{\partial x_i} = -\frac{\hat{\kappa}}{T^2}\frac{\partial T}{\partial x_i} = -\kappa \frac{\partial T}{\partial x_i}$$

note: $e(T)$ and $\eta(T)$ are *local*

$q_i = q_i\left(T, \frac{\partial T}{\partial x_i}\right)$ is *non-local*, no history dependence

Pure Heat Transfer: Extended Irreversible Thermodynamics

[I. Müller, D. Jou, etc]

1st law: conservation of energy e

$$\frac{\partial e}{\partial t} + \frac{\partial q_i}{\partial x_i} = 0$$

local constitutive equations: q_i as additional variable, *local* const. eq.

ansatz for Gibbs equation in non-equilibrium ($a > 0$ for convexity)

$$T d\eta = de - aTq_i dq_i$$

combine Gibbs eq and 1st law $\Longrightarrow$ 2nd law, entropy flux and production

$$\frac{\partial \eta}{\partial t} + \frac{\partial \phi_i}{\partial x_i} = \Sigma \quad \text{with} \quad \phi_i = \frac{q_i}{T} \quad , \quad \Sigma = q_i \left(\frac{\partial \frac{1}{T}}{\partial x_i} - a \frac{\partial q_i}{\partial t} \right) \overset{!!}{\geq} 0$$

eq. for q_i ensures $\sigma \geq 0$ $\Longrightarrow$ Cattaneo eq with $\hat{\kappa} a = \tau$

$$q_i = \hat{\kappa} \left(\frac{\partial \frac{1}{T}}{\partial x_i} - a \frac{\partial q_i}{\partial t} \right) \quad \Longrightarrow \quad \frac{\partial q_i}{\partial t} + \frac{\kappa}{\tau} \frac{\partial T}{\partial x_i} = -\frac{1}{\tau} q_i$$

note: balance law for heat flux accounts for non-locality and history!!

κ, τ from measurements, equations are stable

Rational Extended Thermodynamics [I. Müller, T. Ruggeri, etc]

1st law: conservation of energy e

$$\frac{\partial e}{\partial t} + \frac{\partial q_i}{\partial x_i} = 0$$

postulate: balance law form for flux, and fluxes of fluxes

$$\begin{aligned} \frac{\partial q_i}{\partial t} + \frac{\partial F_{ik}}{\partial x_k} &= P_i \\ \frac{\partial F_{ij}}{\partial t} + \frac{\partial F_{ijk}}{\partial x_k} &= P_{ij} \\ \frac{\partial F_{ijk}}{\partial t} + \cdots \quad &= \end{aligned}$$

general notation: note motivation from kinetic theory!

$$\frac{\partial u_A}{\partial t} + \frac{\partial F_{Ak}}{\partial x_k} = P_A \quad , \quad A = 1, \cdots, N$$

variables $u_A = \{e, q_i, F_{ij}, \ldots\}$

fluxes $F_{Ak} = \{q_i, F_{ik}, F_{ijk}, \ldots\}$

productions $P_A = \{0, P_i, P_{ij}, \ldots\}$

RET demands: *local* constitutive relations

$$F_{Ak} = F_{Ak}\left(u_B\right) \quad , \quad P_A = P_A\left(u_B\right)$$

Rational Extended Thermodynamics **(cont'd)** [I. Müller, T. Ruggeri, etc]

2nd law: must hold for *all solutions* of the field equations

$$\frac{\partial \eta}{\partial t} + \frac{\partial \phi_k}{\partial x_k} = \Sigma \geq 0$$

local constitutive relations: for entropy, flux, production

$$\eta = \eta\left(u_A\right) \ , \quad \phi_k = \phi_k\left(u_A\right) \ , \quad \Sigma\left(u_A\right)$$

convexity:

$$-\frac{\partial^2 \eta}{\partial u_A \partial u_B} \qquad \text{pos.definite}$$

Liu procedure: use Lagrange multipliers Λ_A, so that for *all values* of the fields u_A

$$\frac{\partial \eta}{\partial t} + \frac{\partial \phi_k}{\partial x_k} - \Lambda_A \left(\frac{\partial u_A}{\partial t} + \frac{\partial F_{Ak}}{\partial x_k} - P_A \right) = \Sigma \geq 0$$

$\Rightarrow$ **generalized Gibbs equation**, etc.

$$d\eta = \Lambda_A du_A \quad , \quad d\phi_k = \Lambda_A dF_{Ak} \quad , \quad \sigma = \Lambda_A P_A \geq 0$$

Rational Extended Thermodynamics (cont'd) [I. Müller, T. Ruggeri, etc]

Λ_A **as variables:** Legendre transform

$$\eta' = \Lambda_A u_A - \eta \quad , \quad \Phi'_k = \Lambda_A F_{Ak} - \Phi_k$$

so that

$$d\eta' = u_A d\Lambda_A \quad , \quad d\Phi'_k = F_{Ak} d\Lambda_A$$

symmetry relations

$$\frac{\partial^2 \eta'}{\partial \Lambda_A \partial \Lambda_B} = \frac{\partial u_A}{\partial \Lambda_B} = \frac{\partial u_B}{\partial \Lambda_A} \quad , \quad \frac{\partial^2 \Phi'_k}{\partial \Lambda_A \partial \Lambda_B} = \frac{\partial F_{Ak}}{\partial \Lambda_B} = \frac{\partial F_{Bk}}{\partial \Lambda_A}$$

Lagrange multipliers as variables

$$\frac{\partial u_A}{\partial \Lambda_B} \frac{\partial \Lambda_B}{\partial t} + \frac{\partial \bar{F}_{Ak}}{\partial \Lambda_B} \frac{\partial \Lambda_B}{\partial r_k} = P_A$$

Hyperbolicity: due to symmetry and convexity

$\Rightarrow$ **symmetric hyperbolic system with convex extension**

$\Rightarrow$ **finite speeds of propagation**

$\Rightarrow$ **well-posedness of Initial Value Problems**

Rational Extended Thermodynamics: Success and Problems

- few known systems with full RET structure (Euler, 10 moment)
- no guidelines on choice of variables ⇒ *trial and error*
- boundary conditions widely ignored in ET
- finite speed of propagation ⇒ discontinuities in shocks structures?!
- Extended Irreversible TD is approximation of Rational ET, with less structure
- Existing RET/EIT systems mostly equivalent to Grad-type moment systems.
  ⇒ Thermodynamic structure lost far from equilibrium
- EIT/RET/Grad show good results for linear bulk problems:
  ⇒ dispersion relation, light scattering
- most systems based on kinetic theory of gases, phonons, photons, electrons
- kinetic theory will explain why full RET is difficult (impossible?) to achieve

Use Kinetic Theory
for foundations, workable alternatives, boundary conditions

The Task:

Identify the relevant macroscopic properties/variables and their equations

We need good methods and good principles to guide us

Let's look at the moment method

Back to Kinetic Theory: Moment Method

assumption, as in ET: state described by moments $u_A = \int \varphi_A(c_i) f d\mathbf{c}$, $A = 1, \ldots, N$

$$\frac{\partial u_A}{\partial t} + \frac{\partial F_{Ak}}{\partial x_k} = P_A \quad , \quad A = 1, \ldots, N$$

moment closure problem: need constitutive equations for

$$F_{Ak} = \int \varphi_A(c_i) c_k f d\mathbf{c} \quad , \quad P_A = \frac{1}{\mathrm{Kn}} \int \varphi_A(c_i) \mathcal{S}(f) d\mathbf{c}$$

general ansatz: f depends on (x_k, t) through moments/derivatives, i.e., *non-local*

$$f(x_k, t, c_k) = f\left(u_A(x_k, t), \ldots, \frac{\partial^{r+s} u_A(x_k, t)}{(\partial x_i)^r \partial t^s}, \ldots; c_k\right)$$

special case: *local* constituitve eqs. as in ET

$$f(x_k, t, c_k) = f(u_A(x_k, t); c_k) \implies F_{Ak}(u_B) \quad , \quad P_A(u_B)$$

Questions that will keep us busy:

- **which moments ??**
- **how many moments ??**
- **how to close, ie, how to construct** $f(u_A(x_k, t); c_k)$ **??**

Maximum Entropy Principle = RET

use that phase density that maximizes entropy for given values of u_A!!

introduce Lagrange multipliers, and maximize without constraints

$$\Phi = -\int f \ln \frac{f}{y} d\mathbf{c} - \Lambda_A \left(\int \varphi_A f d\mathbf{c} - u_A \right) \longrightarrow \text{maximum}$$

$$\Rightarrow \quad f_{MEP} = y \exp\left[-1 - \Lambda_A \varphi_A\right]$$

this implies all RET features, e.g. convexity, and

$$d\eta = \Lambda_A du_A \quad , \quad d\phi_k = \Lambda_A dF_{Ak} \quad , \quad \Sigma = \Lambda_A P_A$$

Procedure, in principle,

- find $u_A(\Lambda_B) = \int \varphi_A f_{MEP}(\Lambda_B) \, d\mathbf{c}$
- invert to find $\Lambda_A(u_B)$
- find $F_{Ak}(u_B) = \int \varphi_A c_k f_{MEP}(\Lambda_B(u_C)) \, d\mathbf{c}$
- find $P_A(u_B) = \frac{1}{\mathrm{Kn}} \int \varphi_A \mathcal{S}(f_{MEP}(\Lambda_B(u_C))) \, d\mathbf{c}$
- also can be used to find $\eta = -k \int f \ln \frac{f}{y} d\mathbf{c}$, $\phi_k = -k \int c_k f \ln \frac{f}{y} d\mathbf{c}$ etc

Maximum Entropy Principle = RET

the problem: exponential distribution

$$f_{MEP} = y \exp\left[-1 - \Lambda_A \varphi_A\right]$$

and polynomial base functions

$$\varphi_A = c_{i_1} c_{i_2} \cdots c_{i_n}$$

$\Longrightarrow$ highest polynomial $\varphi_N = c^N$ must be $N = even$

$\Longrightarrow$ no analytical solution for integrals if $N > 2$

$\Longrightarrow$ determine all integrals numerically, on the fly, or in advance: **extremely costly**

and singularity: physically realistic moment states where entropy maximization problem has no solution [Junk, 1998]

McDonald found fit $F_{Ak}(u_C)$, $P_A(u_C)$ for 5 moments in 1D,

works on approximation for 14 moments in 3D ...

... but we'll need more than 14

MEP: Hyperbolicity, characteristic speeds, and shocks

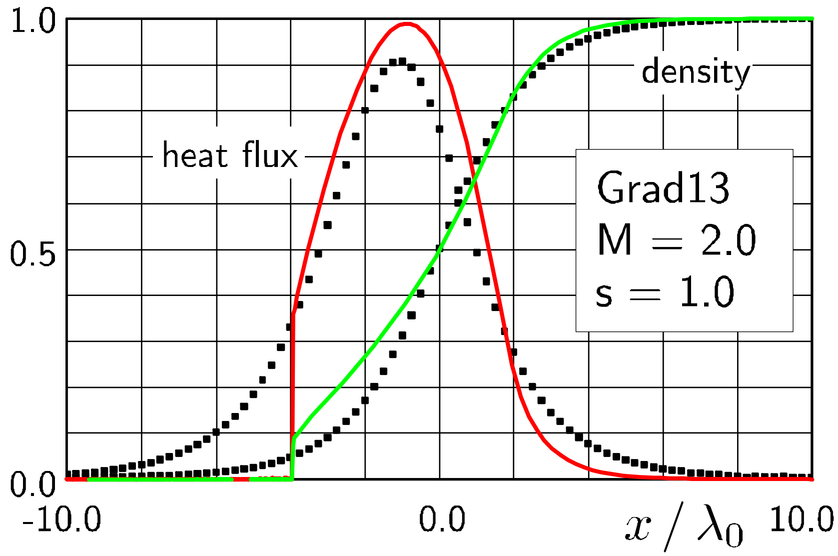
1D equations

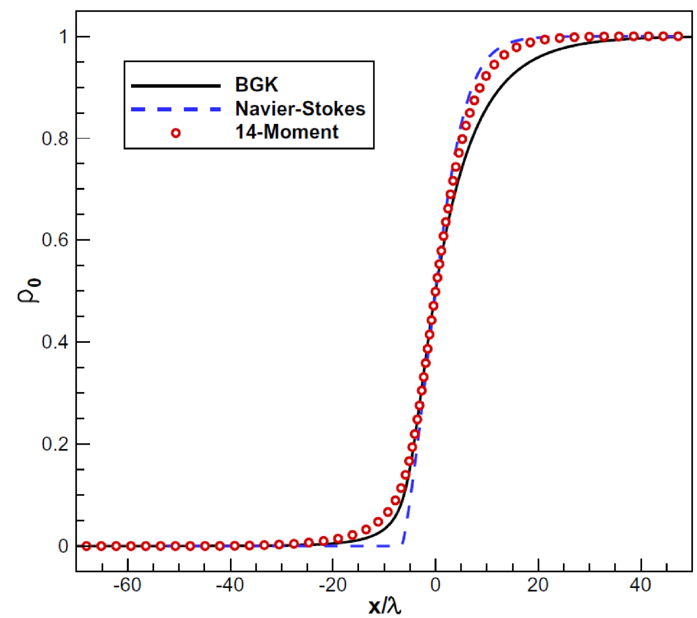
$$\frac{\partial u_A}{\partial t} + \frac{\partial F_{A1}}{\partial u_B}\frac{\partial u_B}{\partial x_1} = P_A$$

Characteristic speeds Γ_A : eigenvalues of $\frac{\partial F_{A1}}{\partial u_B}$

subshocks for $\Gamma_{\max} > \mathrm{Ma}$, eg. 13 moment ET

McDonald's 5 and 14 MEP approx: smooth shocks for all Ma **!**





(a) Normalized density, $\mathrm{Ma} = 8$.

singularity gives $\Gamma_{\max} \to \infty$ **!!!**

[McDonald and Torrilhon, JCP 251, 2013]

Some points to consider

MEP and RET are equivalent—with MEP program extremely difficult, one cannot expect access to RET with larger moment numbers!

Almost all known *Extended Thermodynamic Systems* are approximations which forfeit some thermodynamic or mathematical structure to workability

Typically, 2nd law/entropy can only be approximated

ET proponents emphasize hyperbolicity, but subshocks are not physical.

Approaches to force thermodynamic structure on equations, eg. Öttinger 13 moments, or Torrilhon's R13 with entropy, lead to poorer quality of predicitons

Even good macroscopic approximations to the Boltzmann equations can only approximate its features

Provocative Question:

IF we cannot have both, what do we value higher:

- **accuracy in approximation?**
- **thermodynamic/mathematical structure?**

Grad closure as approximation

MEP exponential f_{MEP} **can't be used** $\Longrightarrow$ rewrite

$$f_{MEP} = y \exp\left[-1 - \frac{1}{k}\Lambda_A \varphi_A\right] = f_{|E} \exp\left[-\frac{1}{k}\lambda_A \varphi_A\right]$$

$f_{|E}$ – Equilibrium (Maxwellian), λ_A – non-eq. part of Λ_A

Expansion for small λ_A

$$f_G \simeq f_{|E}\left[1 - \frac{1}{k}\lambda_A \varphi_A\right]$$

Linear relation

$$u_A - u_{A|E} = -\frac{1}{k}\int f_{|E}\, \varphi_A \varphi_B \, d\mathbf{c}\, \lambda_B = \mathcal{A}_{AB}\lambda_B \quad \Longrightarrow \quad \lambda_B = \mathcal{A}_{BA}^{-1}\left(u_A - u_{A|E}\right)$$

closure $F_{Ak}(u_B)\,,\ P_A = P_A(u_B)$ **straightforward** $\Longrightarrow$

Explicit Grad moment systems for arbitrary number of moments!!

- **Which and how many moments ??**
- **How to reduce a large system to its essence ??**
- **Thermodynamic structure ??**
- **Quality of predictions ??**

Order of magnitude method [HS 2004]

Step 1:

- **set up moment system for arbitrary number of moments** N
- **close with Grad method** (or other . . .)

Step 2:

- **Chapman-Enskog expansion to find leading** $\mathrm{Kn}-$**order of moments**
- **linear combination of moments such that number of moments at given** $\mathrm{Kn}-$**order is minimal**
- **repeat for next order of magnitude**

Step 3:

- **use** $\mathrm{Kn}-$**orders to rescale equations for new moments**
- **use scaling for model reduction to a given order of accuracy**

Overall goal: Reduce large moment system to its essence

Order of magnitude method [HS 2004]

$$\mathrm{Kn} = \frac{\text{mean free path}}{\text{macroscopic lengthscale of process}}$$

Step by step derivation of equations for the collective from Boltzmann

- $\mathcal{O}\left(\mathrm{Kn}^0\right)$: **Euler**
- $\mathcal{O}\left(\mathrm{Kn}^1\right)$: **Navier-Stokes-Fourier**
- $\mathcal{O}\left(\mathrm{Kn}^2\right)$: **Grad 13**
- $\mathcal{O}\left(\mathrm{Kn}^3\right)$: **regularized 13 moment equations (R13)**

- **stable equations at all orders** [HS & MT 2003]
- **accessible for arbitrary interaction potentials** [HS 2005, HS & MT 2013]
- **application to phonon transport** [AM & HS in progress]
- **extension to polyatomic molecules** [BR & HS 2014]
- **extension to mixtures** [V.Gupta 2014]

Base: Moments and their equations

central moments C_i – peculiar velocity

$$u^a_{i_1\cdots i_n} = m\int C^{2a} C_{\langle i_1} C_{i_2}\cdots C_{i_n\rangle} f\, d\mathbf{c}$$

equilibrium values (from Maxwellian)

$$u^a_{|E} = (2a+1)!!\rho\theta^a \quad , \quad u^a_{i_1\cdots i_n|E} = 0 \;\; , \;\; n \geq 1$$

non-equilibrium moments

$$w^a = u^a - u^a_{|E} \quad , \quad u^a_{i_1\cdots i_n} \quad (a \geq 1)$$

general moment equation for central moments (no closure)

$$\frac{Du^a_{i_1\cdots i_n}}{Dt} + 2a u^{a-1}_{i_1\cdots i_n k}\frac{Dv_k}{Dt} + \frac{n}{2n+1}(2a+2n+1)\, u^a_{\langle i_1\cdots i_{n-1}}\frac{Dv_{i_n\rangle}}{Dt} + \frac{\partial u^a_{i_1\cdots i_n k}}{\partial x_k} + \frac{n}{2n+1}\frac{\partial u^{a+1}_{\langle i_1\cdots i_{n-1}}}{\partial x_{i_n\rangle}}$$
$$+ 2a u^{a-1}_{i_1\cdots i_n kl}\frac{\partial v_k}{\partial x_l} + 2a\frac{n+1}{2n+3}u^a_{\langle i_1\cdots i_n}\frac{\partial v_{k\rangle}}{\partial x_k} + 2a\frac{n}{2n+1}u^a_{k\langle i_1\cdots i_{n-1}}\frac{\partial v_k}{\partial x_{i_n\rangle}} + n u^a_{k\langle i_1\cdots i_{n-1}}\frac{\partial v_{i_n\rangle}}{\partial x_k}$$
$$+ u^a_{i_1\cdots i_n}\frac{\partial v_k}{\partial x_k} + \frac{n(n-1)}{4n^2-1}(2a+2n+1)\, u^{a+1}_{\langle i_1\cdots i_{n-2}}\frac{\partial v_{i_{n-1}}}{\partial x_{i_n\rangle}} = -\frac{1}{\mathrm{Kn}}\frac{1}{\tau}\sum_b C^{(n)}_{ab}\theta^{a-b}u^b_{i_1\cdots i_n}$$

mean free time: $\frac{1}{\tau} = \frac{1}{\tau_0}\rho\theta^{1-s}$ **BGK model:** $\mathcal{C}^{(n)}_{ab}$ diagonal **Maxwell molecules:** $\mathcal{C}^{(n)}_{ab}$ triangular

Order of magnitude method [HS 2004]

Step 1:

- set up moment system for arbitrary number of moments N
- close with Grad method (or alternative . . .)

Based on assumption that a large moment system ($N \gg 1$) contains all relevant physics from the kinetic equation.

Goal is to remove all unneccessary terms from the large system, retain the essence

note: closure affects mainly eqs for higher moments; how important are closure details?

Step 1: Grad closure for moment equations (linear, dimless)

Conservation laws

$$\frac{\partial\rho}{\partial t}+\frac{\partial v_k}{\partial x_k}=0 \quad , \quad \frac{\partial v_i}{\partial t}+\frac{\partial\rho}{\partial x_i}+\frac{\partial\theta}{\partial x_i}+\frac{\partial\sigma_{ik}}{\partial x_k}=G_i \quad , \quad \frac{3}{2}\frac{\partial\theta}{\partial t}+\frac{\partial v_k}{\partial x_k}+\frac{\partial q_k}{\partial x_k}=0$$

equations for higher moments (renumbered), $a=1,\ldots,N$

$$\frac{\partial\tilde{w}^a}{\partial t}+\sum_{b=1}^{N}\tilde{\mathcal{R}}_{ab}^{(1)}\frac{\partial\tilde{u}_k^b}{\partial x_k}-(2a+3)!!\frac{2\,(a+1)}{3}\frac{\partial q_k}{\partial x_k}=-\frac{1}{\mathrm{Kn}}\sum_{b=1}^{N}\tilde{\mathcal{C}}_{ab}^{(0)}\tilde{w}^b$$

$$\frac{\partial\tilde{u}_i^a}{\partial t}+\sum_{b=1}^{N}\tilde{\mathcal{R}}_{ab}^{(2)}\frac{\partial\tilde{u}_{ik}^b}{\partial x_k}+\frac{1}{3}\frac{\partial\tilde{w}^a}{\partial x_i}-\frac{(2a+3)!!}{3}\frac{\partial\sigma_{ik}}{\partial x_k}+(2a+3)!!\frac{a}{3}\frac{\partial\theta}{\partial x_i}=-\frac{1}{\mathrm{Kn}}\sum_{b=1}^{N}\tilde{\mathcal{C}}_{ab}^{(1)}\tilde{u}_i^b$$

$$\frac{\partial\tilde{u}_{ij}^a}{\partial t}+\frac{\partial\tilde{u}_{ijk}^a}{\partial x_k}+\frac{2}{5}\frac{\partial\tilde{u}_{\langle i}^a}{\partial x_{j\rangle}}+\frac{2\,(2a+3)!!}{15}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}=-\frac{1}{\mathrm{Kn}}\sum_{b=1}^{N}\tilde{\mathcal{C}}_{ab}^{(2)}\tilde{u}_{ij}^b$$

$$\frac{\partial\tilde{u}_{ijk}^a}{\partial t}+\frac{\partial\tilde{u}_{ijkl}^a}{\partial x_l}+\frac{3}{7}\sum_{b=1}^{N}\tilde{\mathcal{R}}_{ab}^{(2)}\frac{\partial\tilde{u}_{\langle ij}^b}{\partial x_{k\rangle}}=-\frac{1}{\mathrm{Kn}}\sum_{b=1}^{N}\tilde{\mathcal{C}}_{ab}^{(3)}\tilde{u}_{ijk}^b$$

$$etc.$$

$\tilde{w}^a=\tilde{u}^a-\tilde{u}_E^a$: **non-equilibrium part of scalar moments**

$\tilde{\mathcal{R}}_{ab}^{(n)}$: **coefficients from Grad closure** (closure coefficients only for $b=N$)

$\tilde{\mathcal{C}}_{ab}^{(n)}$: **production matrices: collision term + Grad closure** [Gupta & Torrilhon, RGD28]

Order of magnitude method [HS 2004]

Step 2:

- Chapman-Enskog expansion to find leading $\mathrm{Kn}-$order of moments
- linear combination of moments such that number of moments at given $\mathrm{Kn}-$order is minimal
- repeat for next order of magnitude

This step aims at constructing a unique set of variables

Basic moment set must be complete set of polynomials in 3D

Step 2: Order of magnitude of moments [HS 2004]

idea: Chapman-Enskog expansion of **moments**

$$u^a_{i_1\cdots i_n} = \mathrm{Kn}^0 u^a_{i_1\cdots i_n|0} + \mathrm{Kn}^1 u^a_{i_1\cdots i_n|1} + \mathrm{Kn}^2 u^a_{i_1\cdots i_n|2} + \mathrm{Kn}^3 u^a_{i_1\cdots i_n|3} + \cdots$$

$u^a_{i_1\cdots i_n}$ is of leading order λ if $u^a_{i_1\cdots i_n|\beta} = 0$ for all $\beta < \lambda$

order and leading term are of interest, but not higher order terms

Zeroth order of magnitude $\mathcal{O}\left(\mathrm{Kn}^0\right)$

$\Longrightarrow$ conserved quantities ϱ, v_i, θ

First order of magnitude $\mathcal{O}\left(\mathrm{Kn}^1\right)$

$\Longrightarrow$ vectors u^a_i and rank-2 tensors u^a_{ij}

Second order of magnitude $\mathcal{O}\left(\mathrm{Kn}^2\right)$

$\Longrightarrow$ scalars w^a , 3-tensors u^b_{ijk} , 4-tensors u^b_{ijkl}

Step 2: Minimal number of moments of order $\mathcal{O}\left(\mathrm{Kn}^1\right)$ [HS 2004]

heat flux and pressure deviator to first order

$$q_{i|1} = \frac{1}{2}u^1_{i|1} = -\kappa_1 \frac{\partial \theta}{\partial x_i} \quad , \quad \sigma_{ij|1} = u^0_{ij|1} = -2\mu_0 \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$$

$u^a_{i|1}$ and $u^a_{ij|1}$ to first order

$$u^a_{i|1} = -\kappa_a \frac{\partial \theta}{\partial x_i} = \frac{\kappa_a}{\kappa_1} 2 q_{i|1} \quad , \quad u^a_{ij|1} = -\mu_a \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = \frac{\mu_a}{\mu_0}\sigma_{ij|1}$$

new second order moments

$$w^a_i = u^a_i - \frac{\kappa_a}{\kappa_1} 2 q_i \;\; (a \geq 2) \quad , \quad w^a_{ij} = u^a_{ij} - \frac{\mu_a}{\mu_0}\sigma_{ij} \;\; (a \geq 1)$$

$\Longrightarrow$ ϱ, v_i, θ are 0th order

$\Longrightarrow$ σ_{ij}, q_i are 1st order

$\Longrightarrow$ $w^a, w^a_i, w^a_{ij}, u^a_{i_1 \cdots i_n}$ are at least 2nd order

---

$$\kappa_a = \frac{\tau_0}{\theta^{1-s-a}} \sum_{b=1} \left[\mathcal{C}^{(1)}_{ab}\right]^{-1} \frac{b\,(2b+3)!!}{6} \quad , \quad \mu_a = \frac{\tau_0}{\theta^{-s-a}} \sum_{b=0} \left[\mathcal{C}^{(2)}_{ab}\right]^{-1} \frac{(2b+5)!!}{15}$$

Step 2: Minimal number of moments of order $\mathcal{O}\left(\mathrm{Kn}^1\right)$ [HS 2004]

and so on, for higher orders . . .

lots of detail ignored

next only equations for Maxwell molecules, which are simplest by far
(triangular matrices $\mathcal{C}_{ab}^{(\alpha)}$)

Order of magnitude method [HS 2004]

Step 3:

- use $\mathrm{Kn}-$orders to rescale equations for new moments
- use scaling for model reduction to a given order of accuracy

Step 2 assignes Knudsen orders to all terms in all equations, which are now used to remove what is not needed

We proceed backwards, that is add more and more terms

Zeroth order: Euler

delete all terms of order

$$\mathcal{O}\left(\mathrm{Kn}^1\right) \text{ and higher}$$

conservation laws

$$\begin{aligned}
\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} &= 0 \\
\rho\frac{Dv_i}{Dt} + \rho\frac{\partial \theta}{\partial x_i} + \theta\frac{\partial \rho}{\partial x_i} &= 0 \\
\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} &= 0
\end{aligned}$$

equations for pressure deviator and heat flux

First order: Navier-Stokes-Fourier

delete all terms of order

$$\mathcal{O}\left(\mathrm{Kn}^2\right) \text{ and higher}$$

conservation laws

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} = 0$$

$$\rho\frac{Dv_i}{Dt} + \rho\frac{\partial\theta}{\partial x_i} + \theta\frac{\partial\rho}{\partial x_i} + \mathrm{Kn}^1\left[\frac{\partial\sigma_{ik}}{\partial x_k}\right] = 0$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} + \mathrm{Kn}^1\left[\frac{\partial q_k}{\partial x_k} + \sigma_{kl}\frac{\partial v_k}{\partial x_l}\right] = 0$$

equations for pressure deviator and heat flux

$$0 = -\rho\theta\mathrm{Kn}^1\left[\sigma_{ij} + 2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

$$0 = -\frac{5}{2}\rho\theta\mathrm{Kn}^1\left[q_i + \kappa\frac{\partial\theta}{\partial x_i}\right]$$

2nd order: Grad 13 moments

delete all terms of order

$$\mathcal{O}\left(\mathrm{Kn}^3\right) \text{ and higher}$$

conservation laws

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} = 0$$

$$\rho\frac{Dv_i}{Dt} + \rho\frac{\partial \theta}{\partial x_i} + \theta\frac{\partial \rho}{\partial x_i} + \mathrm{Kn}^1\left[\frac{\partial \sigma_{ik}}{\partial x_k}\right] = 0$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} + \mathrm{Kn}^1\left[\frac{\partial q_k}{\partial x_k} + \sigma_{kl}\frac{\partial v_k}{\partial x_l}\right] = 0$$

equations for pressure deviator and heat flux

$$\mathrm{Kn}^2\mu\left[\frac{D\sigma_{ij}}{Dt} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k}\right] + \qquad = -\rho\theta\mathrm{Kn}^1\left[\sigma_{ij} + 2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

$$\mathrm{Kn}^2\kappa\left[\frac{Dq_i}{Dt} + \frac{5}{2}\sigma_{ik}\frac{\partial \theta}{\partial x_k} - \sigma_{ik}\theta\frac{\partial \ln\rho}{\partial x_k} + \theta\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i}\right]$$
$$= -\frac{5}{2}\rho\theta\mathrm{Kn}^1\left[q_i + \kappa\frac{\partial \theta}{\partial x_i}\right]$$

3rd order: R13 equations

delete all terms of order

$$\mathcal{O}\left(\mathrm{Kn}^4\right) \text{ and higher}$$

conservation laws

$$\frac{D\rho}{Dt}+\rho\frac{\partial v_k}{\partial x_k}=0$$

$$\rho\frac{Dv_i}{Dt}+\rho\frac{\partial\theta}{\partial x_i}+\theta\frac{\partial\rho}{\partial x_i}+\mathrm{Kn}^1\left[\frac{\partial\sigma_{ik}}{\partial x_k}\right]=0$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt}+\rho\theta\frac{\partial v_k}{\partial x_k}+\mathrm{Kn}^1\left[\frac{\partial q_k}{\partial x_k}+\sigma_{kl}\frac{\partial v_k}{\partial x_l}\right]=0$$

equations for pressure deviator and heat flux

$$\mathrm{Kn}^2\mu\left[\frac{D\sigma_{ij}}{Dt}+\frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}}+2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k}+\sigma_{ij}\frac{\partial v_k}{\partial x_k}\right]+\mathrm{Kn}^3\mu\left[\frac{\partial m_{ijk}}{\partial x_k}\right]=-\rho\theta\mathrm{Kn}^1\left[\sigma_{ij}+2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

$$\mathrm{Kn}^2\kappa\left[\frac{Dq_i}{Dt}+\frac{5}{2}\sigma_{ik}\frac{\partial\theta}{\partial x_k}-\sigma_{ik}\theta\frac{\partial\ln\rho}{\partial x_k}+\theta\frac{\partial\sigma_{ik}}{\partial x_k}+\frac{7}{5}q_i\frac{\partial v_k}{\partial x_k}+\frac{7}{5}q_k\frac{\partial v_i}{\partial x_k}+\frac{2}{5}q_k\frac{\partial v_k}{\partial x_i}\right]$$
$$+\mathrm{Kn}^3\kappa\left[\frac{1}{2}\frac{\partial R_{ij}}{\partial x_k}+\frac{1}{6}\frac{\partial\Delta}{\partial x_i}+m_{ikl}\frac{\partial v_k}{\partial x_l}-\frac{\sigma_{ik}}{\rho}\frac{\partial\sigma_{kl}}{\partial x_l}\right]=-\frac{5}{2}\rho\theta\mathrm{Kn}^1\left[q_i+\kappa\frac{\partial\theta}{\partial x_i}\right]$$

+ higher moment equations for $m_{ijk}=u^0_{ijk}$, $R_{ij}=u^1_{ij}-\mu_1\sigma_{ij}$, $\Delta=u^2-u^2_{|E}$

R13 equations (non-linear) [HS & MT 2003, HS 2004]

(Euler / NSF / Grad13 / R13)

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} = 0$$

$$\rho\frac{Dv_i}{Dt} + \rho\frac{\partial \theta}{\partial x_i} + \theta\frac{\partial \rho}{\partial x_i} + \left[\frac{\partial \sigma_{ik}}{\partial x_k}\right] = \rho G_i$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} + \left[\frac{\partial q_k}{\partial x_k} + \sigma_{kl}\frac{\partial v_k}{\partial x_l}\right] = 0$$

$$\left[\frac{D\sigma_{ij}}{Dt} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k}\right] + \left[\frac{\partial m_{ijk}}{\partial x_k}\right] = -\rho\theta\left[\frac{\sigma_{ij}}{\mu} + 2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

$$\left[\frac{Dq_i}{Dt} + \frac{5}{2}\sigma_{ik}\frac{\partial \theta}{\partial x_k} - \sigma_{ik}\theta\frac{\partial \ln\rho}{\partial x_k} + \theta\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i}\right]$$
$$+\left[-\frac{\sigma_{ij}}{\varrho}\frac{\partial \sigma_{jk}}{\partial x_k} + \frac{1}{2}\frac{\partial R_{ik}}{\partial x_k} + \frac{1}{6}\frac{\partial \Delta}{\partial x_i} + m_{ijk}\frac{\partial v_j}{\partial x_k}\right] = -\frac{5}{2}\rho\theta\left[\frac{q_i}{\kappa} + \frac{\partial \theta}{\partial x_i}\right]$$

$$\Delta = -\frac{\sigma_{ij}\sigma_{ij}}{\rho} - 12\frac{\mu}{p}\left[\theta\frac{\partial q_k}{\partial x_k} + \theta\sigma_{kl}\frac{\partial v_k}{\partial x_l} + \frac{7}{2}q_k\frac{\partial \theta}{\partial x_k} - q_k\frac{\theta}{p}\frac{\partial p}{\partial x_k}\right]$$

$$R_{ij} = -\frac{4}{7}\frac{1}{\rho}\sigma_{k\langle i}\sigma_{j\rangle k} - \frac{24}{5}\frac{\mu}{p}\left[\theta\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2q_{\langle i}\frac{\partial \theta}{\partial x_{j\rangle}} + \frac{5}{7}\theta\left(\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \sigma_{k\langle i}\frac{\partial v_k}{\partial x_{j\rangle}} - \frac{2}{3}\sigma_{ij}\frac{\partial v_k}{\partial x_k}\right) - \frac{\theta}{p}q_{\langle i}\frac{\partial p}{\partial x_{j\rangle}}\right]$$

$$m_{ijk} = -2\frac{\mu}{p}\left[\theta\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} + \sigma_{\langle ij}\frac{\partial \theta}{\partial x_{k\rangle}} + \frac{4}{5}q_{\langle i}\frac{\partial v_j}{\partial x_{k\rangle}} - \sigma_{\langle ij}\frac{\theta}{p}\frac{\partial p}{\partial x_{k\rangle}}\right]$$

Chapman-Enskog expansion of R13 $\Rightarrow$ Euler / NSF / Burnett / super-Burnett

Euler / NSF / Grad13 / R13 (linearized) [HS & MT 2003]

$$\partial_t \rho + \rho_0 \nabla \cdot \mathbf{v} = 0$$

$$\rho_0 \partial_t \mathbf{v} + \nabla p + \nabla \cdot \sigma = \rho_0 \mathbf{G}$$

$$\frac{3}{2}\rho_0 \partial_t \theta + p_0 \nabla \cdot \mathbf{v} + \nabla \cdot \mathbf{q} = 0$$

$$\partial_t \sigma + \frac{4}{5}\langle \nabla \mathbf{q} \rangle + 2p_0 \langle \nabla \mathbf{v} \rangle = -\frac{p_0}{\mu_0}\sigma + \frac{2}{3}\frac{\mu_0}{p_0}\left[\triangle \sigma + \frac{6}{5}\langle \nabla (\nabla \cdot \sigma) \rangle \right]$$

$$\partial_t \mathbf{q} + \nabla \cdot \sigma + \frac{5}{2}\nabla \theta = -\frac{2}{3}\frac{p_0}{\mu_0}\mathbf{q} + \frac{6}{5}\frac{\mu_0}{p_0}\left[\triangle \mathbf{q} + 2\nabla (\nabla \cdot \mathbf{q}) \right]$$

$\langle \phi \rangle$ – symmetric tracefree tensors

blue terms: diffusion; green terms: wave-like; red + blue terms: Knudsen layers.

Stability in time: Grad13, R13 are stable

disturbance in space: k real, $\Omega = \Omega_r(k) + i\Omega_i(k)$ complex

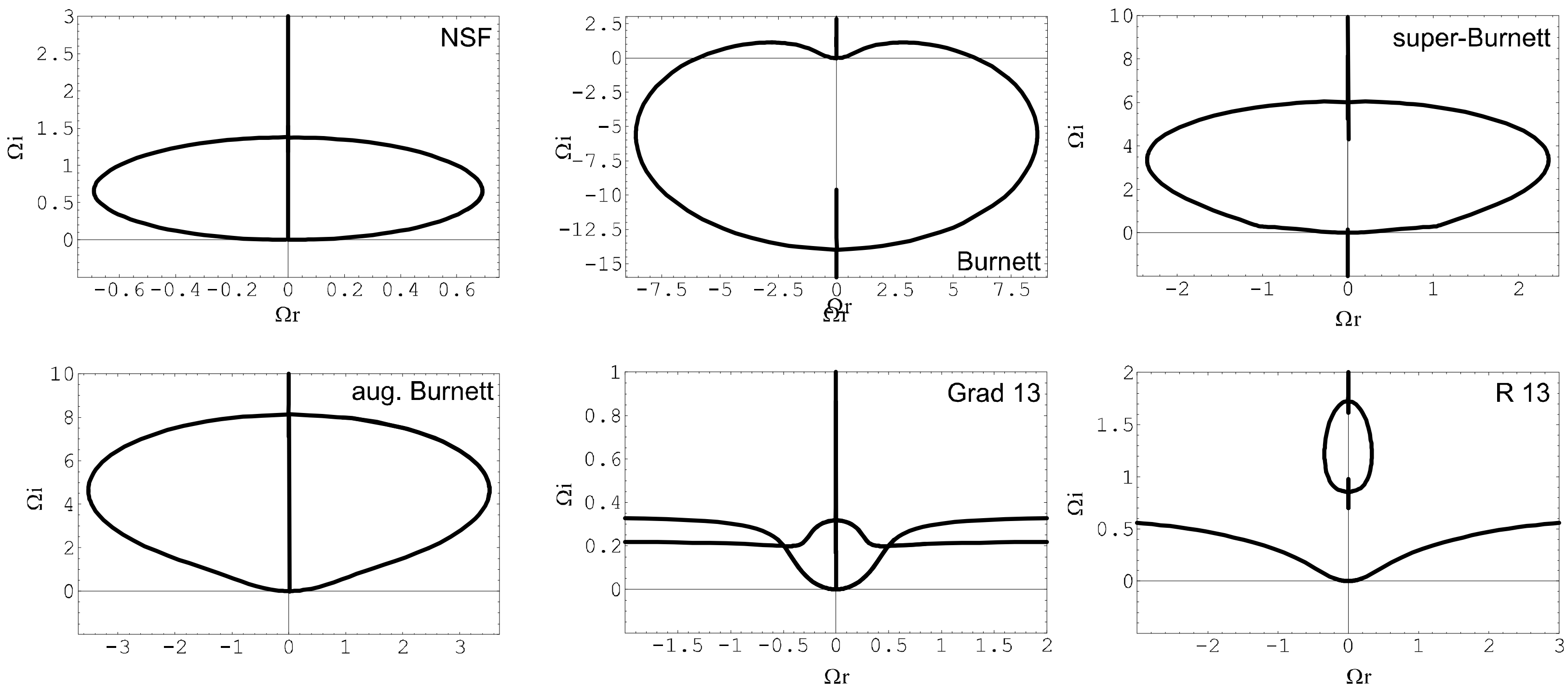
$$u_A = \tilde{u}_A \exp\left[i\left(\Omega t - kx\right)\right] = \tilde{u}_A \exp\left[-\alpha t\right] \exp\left[ik\left(v_{ph}t - x\right)\right]$$

phase velocity and damping:

$$v_{ph} = \frac{\Omega_r(k)}{k} \quad \text{and} \quad \alpha = \Omega_i(k)$$

stability:

$$\Omega_i(k) \geq 0$$



H-Theorem for linear R13 equations [HS & MT 2007]

entropy balance

$$\frac{D\eta}{Dt} + \frac{\partial \phi_k}{\partial x_k} = \Sigma \geq 0$$

convex dimensionless entropy density similar to [Bobylev 2007]

(ρ, v_i, θ are dimless deviations from equilibrium state ρ_0, $v_i^0 = 0$, θ_0)

$$\eta = \eta_0 - \frac{1}{2}\rho^2 - \frac{1}{2}v_i v_i - \frac{3}{4}\theta^2 - \frac{1}{4}\sigma_{ij}\sigma_{ij} - \frac{1}{5}q_i q_i$$

entropy flux $\left[w_{ij} = R_{ij} + \frac{\Delta}{3}\delta_{ij}\right]$

$$\phi_k = -(\rho + \theta)\, v_k - v_i \sigma_{ik} - \theta q_k - \frac{2}{5} q_i \sigma_{ik} - \frac{1}{2}\sigma_{ij} m_{ijk} - \frac{1}{5} q_i w_{ik}$$

bulk entropy generation rate

$$\Sigma = \frac{\sigma_{ij}\sigma_{ij}}{2\mathrm{Kn}} + \frac{4}{15}\frac{q_i q_i}{\mathrm{Kn}} - \frac{1}{2} m_{ijk} \frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} - \frac{1}{5} w_{ik} \frac{\partial q_i}{\partial x_k} \overset{!}{\geq} 0$$

regularizing constitutive equations guarantee $\Sigma \geq 0$ and linear stability

$$w_{ij} = R_{ij} + \frac{\Delta}{3}\delta_{ij} = -\frac{24}{5}\mathrm{Kn}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - 4\mathrm{Kn}\frac{\partial q_k}{\partial x_k}\delta_{ij} \quad , \quad m_{ijk} = -2\mathrm{Kn}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}}$$

extension to non-linear case: [Torrilhon 2011]

H-Theorem & boundary conditions [HS & MT 2007]

first and second law for solid wall at rest, temperature θ_W

$$c_v \frac{\partial \theta_W}{\partial t} + \frac{\partial q_k}{\partial x_k} = 0 \quad , \qquad \frac{\partial \eta_W}{\partial t} + \frac{\partial \phi_k^W}{\partial x_k} = \Sigma_W$$

with $\eta_W = \eta_W^0 - \frac{c_v}{2}\theta_W^2$, $\phi_k^W = -\theta_W q_k$, $\Sigma_W = -q_k \frac{\partial \theta_W}{\partial x_k}$

entropy generation at wall: $\Sigma_W = \left(\phi_k^W - \phi_k\right) n_k \geq 0$

$$\Sigma_W = \bar{\sigma}_{ni}\left[v_i - v_i^W + \left(\frac{2}{5} - \alpha\right)\bar{q}_i + m_{inn}\right] + \bar{q}_i\left[\alpha\bar{\sigma}_{ni} + \frac{1}{5}w_{in}\right]$$
$$+ q_n\left[\theta - \theta_W + \left(\frac{2}{5} - \beta\right)\sigma_{nn} + \frac{1}{5}w_{nn}\right] + \sigma_{nn}\left[\beta q_n + \frac{3}{4}m_{nnn}\right] + \frac{1}{2}\bar{\sigma}_{ij}u_{ijn}^0 \geq 0$$

phenomenological boundary conditions guarantee $\Sigma_W \geq 0$

$$\bar{\sigma}_{ni} = \gamma_1\left[v_i - v_i^W + \left(\frac{2}{5} - \alpha\right)\bar{q}_i + m_{inn}\right] \qquad \bar{q}_i = \gamma_2\left[\alpha\bar{\sigma}_{ni} + \frac{1}{5}w_{ni}\right]$$

$$q_n = \gamma_4\left[\theta - \theta_W + \left(\frac{2}{5} - \beta\right)\sigma_{nn} + \frac{1}{5}w_{nn}\right] \qquad \sigma_{nn} = \gamma_3\left[\beta q_n + \frac{1}{2}m_{nnn}\right] \qquad \bar{\sigma}_{ij} = \gamma_5\left[\frac{1}{2}m_{ijn}\right]$$

with phenomenological coefficients $\gamma_1 - \gamma_5$, α, β

How many BC do we need anyway?

Write set of eqs as n, τ – normal/tangential to wall

$$\mathcal{D}_{AB}\frac{\partial u_B}{\partial t} + \mathcal{A}_{AB}\frac{\partial u_B}{\partial x_n} + \mathcal{B}_{AB}\frac{\partial u_B}{\partial x_\tau} = P_A$$

How many space integrations?

$$\# \text{ of constants for } x_n\text{-integration} = \# \text{ of eigenvalues of } \mathcal{A}_{AB}$$

Interesting problem:

Grad 13 linear, non-linear need different number of BC!

same for orginal R13!!

Fix # of BC for R13 (Maxwell molecules) [AR & HS, 2014]

rewrite: with $\sigma_{ij}^{NSF} = -2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$, $q_i^{NSF} = -\frac{15}{4}\mu\frac{\partial\theta}{\partial x_i}$

$$\Delta = -\frac{\sigma_{ij}\sigma_{ij}}{\rho} + 6\frac{\sigma_{kl}\sigma_{kl}^{NSF}}{\rho} + \frac{56}{5}\frac{q_k q_k^{NSF}}{p} - 12\mu\theta\frac{\partial}{\partial x_k}\left(\frac{q_k}{p}\right)$$

$$R_{ij} = -\frac{4}{7}\frac{\sigma_{k\langle i}\sigma_{j\rangle k}}{\rho} + \frac{24}{7}\frac{\sigma_{k\langle i}\sigma_{jk\rangle}^{NSF}}{\rho} + \frac{64}{25}\frac{q_{\langle i}q_{j\rangle}^{NSF}}{p} - \frac{24}{5}\mu\theta\frac{\partial}{\partial x_{\langle i}}\left(\frac{q_{j\rangle}}{p}\right)$$

$$m_{ijk} = \frac{8}{15}\frac{1}{p}\sigma_{\langle ij}q_{k\rangle}^{NSF} + \frac{4}{5}\frac{1}{p}q_{\langle i}\sigma_{jk\rangle}^{NSF} - 2\mu\theta\frac{\partial}{\partial x_{\langle i}}\left(\frac{\sigma_{jk\rangle}}{p}\right)$$

replace: $\sigma_{ij}^{NSF} \longrightarrow \sigma_{ij}$, $q_i^{NSF} \longrightarrow q_i$

- **# of BC the same for linear and non-linear eqs.**
- **assymptotics remain, i.e., R13 system remains** $\mathcal{O}\left(\mathrm{Kn}^3\right)$
- **non-linear behavior has changed (shocks!!) . . . under investigation**
- **no equivalent procedure for Grad 13**

Boundary conditions for moments [MT & HS 2008]

derived from Maxwell boundary conditions for Boltzmann eq.

kinetic BC for odd fluxes (at left and right boundary)

slip $$\sigma_{tn} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[P\left(v_t - v_t^W\right) + \frac{1}{5}q_t + \frac{1}{2}m_{tnn}\right]n_n$$

jump $$q_n = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[2P\left(\theta-\theta_W\right) - \frac{1}{2}PV^2 + \frac{1}{2}\theta\sigma_{nn} + \frac{1}{15}\Delta + \frac{5}{28}R_{nn}\right]n_n$$

$$m_{ttn} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[\frac{1}{14}R_{tt} + \theta\sigma_{tt} - \frac{1}{5}\theta\sigma_{nn} + \frac{1}{5}P\left(\theta-\theta_W\right) - \frac{4}{5}PV^2 + \frac{1}{150}\Delta\right]n_n$$

$$m_{nnn} = \frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[\frac{2}{5}P\left(\theta-\theta_W\right) - \frac{3}{5}PV^2 - \frac{7}{5}\theta\sigma_{nn} + \frac{1}{75}\Delta - \frac{1}{14}R_{nn}\right]n_n$$

$$R_{tn} = \frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[P\theta\left(v_t - v_t^W\right) - \frac{11}{5}q_t - \frac{1}{2}\theta m_{tnn} - PV^3 + 6PV\left(\theta-\theta_W\right)\right]n_n$$

$$V_t = v_t - v_t^W \;,\; v_n = 0 \;,\; P = \rho\theta + \tfrac{1}{2}\sigma_{nn} - \tfrac{1}{120}\tfrac{\Delta}{\theta} - \tfrac{1}{28}\tfrac{R_{nn}}{\theta}$$

χ accommodation coefficient

indices n, t: normal/tangential components

$\Longrightarrow$ **purely local BC, well-posed problem!**

H-Theorem at wall in linear case [HS & MT 2007]

2nd order BC for NSF in limit $\mathcal{O}\left(\mathrm{Kn}^2\right)$ [HS & MT 2009]

[Gu&Emerson 2007]: kinetic BC for R13, but too many BC lead to spurious wall layers

A remark on temperature in kinetic theory

internal energy and pressure tensor

$$\rho u = \frac{m}{2}\int C^2 f d\mathbf{c} \quad , \quad p_{ij} = m\int C_i C_j f d\mathbf{c}$$

$\Longrightarrow$ **pressure**

$$p = \frac{1}{3}p_{kk} = \frac{1}{3}m\int C_k C_k f d\mathbf{c} = \frac{2}{3}\frac{m}{2}\int C^2 f d\mathbf{c} = \frac{2}{3}\rho u$$

non-equilibrium temperature defined through energy as in equilibrium

$$\rho u = \frac{3}{2}\rho RT = \frac{3}{2}\rho\theta \qquad \Rightarrow \quad p = \frac{2}{3}\rho u = \rho\theta$$

but what do we measure? from jump condition

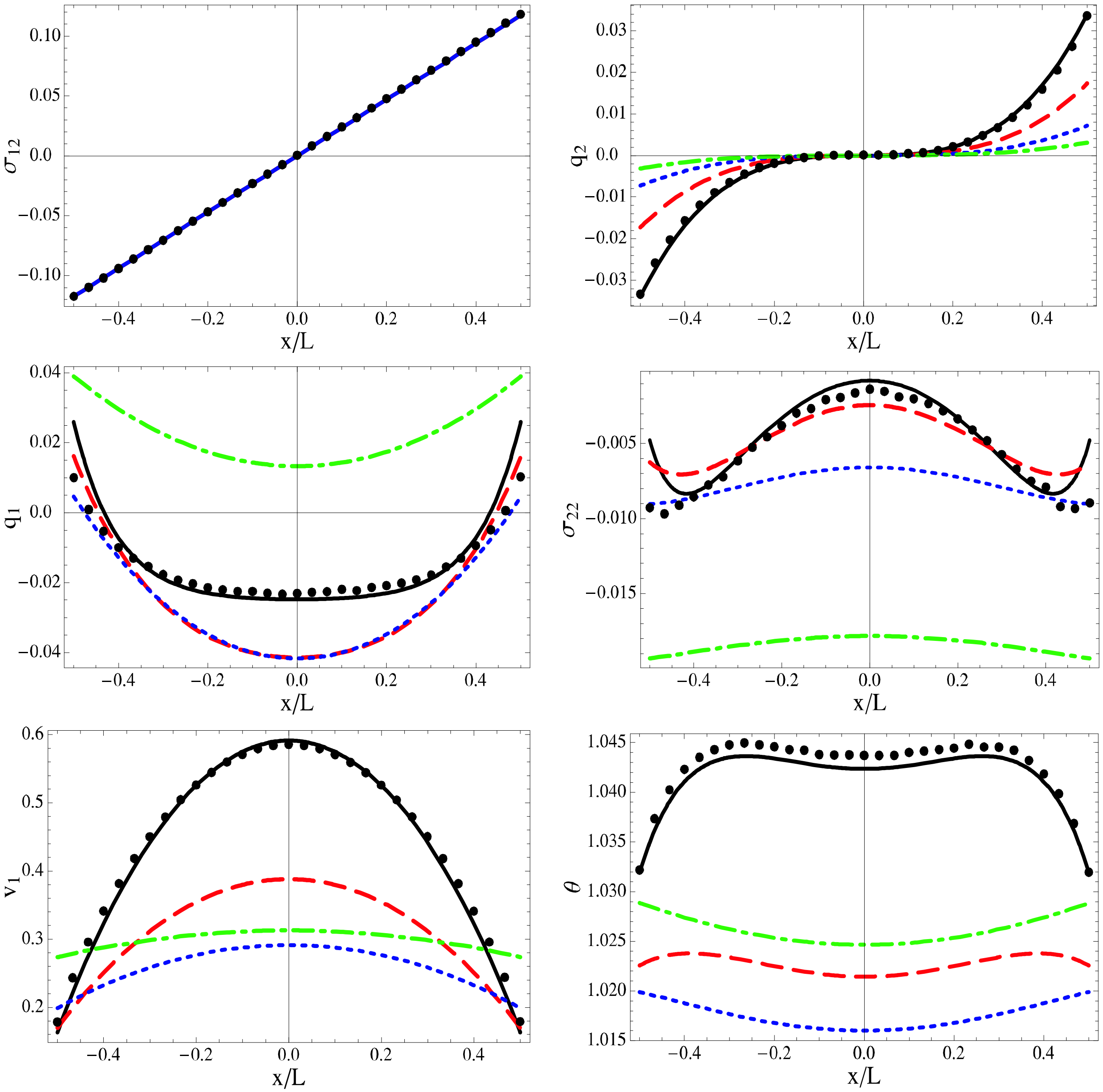
$$\theta_W = \theta + \frac{2-\chi}{2\chi}\sqrt{\frac{\pi\theta}{2}}\frac{q_n}{P} - \frac{1}{4}V^2 + \frac{1}{4}\frac{\theta\sigma_{nn}}{P} + \frac{1}{30}\frac{\Delta}{P} + \frac{5}{56}\frac{R_{nn}}{P}$$

θ_W **is thermometer temperature,** θ **is gas temperature!**

$\Longrightarrow$ **gas temperature cannot be measured easily**

Force driven Poiseuille flow [PT, MT & HS 2008]

R13 equations exhibit temperature dip [Tij & Santos 1994/98, Xu 2003]



$$\theta = \mathsf{C}_4 - \frac{G_1^2}{\mathrm{Kn}^2}\left[\frac{y^4}{45} - \frac{488}{525}\,\mathrm{Kn}^2 y^2\right]$$

$$- \mathsf{C}_3\,\frac{2}{5}\,\cosh\left[\frac{\sqrt{5}y}{\sqrt{6}\mathrm{Kn}}\right]$$

$$+ \mathsf{C}_2\,\frac{956}{375}\,G_1\,\mathrm{Kn}\,\cosh\left[\frac{\sqrt{5}y}{3\mathrm{Kn}}\right]$$

$$+ \mathsf{C}_2\,\frac{32}{35\sqrt{5}}\,\sigma_{12}\,\sinh\left[\frac{\sqrt{5}y}{3\mathrm{Kn}}\right]$$

superposition of

bulk solution

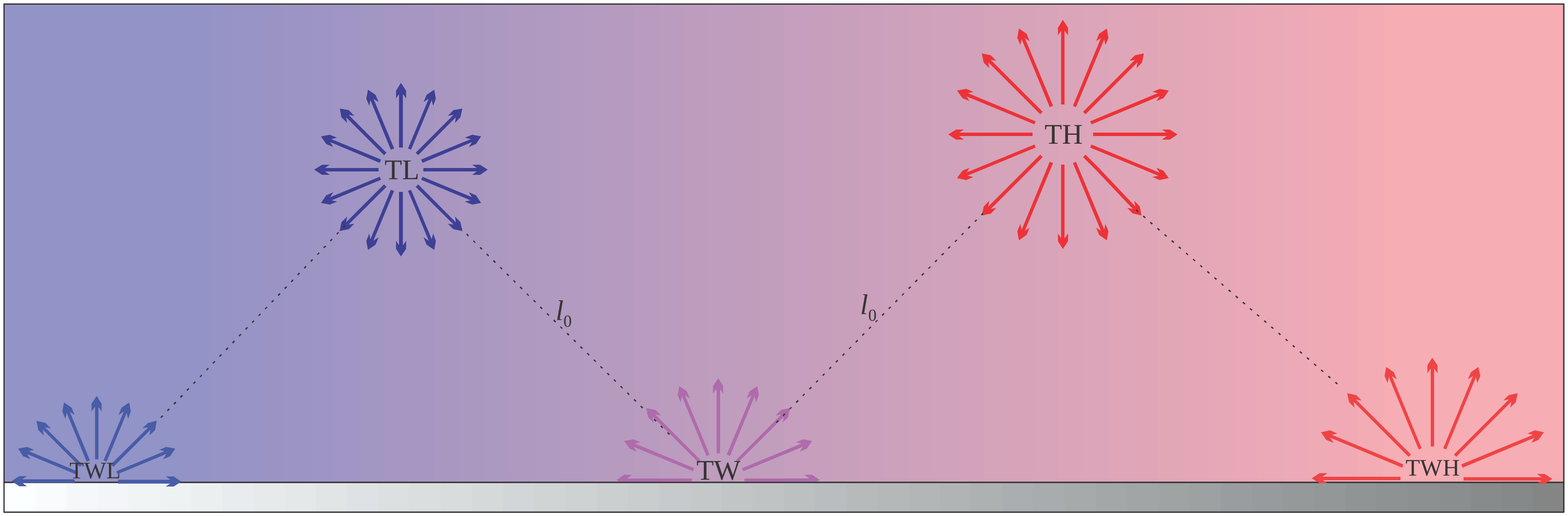
Knudsen layers

$\mathrm{Kn} = 0.072, 0.15, 0.4, 1.0$

constants C_α from BC

Transpiration flow

Flow driven by temperature gradient

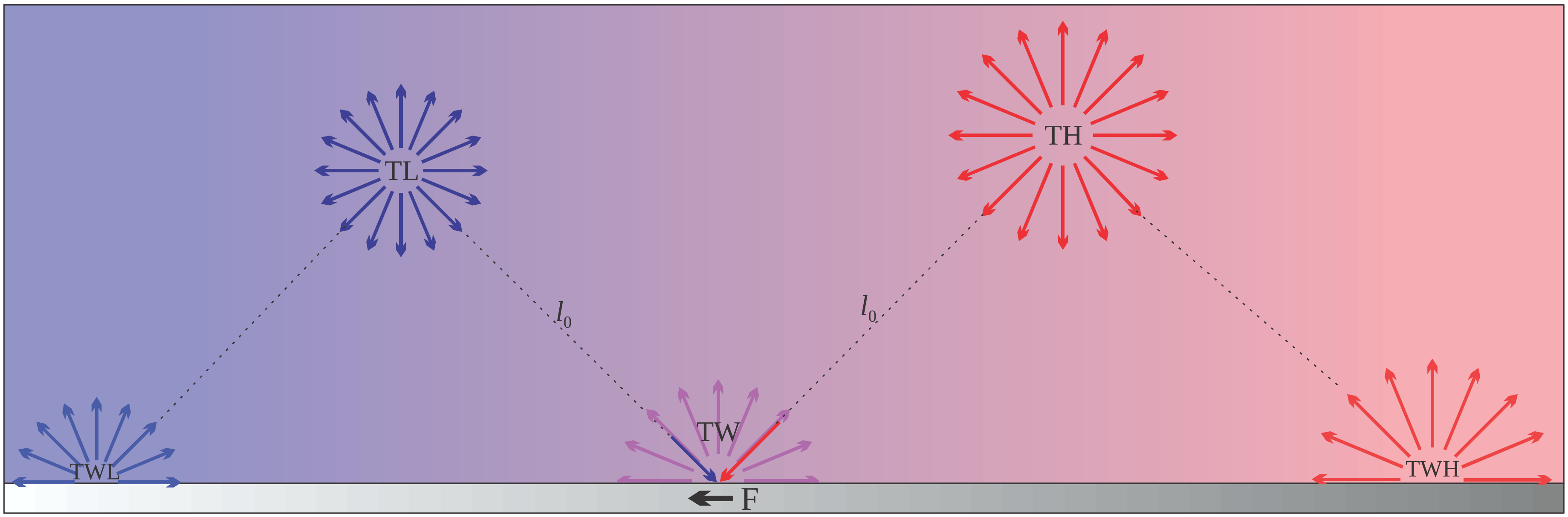


gas particles thermalize at wall

T-gradient in the wall induces T-gradient in gas

Transpiration flow

Flow driven by temperature gradient



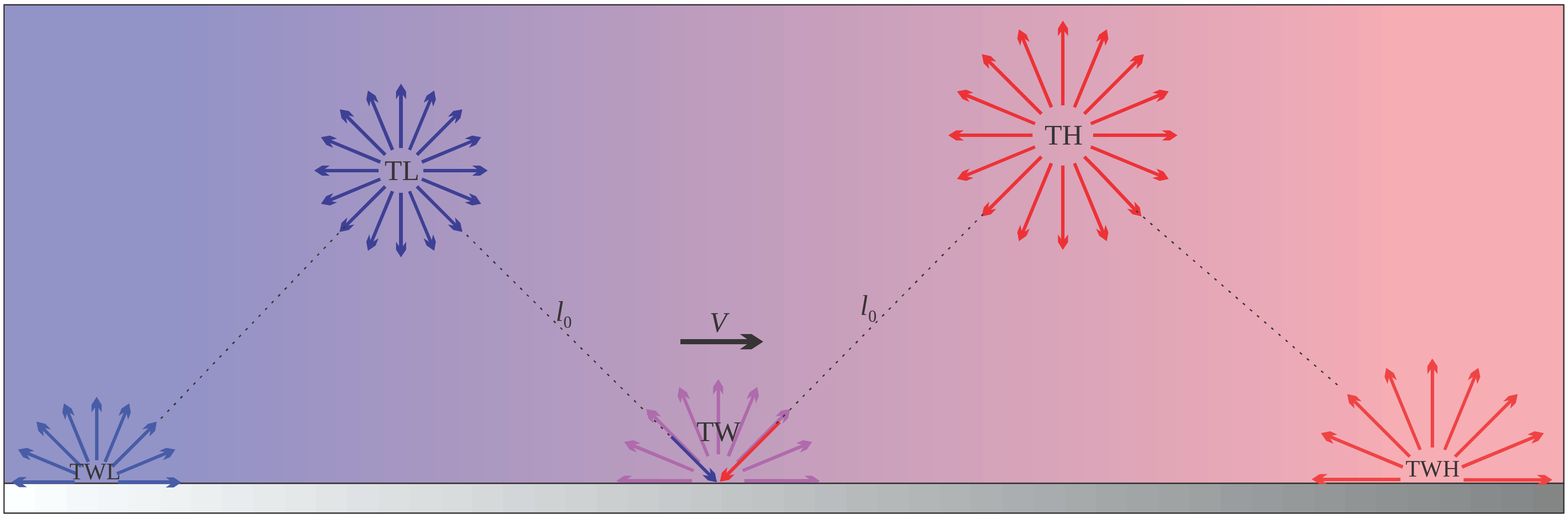
gas particles thermalize at wall

T-gradient in the wall induces T-gradient in gas

gas-wall interaction: wall pushed towards cold side

Transpiration flow

Flow driven by temperature gradient



gas particles thermalize at wall

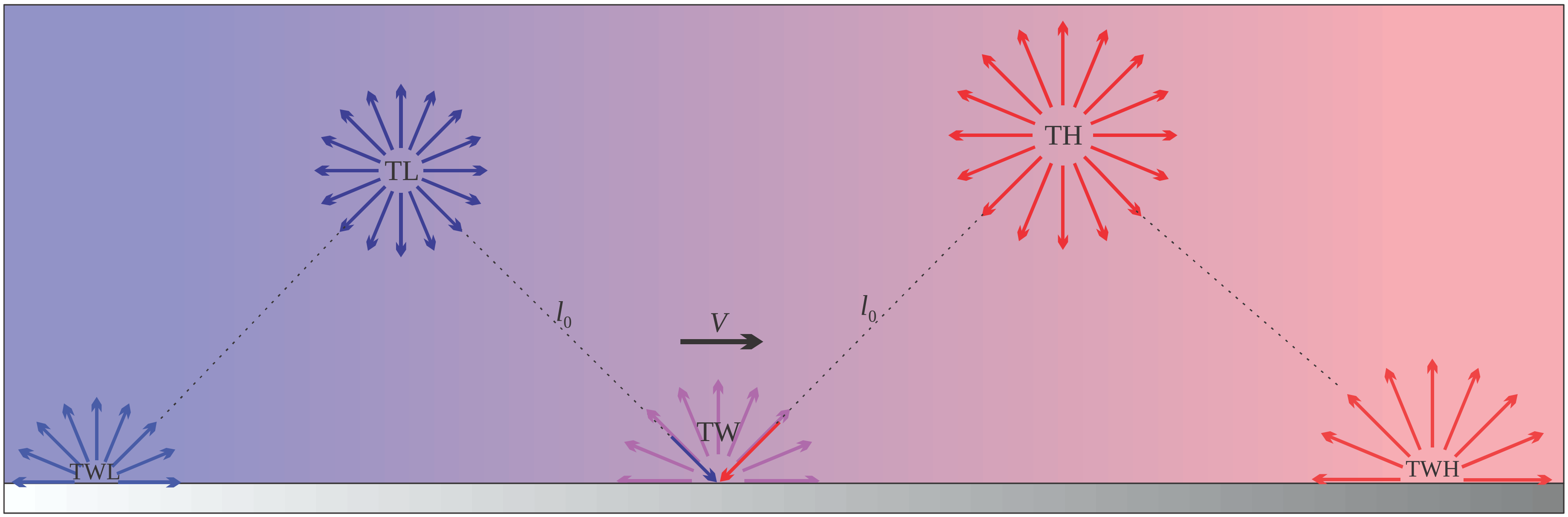
T-gradient in the wall induces T-gradient in gas

gas-wall interaction: wall pushed towards cold side

actio = reactio: if wall at rest, gas moves towards warm side

Transpiration flow

Flow driven by temperature gradient



gas particles thermalize at wall

T-gradient in the wall induces T-gradient in gas

gas-wall interaction: wall pushed towards cold side

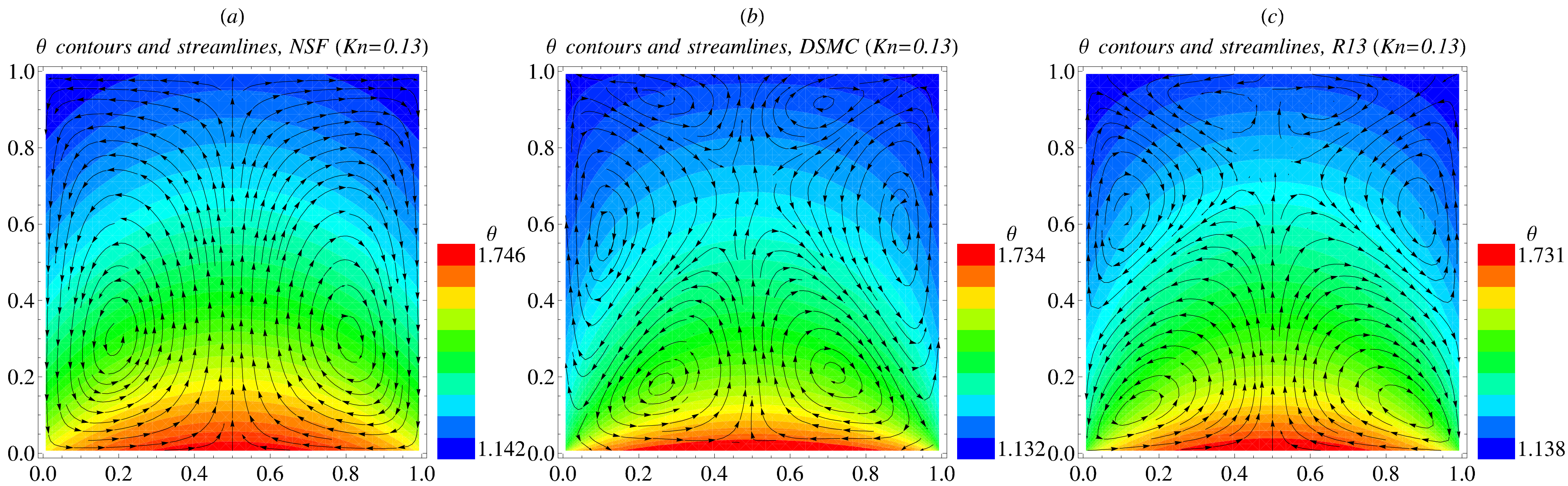
actio = reactio: if wall at rest, gas moves towards warm side

surface force: moves only for small volume/area $\Longrightarrow$ transition regime

Example (failure of hydrodynamics):

2D Bottom heated cavity, Kn=0.13

temperature contures and velocity streamlines



[Rana et al., Cont. Mech. Thermodyn. **27**, 2015]

Middle: DSMC solution of Boltzmann equation, exact, but takes days

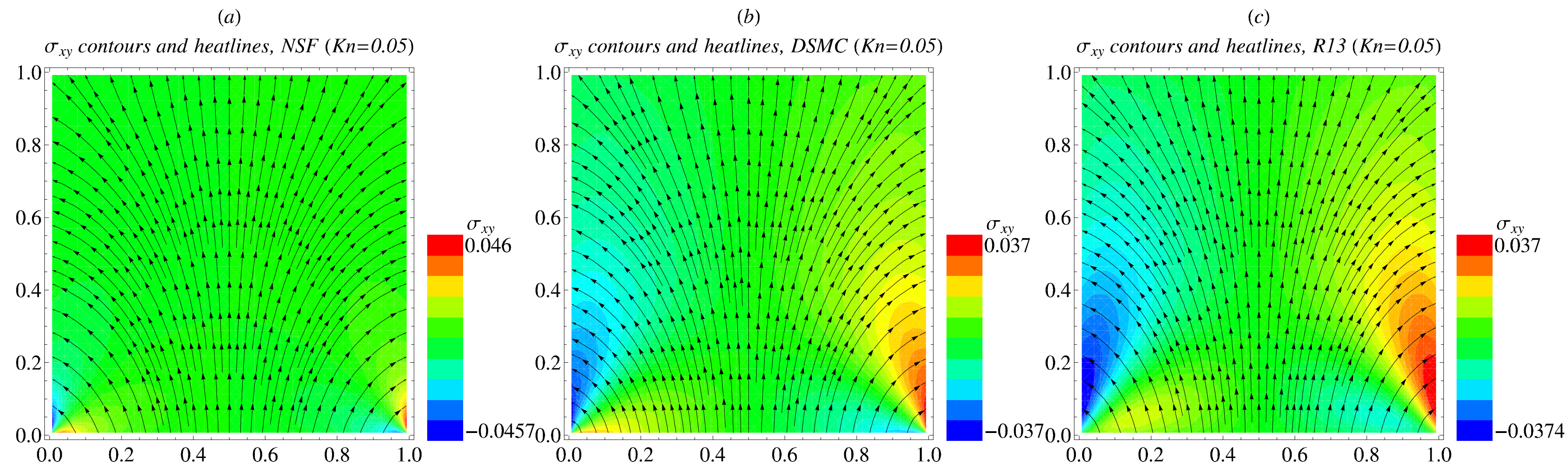
Left: Classical Hydrodynamics (jump/slip NSF): minutes, but misses flow details

Right: Extended Thermodynamics (R13 eqs): minutes, has all details (approx)!!

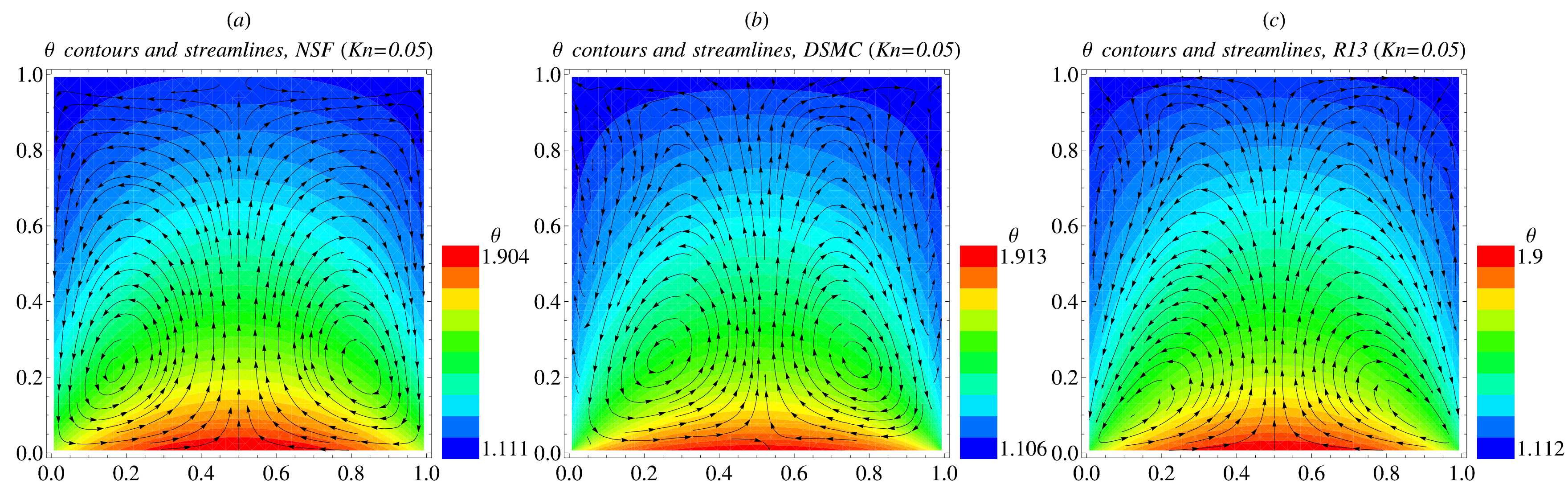
R13: 2D Bottom heated plate (MM) [AR, AM, HS 2015]

comparison of NSF, DSMC, R13

Kn=0.05: heat flux and shear stress



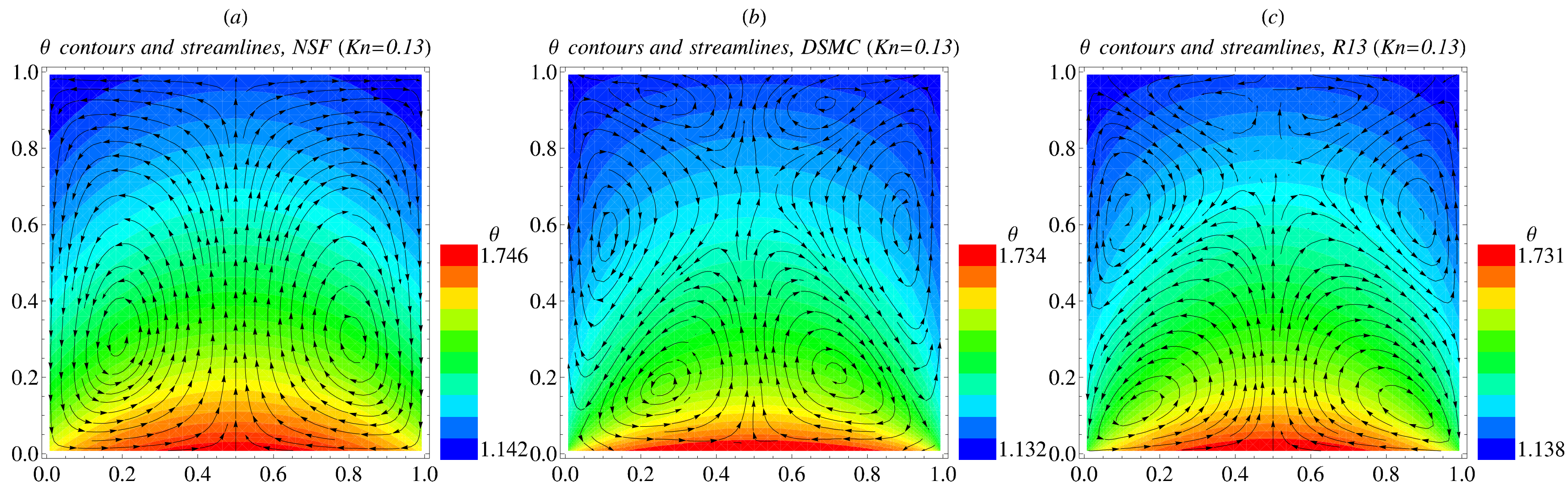
Kn=0.05: temperature and streamlines



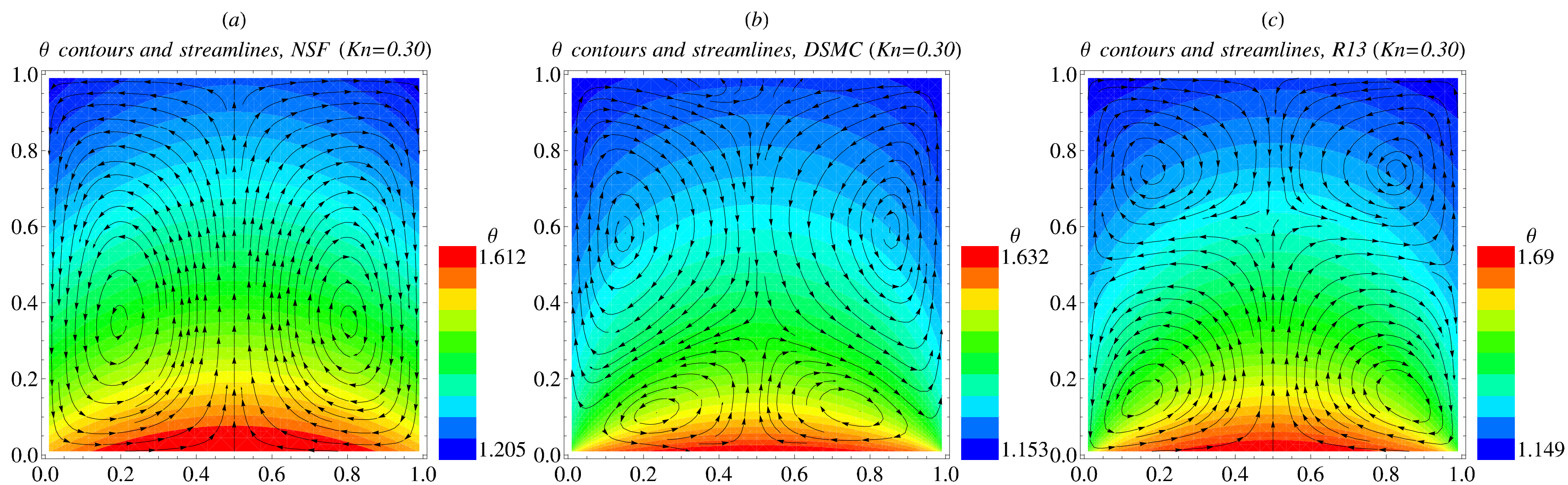
R13: 2D Bottom heated plate (MM) [AR, AM, HS submitted]

comparison of NSF, DSMC, R13: temperature and streamlines

Kn=0.13



Kn=0.3

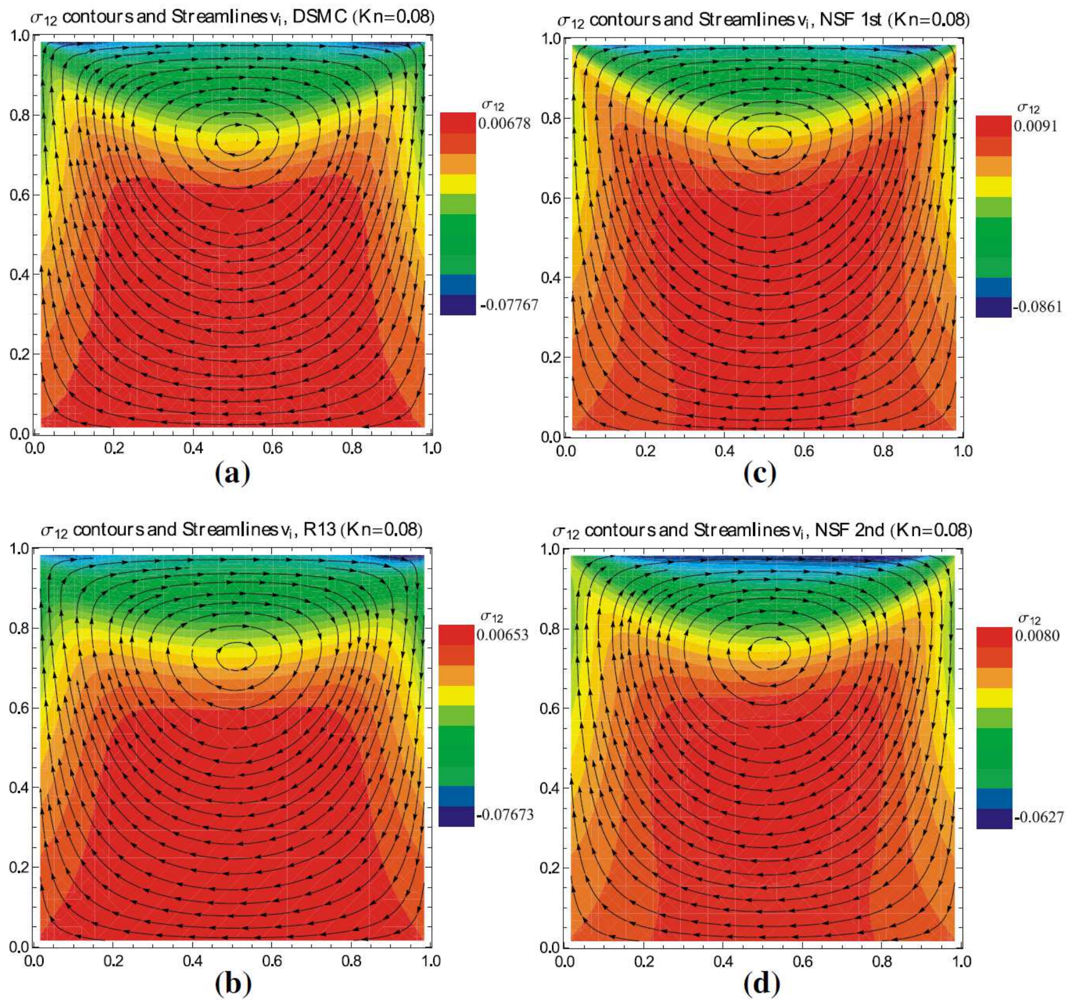


Fun excursion:

play with BC: inverted transpiration

R13: Lid-driven cavity flow (MM) [AR, MT, HS 2013]

velocity streamlines and stress contours $\mathrm{Kn} = 0.08,\ v_{lid} = 50\frac{\mathrm{m}}{\mathrm{s}}$

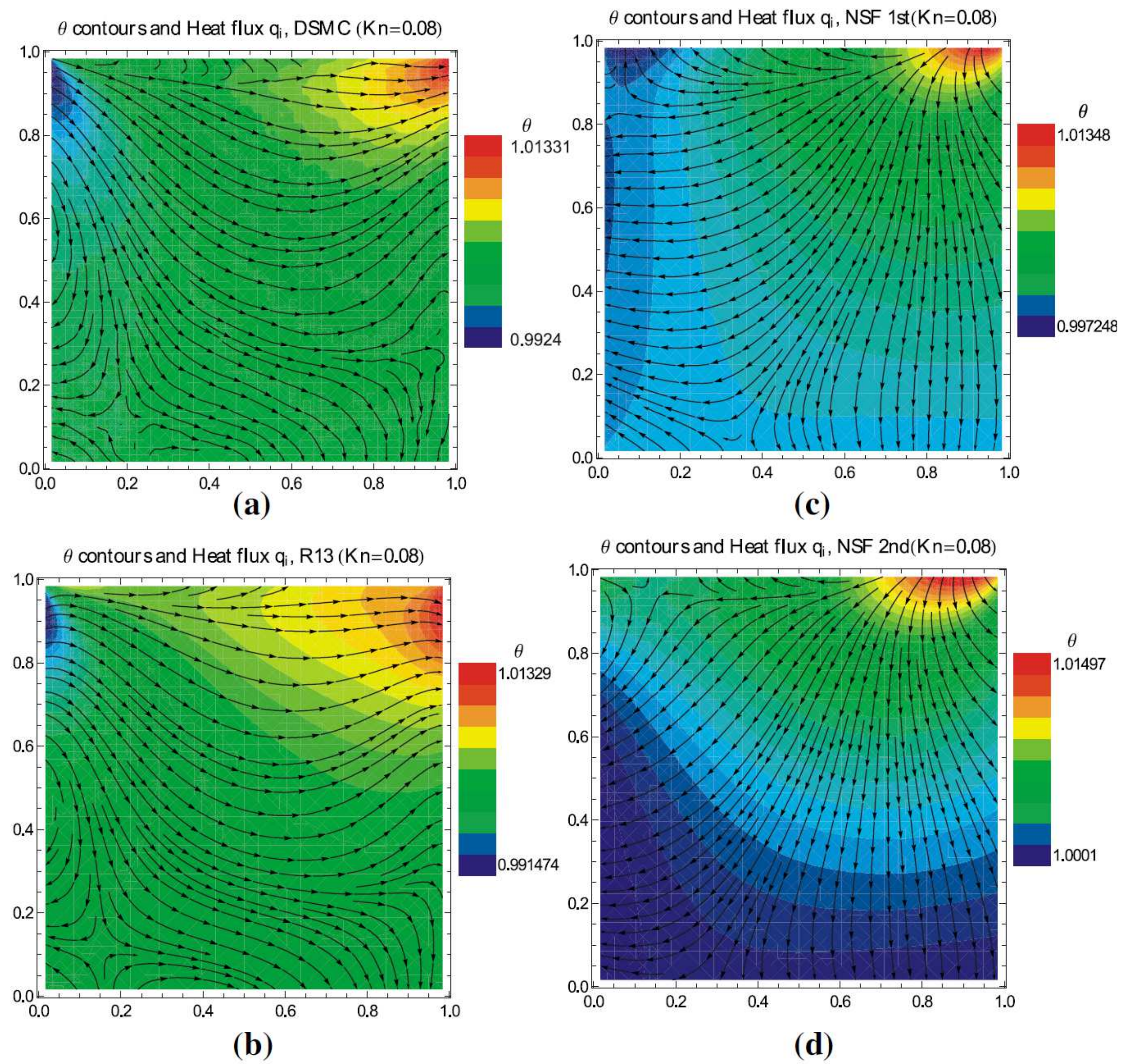


Dimensionless shear stress, D on the moving wall vs Knudsen number for R13, NSF with 1st order BCs (NSF1) and 2nd order BCs (NSF2).

Kn	δ	D [6]	D (R13)	D (NSF1)	D (NSF2)
0.010	70.7	–	0.1585	0.1476	0.1416
0.071	10	0.415 – –0.417	0.4271	0.4967	0.4000
0.141	5	0.502 – –0.507	0.5084	0.6613	0.4474
0.354	2	0.580 – –0.592	0.5644	0.8554	0.3717
0.707	1	0.620 – –0.631	0.5722	0.9619	0.2533

R13: Lid-driven cavity flow (MM) [AR, MT, HS 2013]

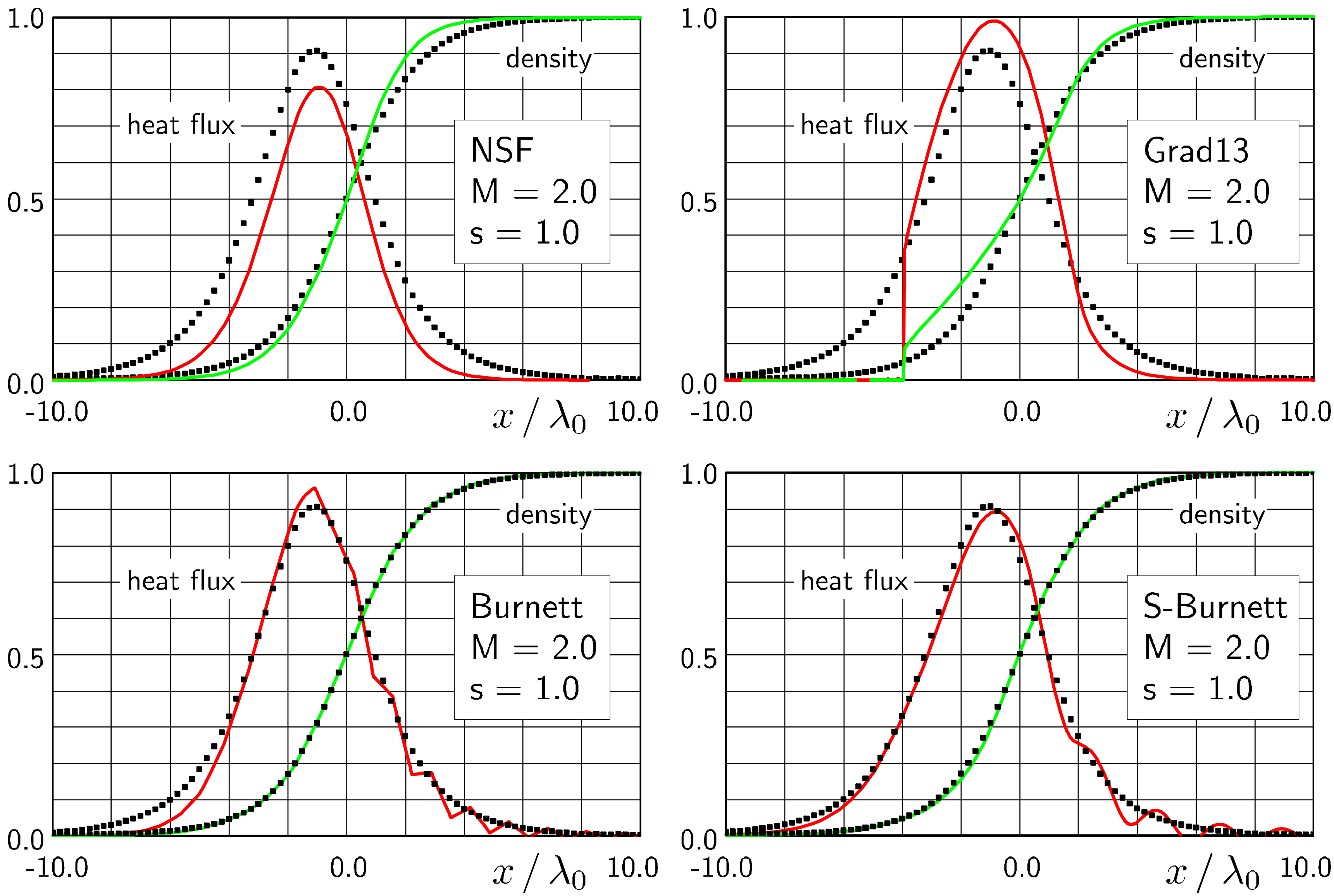
temperature contours and heat flux streamlines $\mathrm{Kn} = 0.08$, $v_{lid} = 50\frac{\mathrm{m}}{\mathrm{s}}$



DSMC, R13: heat flux from hot to cold!

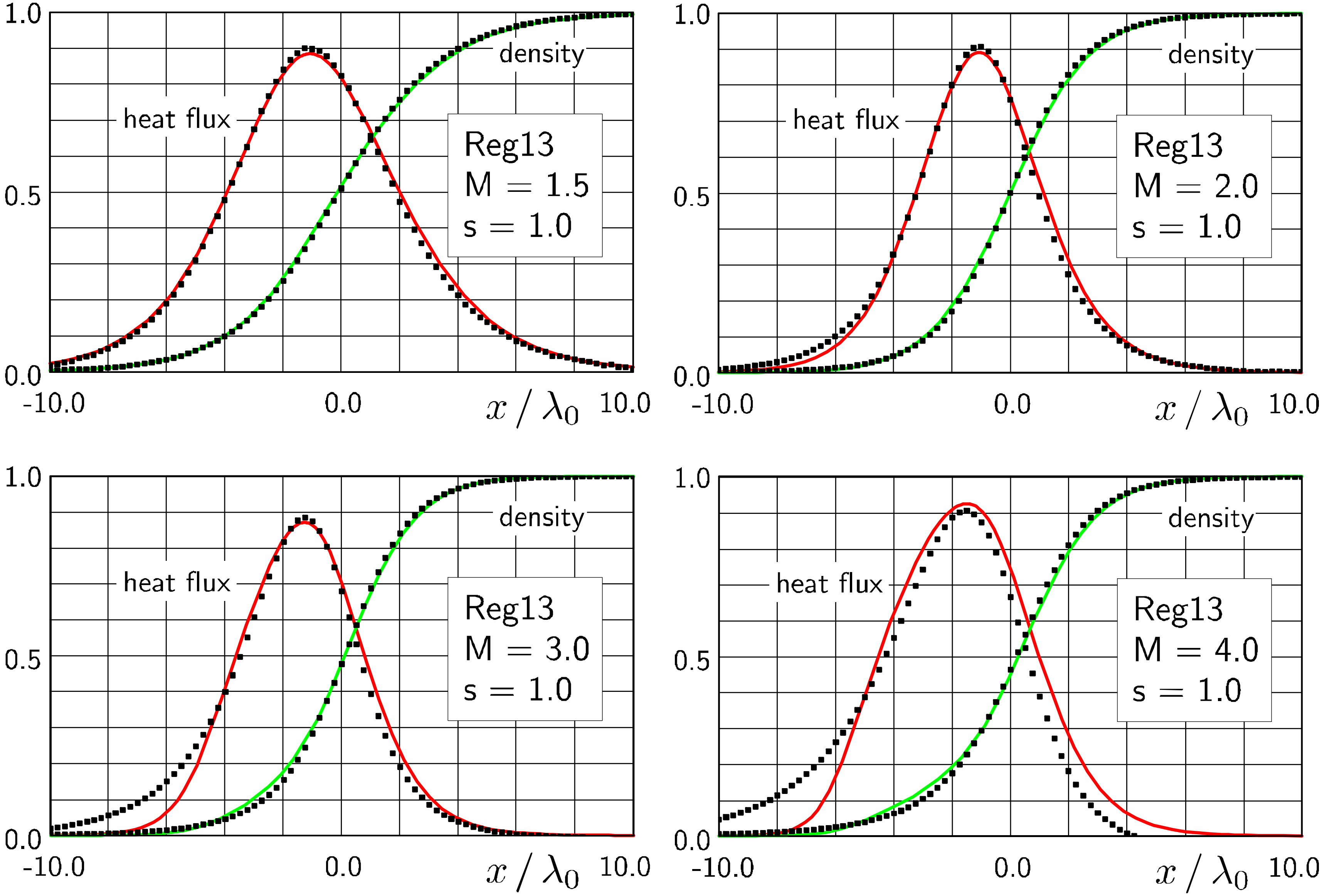
Shocks: Comparison with DSMC results [MT & HS 2004]

Failure of NSF, Burnett, super-Burnett, and Grad13



Shocks: Comparison with DSMC results [MT & HS 2004]

Success of R13



Let's take a step back, and summarize

- **close to equilibrium**
  - LIT and Chapman-Enskog expansion agree
  - classical hydrodynamics: Navier-Stokes-Fourier
  - thermodynamic structure within range of validity $\mathcal{O}\left(\mathrm{Kn}^1\right)$
- **away from equilibrium**
  - Extended Thermodynamics has great structure, but almost impossible
  - Chapman-Enskog to higher orders leads to bad equations (Burnett, s-Burnett)
  - Grad method/regularization gives good results, loss of thermodyn. structure
- **choice of variables**
  - ET: by prejudice, expectation, trial & error
  - Order of Magnitude: arbitrary system is reduced to its **essence**

Boltzmann Equation and the Collective

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} + G_k \frac{\partial f}{\partial c_k} = \frac{1}{\mathrm{Kn}} \int \int_0^{2\pi} \int_0^{\pi/2} \left(f' f^{1\prime} - f f^1 \right) \, g \, \sigma_{coll} \sin\Theta \, d\Theta \, d\varepsilon \, d\mathbf{c}^1$$

The Equilibrium Collective: $\mathrm{Kn} \mapsto 0$

Maxwell distribution: $C_i = c_i - v_i \ , \ \ \xi_i = C_i / \sqrt{2\theta}$

$$f_{|E}\left(\rho, v_i, T\right) = \frac{\rho}{m} \frac{1}{\sqrt{2\pi\theta}^3} \exp\left[-\frac{\xi^2}{2\theta} \right]$$

The Weakly Non-Equilibrium Collective: $\mathrm{Kn} \ll 1$

1st order Chapman-Enskog distribution: Sonine polynomials $S^{(r)}_{l+\frac{1}{2}}\left(\xi^2\right)$

$$f\left(\rho, v_i, T; \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \frac{\partial \theta}{\partial x_i}; \sigma\right) = f_{|E} \left[1 + \sum_{r=0}^{n_b} a_r S^{(r)}_{\frac{5}{2}} \xi_{\langle i} \xi_{j\rangle} \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + \sum_{r=1}^{n_a} b_r S^{(r)}_{\frac{3}{2}} \xi_i \sqrt{\frac{2}{\theta}} \frac{\partial \theta}{\partial x_i} \right]$$

coefficients a_r, b_r depend on cross section σ_{coll}, determine μ, κ

Hydrodynamics vs. Grad 13 moments

Hydrodynamics: variables ρ, v_i, θ; constitutive equations for σ_{ij}, q_i

CE distribution

$$f\left(\rho, v_i, T; \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \frac{\partial \theta}{\partial x_i}; \sigma\right) = f_M \left[1 + \sum_{r=0}^{n_b} a_r S_{\frac{5}{2}}^{(r)} \xi_{\langle i}\xi_{j\rangle} \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + \sum_{r=1}^{n_a} b_r S_{\frac{3}{2}}^{(r)} \xi_i \sqrt{\frac{2}{\theta}} \frac{\partial \theta}{\partial x_i}\right]$$

Grad 13 moments: variables ρ, v_i, θ, σ_{ij}, q_i; constitutive eqns for higher moments

Grad distribution

$$f_{|13}\left(\rho,\ v_i, \theta; \sigma_{ij}, q_i\right) = f_M \left[1 + \xi_{\langle i}\xi_{j\rangle} \frac{\sigma_{ij}}{p} + \frac{2\sqrt{2}}{5}\left(\xi^2 - \frac{2}{5}\right)\xi_k \frac{q_k}{p\sqrt{\theta}}\right]$$

$\Longrightarrow$ **CE distribution function has more complexity than Grad 13!!**

CE distribution function has more complexity than Grad 13 . . .

. . . but Grad 13 has more complex equations

Hydrodynamics

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} = 0$$

$$\rho\frac{Dv_i}{Dt} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = G_i$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \frac{\partial q_k}{\partial x_k} = -\left(p\delta_{ik} + \sigma_{ik}\right)\frac{\partial v_i}{\partial x_k}$$

$$\sigma_{ik} = -2\mu\frac{\partial v_{\langle i}}{\partial x_{k\rangle}}$$

$$q_i = -\kappa\frac{\partial \theta}{\partial x_i}$$

Grad's 13 moments

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} = 0$$

$$\rho\frac{Dv_i}{Dt} + \frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = G_i$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \frac{\partial q_k}{\partial x_k} = -\left(p\delta_{ik} + \sigma_{ik}\right)\frac{\partial v_i}{\partial x_k}$$

$$\frac{D\sigma_{ij}}{Dt} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k} + 2p\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\frac{p}{\mu}\sigma_{ij}$$

$$\frac{Dq_i}{Dt} + \frac{5}{2}\sigma_{ik}\frac{\partial \theta}{\partial x_k} - \sigma_{ik}\theta\frac{\partial \ln \rho}{\partial x_k} - \frac{\sigma_{ik}}{\rho}\frac{\partial \sigma_{kl}}{\partial x_l} + \theta\frac{\partial \sigma_{ik}}{\partial x_k} + \\ + \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i} + \frac{5}{2}p\frac{\partial \theta}{\partial x_i} = -\frac{5}{2}\frac{p}{\kappa}q_i$$

Is that enough??

CE expansion to 2nd order: Burnett equations

$$\sigma_{ij} = \sigma_{ij}^{(1)} + \sigma_{ij}^{(2)} \quad , \quad q_i = q_i^{(1)} + q_i^{(2)}$$

$$\sigma_{ij}^{(1)} = -2\mu S_{ij} \;\; \text{and} \;\; q_i^{(1)} = -\kappa \frac{\partial \theta}{\partial x_i} \qquad \text{with} \qquad \mu = \mu_0 \left(\frac{\theta}{\theta_0}\right)^{\omega} \; , \; \kappa = \frac{5}{2}\frac{\mu}{\Pr} \; , \; S_{ij} = \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$$

$$\sigma_{ij}^{(2)} = \frac{\mu^2}{p}\left[\varpi_1 \frac{\partial v_k}{\partial x_k} S_{ij} - \varpi_2 \left(\frac{\partial}{\partial x_{\langle i}}\left(\frac{1}{\rho}\frac{\partial p}{\partial x_{j\rangle}}\right) + \frac{\partial v_k}{\partial x_{\langle i}}\frac{\partial v_{j\rangle}}{\partial x_k} + 2\frac{\partial v_k}{\partial x_{\langle i}} S_{j\rangle k}\right) + \varpi_3 \frac{\partial^2 \theta}{\partial x_{\langle i}\partial x_{j\rangle}} + \varpi_4 \frac{\partial \theta}{\partial x_{\langle i}}\frac{\partial \ln p}{\partial x_{j\rangle}} + \varpi_5 \frac{1}{\theta}\frac{\partial \theta}{\partial x_{\langle i}}\frac{\partial \theta}{\partial x_{j\rangle}} + \varpi_6 S_{k\langle i}S_{j\rangle k}\right]$$

$$q_i^{(2)} = \frac{\mu^2}{\rho}\left[\theta_1 \frac{\partial v_k}{\partial x_k}\frac{\partial \ln \theta}{\partial x_i} - \theta_2 \left(\frac{2}{3}\frac{\partial^2 v_k}{\partial x_k \partial x_i} + \frac{2}{3}\frac{\partial v_k}{\partial x_k}\frac{\partial \ln \theta}{\partial x_i} + 2\frac{\partial v_k}{\partial x_i}\frac{\partial \ln \theta}{\partial x_k}\right) + \theta_3 S_{ik}\frac{\partial \ln p}{\partial x_k} + \theta_4 \frac{\partial S_{ik}}{\partial x_k} + 3\theta_5 S_{ik}\frac{\partial \ln \theta}{\partial x_k}\right]$$

Burnett coefficients for power potentials [Reinecke & Kremer]

γ	ω	ϖ_1	ϖ_2	ϖ_3	ϖ_4	ϖ_5	ϖ_6	θ_1	θ_2	θ_3	θ_4	θ_5
ES-BGK		$\frac{4}{3}\left(\frac{7}{2}-\omega\right)$	2	$\frac{2}{\Pr}$	0	$\frac{2\omega}{\Pr}$	8	$\frac{5}{3}\frac{1}{\Pr^2}\left(\frac{7}{2}-\omega\right)$	$\frac{5}{2}\frac{1}{\Pr^2}$	$-\frac{2}{\Pr}$	$\frac{2}{\Pr}$	$\frac{7}{3}\frac{1}{\Pr}\left(1+\frac{1}{\Pr}+\frac{2\omega}{7}\right)$
5	1	3.333	2	3	0	3	8	9.375	5.625	−3	3	9.75
	ES	3.333	2	3	0	3	8	9.375	5.625	−3	3	9.75
7	0.833	3.561	2.003	2.793	0.217	1.942	7.781	10.038	5.647	−3.010	2.793	9.113
7.66	0.8	3.600	2.004	2.761	0.254	1.784	7.748	10.160	5.656	−3.014	2.761	9.019
9	0.75	3.679	2.007	2.695	0.328	1.466	7.681	10.402	5.674	−3.023	2.695	8.829
17	0.625	3.863	2.016	2.553	0.500	0.814	7.543	10.995	5.736	−3.053	2.553	8.442
∞	0.5	4.056	2.028	2.418	0.681	0.219	7.424	11.644	5.822	−3.09	2.418	8.286
	ES	4	2	3	0	1.5	8	11.25	5.625	−3	3	9.25

2nd order expansion of Grad 13 gives ES-BGK/Maxwell-model coefficients!!

Dependence of moments on molecular interaction model

Couette flow at Kn=0.25, DSMC with different collision models (VHS, VSS, Maxwell)

Hydrodynamic quantities: not much affected

velocity

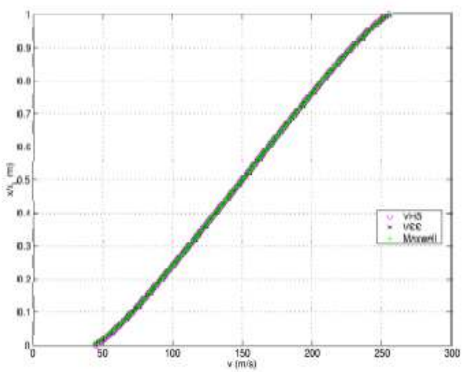


Figure 64: u (m/s) versus x/x_l

temperature

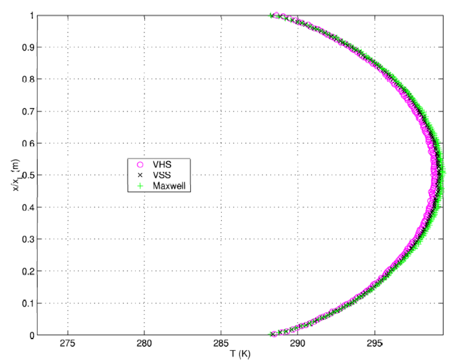


Figure 65: T (K) versus x/x_l

shear stress

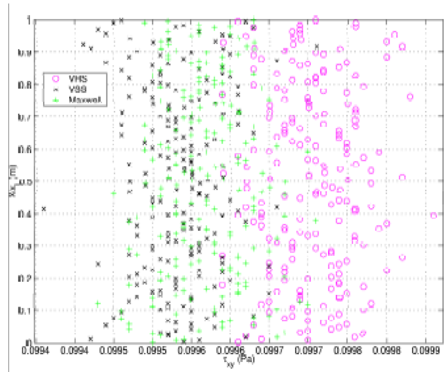


Figure 71: τ_{xy} (Pa) versus x/x_l

normal heat flux

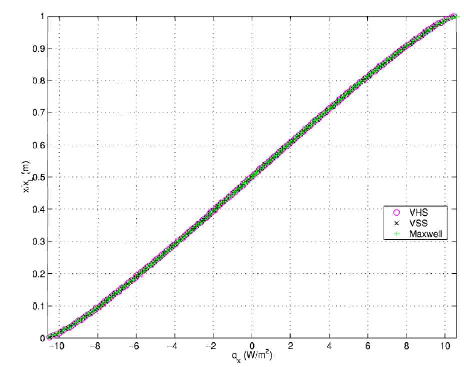


Figure 67: q_x (W/m^2) versus x/x_l

Rarefaction quantities (Burnett etc.): visible dependence on molecular model

parallel heat flux

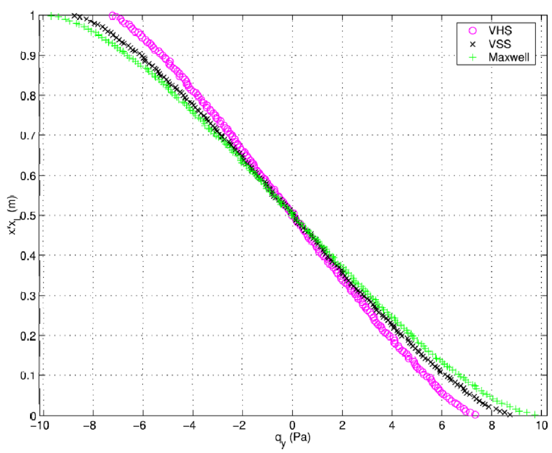


Figure 68: q_y (W/m^2) versus x/x_l

pressure

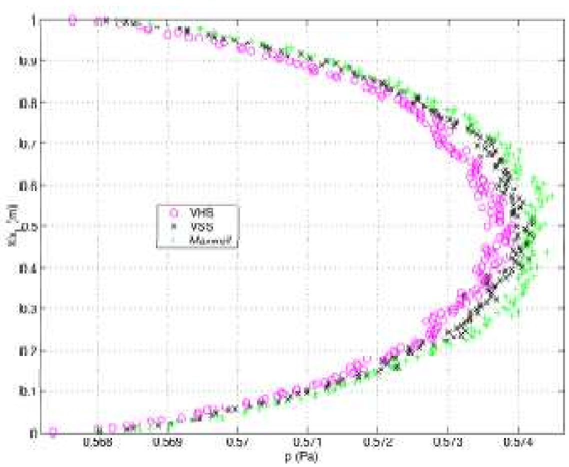


Figure 72: p (Pa) versus x/x_l

normal stress

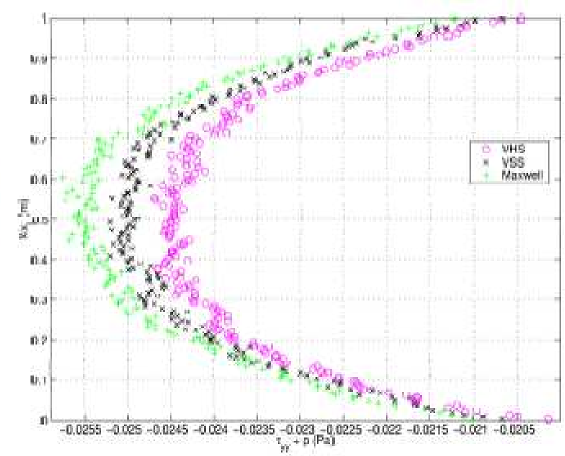
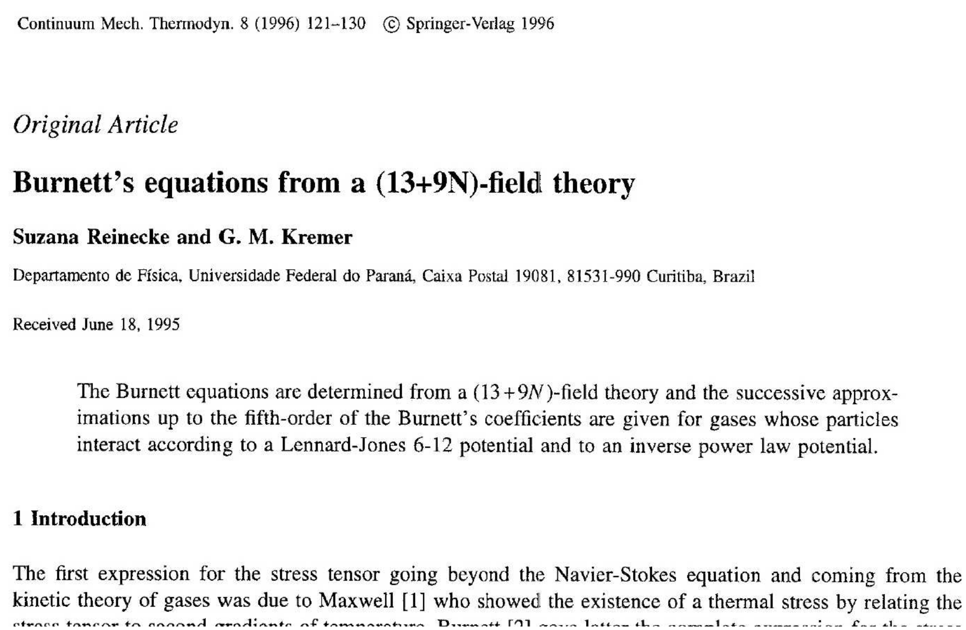


Figure 70: $\tau_{yy} + p$ (Pa) versus x/x_l

Non-Maxwellian molecules with moment method??

Answer 1: Brute force—many moments


Continuum Mech. Thermodyn. 8 (1996) 121–130

Original Article

Burnett's equations from a (13+9N)-field theory

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Received June 18, 1995

The Burnett equations are determined from a $(13+9N)$-field theory and the successive approximations up to the fifth-order of the Burnett's coefficients are given for gases whose particles interact according to a Lennard-Jones 6-12 potential and to an inverse power law potential.

1 Introduction

The first expression for the stress tensor going beyond the Navier-Stokes equation and coming from the kinetic theory of gases was due to Maxwell [1] who showed the existence of a thermal stress by relating the

Burnett is unstable, moment equations are stable

same accuracy with moments requires 13+9N moments $(N \simeq 3 \Longrightarrow 40)$

$\Longrightarrow$ **large computational overhead**

Answer 2: Reduce large moment system to its essence

$\Longrightarrow$ **Order of Magnitude Method**

Regularized 13 moment equations (linear)

coefficients $a^{(\alpha,\beta)}$ determined through Grad closure, collision term

$$\frac{\partial q_i}{\partial t} + a^{(1,1)}\frac{\partial \sigma_{ik}}{\partial x_k} - a^{(1,2)}\frac{\partial}{\partial x_k}\left[\sigma_{ik} + 2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{k\rangle}}\right] - a^{(1,3)}\varepsilon\frac{\partial}{\partial x_k}\frac{\partial q_{\langle i}}{\partial x_{k\rangle}} - a^{(1,4)}\varepsilon\frac{\partial}{\partial x_i}\frac{\partial q_k}{\partial x_k} = -\frac{1}{\varepsilon}a^{(1,0)}\left[q_i + \frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial \theta}{\partial x_i}\right]$$

$$\frac{\partial \sigma_{ij}}{\partial t} + a^{(2,1)}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - a^{(2,2)}\frac{\partial}{\partial x_{\langle i}}\left[q_{j\rangle} + \frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial \theta}{\partial x_{j\rangle}}\right] - a^{(2,3)}\varepsilon\frac{\partial}{\partial x_k}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} - a^{(2,4)}\varepsilon\frac{\partial^2 \sigma_{ij}}{\partial x_k \partial x_k} = -\frac{1}{\varepsilon}a^{(2,0)}\left[\sigma_{ij} + 2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

	Maxwell	hard spheres	BGK
Pr	$\frac{2}{3} = 0.6667$	0.660851	1
$a^{(1,0)}$	$\frac{2}{3} = 0.6667$	0.650061	1
$a^{(1,1)}$	1	0.786941	1
$a^{(1,2)}$	0	0.186614	0
$a^{(1,3)}$	$\frac{12}{5} = 2.4$	2.10417	$\frac{14}{5} = 2.8$
$a^{(1,4)}$	2	1.47742	$\frac{4}{3} = 1.3333$
$a^{(2,0)}$	1	0.98632	1
$a^{(2,1)}$	$\frac{4}{5} = 0.8$	0.631247	$\frac{4}{5} = 0.8$
$a^{(2,2)}$	0	0.0925568	0
$a^{(2,3)}$	2	2.15033	3
$a^{(2,4)}$	0	-0.102588	0

Regularized 13 moment equations (linear)

coefficients $a^{(\alpha,\beta)}$ determined through Grad closure, collision term

$$\kappa_a = \sum_{b=1}^{N} \left[\tilde{\mathcal{C}}^{(1)}\right]^{-1}_{ab} (2b+3)!!\frac{b}{3} \quad , \quad \mu_a = \sum_{a=1}^{N} \left[\tilde{\mathcal{C}}^{(2)}\right]^{-1}_{ab} \frac{2\,(2b+3)!!}{15}$$

$$\zeta_c = \sum_{a=1}^{N} \left[\tilde{\mathcal{C}}^{(0)}\right]^{-1}_{ca} \left[2\sum_{b=1}^{N} \tilde{\mathcal{R}}^{(1)}_{ab}\frac{\kappa_b}{\kappa_1} - (2a+3)!!\frac{2\,(a+1)}{3}\right] \quad , \quad \vartheta_b = \sum_{a=2}^{N} \left[\tilde{\mathcal{D}}^{(1)}\right]^{-1}_{ba} \left[\sum_{c=1}^{N} \tilde{\mathcal{R}}^{(2)}_{ac}\frac{\mu_c}{\mu_1} - \frac{(2a+3)!!}{3} - \frac{\kappa_a}{\kappa_1}\left[\frac{\mu_2}{\mu_1} - 5\right]\right]$$

$$\eta_b = \frac{2}{\kappa_1}\sum_{a=2}^{N} \left[\tilde{\mathcal{D}}^{(1)}\right]^{-1}_{ba} \left[\frac{a\,(2a+3)!!}{3} - 5\frac{\kappa_a}{\kappa_1}\right] \quad , \quad \tilde{\mathcal{D}}^{(1)}_{ab} = \tilde{\mathcal{C}}^{(1)}_{ab} - \frac{\kappa_a}{\kappa_1}\tilde{\mathcal{C}}^{(1)}_{1b} \quad , \quad \varphi_b = \frac{4}{5}\sum_{a=2}^{N} \left[\tilde{\mathcal{D}}^{(2)}\right]^{-1}_{ba} \left[\frac{\kappa_a}{\kappa_1} - \frac{\mu_a}{\mu_1}\right]$$

$$\phi_b = \frac{2}{\mu_1}\sum_{a=2}^{N} \left[\tilde{\mathcal{D}}^{(2)}\right]^{-1}_{ba} \left[\frac{(2a+3)!!}{15} - \frac{\mu_a}{\mu_1}\right] \quad , \quad \tilde{\mathcal{D}}^{(2)}_{ab} = \tilde{\mathcal{C}}^{(2)}_{ab} - \frac{\mu_a}{\mu_1}\tilde{\mathcal{C}}^{(2)}_{1b} \quad , \quad \xi_b = \frac{3}{7}\sum_{a=1}^{N} \left[\tilde{\mathcal{C}}^{(3)}\right]^{-1}_{ba} \sum_{c=1}^{N} \tilde{\mathcal{R}}^{(2)}_{ac}\frac{\mu_c}{\mu_1}$$

$$a^{(1,0)} = \frac{5}{\kappa_1} - \frac{1}{2}\sum_{b=2}^{3} \tilde{\mathcal{C}}^{(1)}_{1b}\eta_b \, , \quad a^{(1,1)} = \frac{\mu_2}{2\mu_1} - \frac{5}{2} - \frac{1}{2}\sum_{b=2}^{3} \tilde{\mathcal{C}}^{(1)}_{1b}\vartheta_b \, , \quad a^{(1,4)} = \frac{\zeta_1}{6} - \frac{1}{2}\sum_{a,b=2}^{N} \tilde{\mathcal{C}}^{(1)}_{1b}\left[\tilde{\mathcal{D}}^{(1)}_{ba}\right]^{-1}\left[\frac{\zeta_a}{3} - \frac{\kappa_a}{\kappa_1}\frac{\zeta_1}{3}\right]$$

$$a^{(1,2)} = \frac{\phi_2}{2} - \frac{1}{2}\sum_{a,b=2}^{N} \tilde{\mathcal{C}}^{(1)}_{1b}\left[\tilde{\mathcal{D}}^{(1)}_{ba}\right]^{-1}\left\{\sum_{c=2}^{3} \tilde{\mathcal{R}}^{(2)}_{ac}\phi_c - \frac{\kappa_a}{\kappa_1}\phi_2 - a^{(2,0)}\left[\vartheta_a - \eta_a\left[\frac{a^{(1,1)}}{a^{(1,0)}} - \frac{5}{4\,\mathrm{Pr}\,a^{(1,0)}}\right]\right]\right\}$$

$$a^{(1,3)} = \frac{\varphi_2}{2} - \frac{1}{2}\sum_{a,b=2}^{N} \tilde{\mathcal{C}}^{(1)}_{1b}\left[\tilde{\mathcal{D}}^{(1)}_{ba}\right]^{-1}\left\{\sum_{c=2}^{3} \tilde{\mathcal{R}}^{(2)}_{ac}\varphi_c - \frac{\kappa_a}{\kappa_1}\varphi_2 - a^{(2,1)}\left[\vartheta_a - \eta_a\left[\frac{a^{(1,1)}}{a^{(1,0)}} - \frac{5}{4\,\mathrm{Pr}\,a^{(1,0)}}\right]\right]\right\}$$

$$a^{(2,0)} = \frac{2}{\mu_1} - \sum_{b=2}^{3} \tilde{\mathcal{C}}^{(2)}_{1b}\phi_b \, , \quad a^{(2,1)} = \frac{4}{5} - \sum_{b=2}^{2} \tilde{\mathcal{C}}^{(2)}_{1b}\varphi_b \, ,$$

$$a^{(2,2)} = \sum_{a,b=2}^{3} \tilde{\mathcal{C}}^{(2)}_{1b}\left[\tilde{\mathcal{D}}^{(2)}\right]^{-1}_{ba}\left\{-\frac{2}{5}\eta_a + a^{(1,0)}\left[\varphi_a + \phi_a\left[\frac{2\,\mathrm{Pr}}{a^{(2,0)}} - \frac{a^{(2,1)}}{a^{(2,0)}}\right]\right]\right\}$$

$$a^{(2,3)} = \xi_1 - \sum_{a,b=2}^{3} \tilde{\mathcal{C}}^{(2)}_{1b}\left[\tilde{\mathcal{D}}^{(2)}_{ba}\right]^{-1}\left\{\xi_a + \vartheta_a - \xi_1\frac{\mu_a}{\mu_1} - \frac{5}{2}a^{(1,1)}\left[\varphi_a + \phi_a\left[\frac{2\,\mathrm{Pr}}{a^{(2,0)}} - \frac{a^{(2,1)}}{a^{(2,0)}}\right]\right]\right\}$$

$$a^{(2,4)} = \frac{1}{3}\sum_{a,b=2}^{3} \tilde{\mathcal{C}}^{(2)}_{1b}\left[\tilde{\mathcal{D}}^{(2)}_{ba}\right]^{-1}\left\{\vartheta_a - \frac{5}{2}a^{(1,1)}\left[\varphi_a + \phi_a\left[\frac{2\,\mathrm{Pr}}{a^{(2,0)}} - \frac{a^{(2,1)}}{a^{(2,0)}}\right]\right]\right\}$$

Burnett and super-Burnett equations

CE expansion of generalized R13 (linear)

$$q_i = -\frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial\theta}{\partial x_i}+\varepsilon^2\left[\frac{\theta_4^B}{2}\frac{\partial^2 v_i}{\partial x_k\partial x_k}+\frac{2}{3}\left(\frac{\theta_4^B}{4}-\theta_2^B\right)\frac{\partial^2 v_k}{\partial x_k\partial x_i}\right]-\varepsilon^3\left[\theta_1^{sB}\frac{\partial^3\rho}{\partial x_i\partial x_k\partial x_k}+\theta_2^{sB}\frac{\partial^3\theta}{\partial x_k\partial x_k\partial x_i}\right]$$

$$\sigma_{ij} = -2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}-\varepsilon^2\left[\varpi_2^B\frac{\partial^2\rho}{\partial x_{\langle i}\partial x_{j\rangle}}+\left(\varpi_2^B-\varpi_3^B\right)\frac{\partial^2\theta}{\partial x_{\langle i}\partial x_{j\rangle}}\right]+\varepsilon^3\left[\varpi_1^{sB}\frac{\partial^2}{\partial x_{\langle i}\partial x_{j\rangle}}\frac{\partial v_k}{\partial x_k}-\varpi_2^{sB}\frac{\partial^2}{\partial x_k\partial x_k}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

	Maxwell	hard spheres	BGK	ES-BGK (HS)
Pr	$\frac{2}{3} = 0.6667$	0.660851	1	0.660851
θ_2^B	$\frac{45}{8} = 5.625$	5.81945	$\frac{5}{2} = 2.5$	$\frac{5}{2}\frac{1}{\mathrm{Pr}^2} = 5.724$
θ_4^B	3	2.42113	2	$\frac{2}{\mathrm{Pr}} = 3.026$
ϖ_2^B	2	2.02774	2	2
ϖ_3^B	3	2.42113	2	$\frac{2}{\mathrm{Pr}} = 3.026$
θ_1^{sB}	$\frac{5}{8} = 0.625$	2.23673	-1	
θ_2^{sB}	$\frac{157}{16} = 9.813$	5.81182	$\frac{25}{6} = 4.1667$	
ϖ_1^{sB}	$\frac{5}{3} = 1.6667$	0.493778	$-\frac{2}{3} = -0.6667$	
ϖ_2^{sB}	$\frac{4}{3} = 1.3333$	1.16695	2	

Burnett coefficients agree with literature

super-Burnett coefficients for non-Maxwellian molecules: first time

R13 nonlinear

non-linear 2nd order [HS 2004] with linear 3rd order contributions

$$\frac{D\rho}{Dt}+\rho\frac{\partial v_k}{\partial x_k}=0 \quad , \quad \rho\frac{Dv_i}{Dt}+\frac{\partial\rho\theta}{\partial x_i}+\frac{\partial\sigma_{ik}}{\partial x_k}=\rho G_i \quad , \quad \frac{3}{2}\rho\frac{D\theta}{Dt}+\frac{\partial q_k}{\partial x_k}+p\frac{\partial v_k}{\partial x_k}+\sigma_{ij}\frac{\partial v_i}{\partial x_j}=0$$

$$\frac{Dq_i}{Dt}+q_k\frac{\partial v_i}{\partial x_k}+\frac{5}{3}q_i\frac{\partial v_k}{\partial x_k}+a^{(1,1)}\theta\frac{\partial\sigma_{ik}}{\partial x_k} - a^{(1,2)}\frac{\partial}{\partial x_k}\left(\theta\left[\sigma_{ik}+2\mu\frac{\partial v_{\langle i}}{\partial x_{k\rangle}}\right]\right)-a^{(1,3)}\frac{\partial}{\partial x_k}\left(\frac{\mu}{\rho}\frac{\partial q_{\langle i}}{\partial x_{k\rangle}}\right)-a^{(1,4)}\frac{\partial}{\partial x_i}\left(\frac{\mu}{\rho}\frac{\partial q_k}{\partial x_k}\right) - a^{(1,5)}\theta\sigma_{ik}\frac{\partial\ln p}{\partial x_k}-a^{(1,6)}\frac{\sigma_{ik}q_k}{\mu}=-a^{(1,0)}\frac{p}{\mu}\left[q_i+\frac{5}{2\,\mathrm{Pr}}\mu\frac{\partial\theta}{\partial x_i}\right]$$

$$\frac{D\sigma_{ij}}{Dt}+2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k}+\sigma_{ij}\frac{\partial v_k}{\partial x_k}+a^{(2,1)}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - a^{(2,2)}\frac{\partial}{\partial x_{\langle i}}\left[q_{j\rangle}+\frac{5}{2\,\mathrm{Pr}}\mu\frac{\partial\theta}{\partial x_{j\rangle}}\right]-a^{(2,3)}\frac{\partial}{\partial x_k}\left(\frac{\mu}{\rho}\frac{\partial\sigma_{\langle ij}}{\partial x_{k\rangle}}\right)-a^{(2,4)}\frac{\partial}{\partial x_k}\left(\frac{\mu}{\rho}\frac{\partial\sigma_{ij}}{\partial x_k}\right) + a^{(2,5)}q_{\langle i}\frac{\partial\ln p}{\partial x_{j\rangle}}+a^{(2,6)}\frac{\sigma_{k\langle i}\sigma_{j\rangle k}}{\mu}+a^{(2,7)}\frac{q_{\langle i}q_{j\rangle}}{\theta\mu}=-a^{(2,0)}\frac{p}{\mu}\left[\sigma_{ij}+2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

	Pr	$a^{(1,0)}$	$a^{(1,1)}$	$a^{(1,2)}$	$a^{(1,3)}$	$a^{(1,4)}$	$a^{(1,5)}$	$a^{(1,6)}$
MM	0.66667	0.66667	1.0	0.0	2.4	2.0	1.0	1.33333
HS	0.66085	0.65006	0.78694	0.17693	2.09248	1.50489	1.00504	0.98678

	$a^{(2,0)}$	$a^{(2,1)}$	$a^{(2,2)}$	$a^{(2,3)}$	$a^{(2,4)}$	$a^{(2,5)}$	$a^{(2,6)}$	$a^{(2,7)}$
MM	1.0	0.8	0.0	2.0	0.0	0.0	0.0	0.0
HS	0.98632	0.63125	0.09466	2.19368	0.11447	0.23128	0.35548	0.10270

Example: Couette flow $\varepsilon = 0.1,\ \chi = 1$ preliminary results, BC not shown

solution of semi-linear R13, similar to [PT,MT&HS 2009]

shear stress

$$\sigma_{xy} = -C_0\,\mathrm{Kn}$$

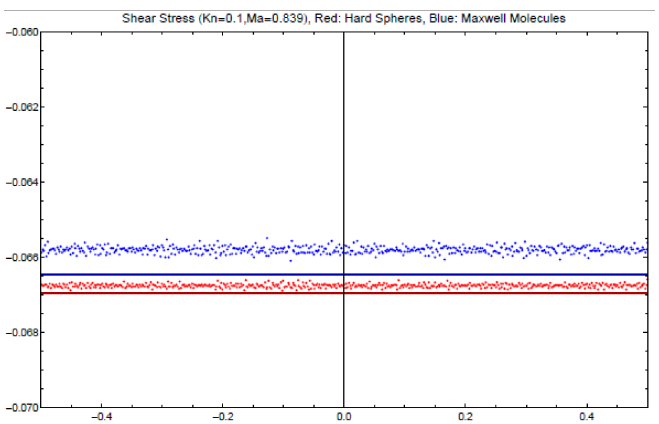
velocity

$$v_x\left(y\right) = -\frac{a^{(2,0)}}{a^{(2,0)}}\frac{1}{\mathrm{Kn}}C_1\ y - \frac{a^{(2,1)} - a^{(2,2)}}{2a^{(2,0)}}q_x\left(y\right)$$

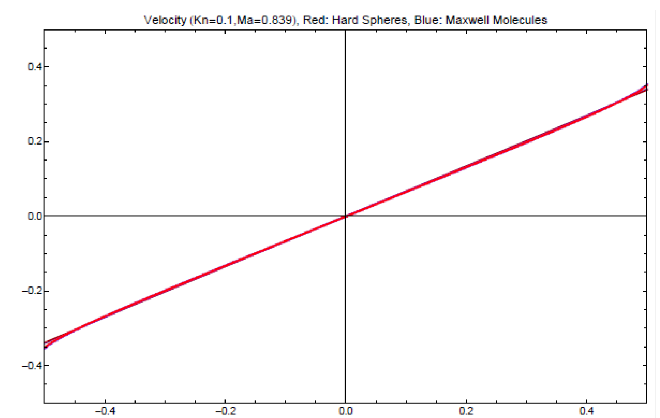
heat flux parallel to wall

$$q_x(y) = -\frac{1 + a^{(1,6)}}{a^{(1,0)}}\mathrm{Kn}^2\,C_0^3\ y + C_2\sinh\left[\sqrt{\frac{2a^{(1,0)}a^{(2,0)}}{a^{(1,3)}a^{(2,0)} - a^{(1,2)}a^{(2,1)} + a^{(1,2)}a^{(2,2)}}}\frac{y}{\mathrm{Kn}}\right]$$

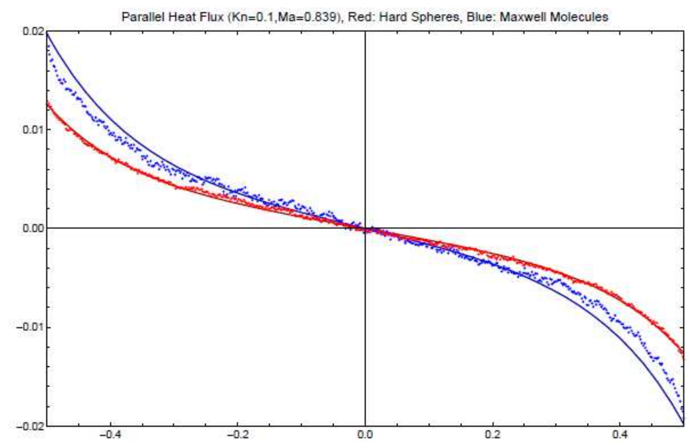
shear stress



velocity



heat flux parallel to wall



constants of integration C_α from BC

Example: Couette flow $\varepsilon = 0.1,\ \chi = 1$ preliminary results, BC not shown

solution of semi-linear R13, similar to [PT,MT&HS 2009]

temperature

$$\theta\left(y\right) = C_4 - \frac{\Pr}{5} C_0^2\, y^2 - 2\Pr\frac{a^{(1,1)} - a^{(1,2)}}{5a^{(1,0)}}\sigma_{yy}$$

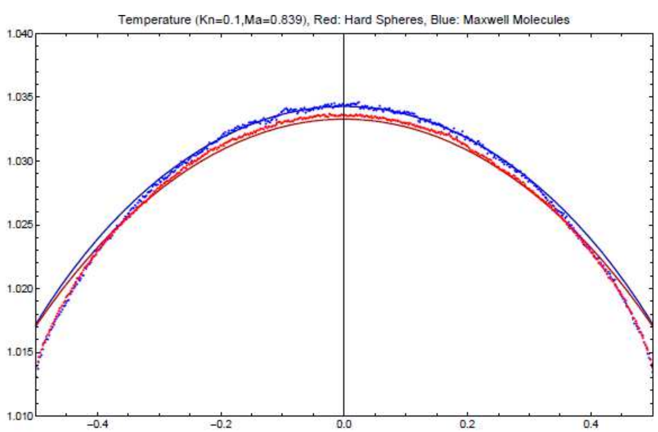
pressure

$$p = P_0 - \sigma_{yy}\left(y\right)$$

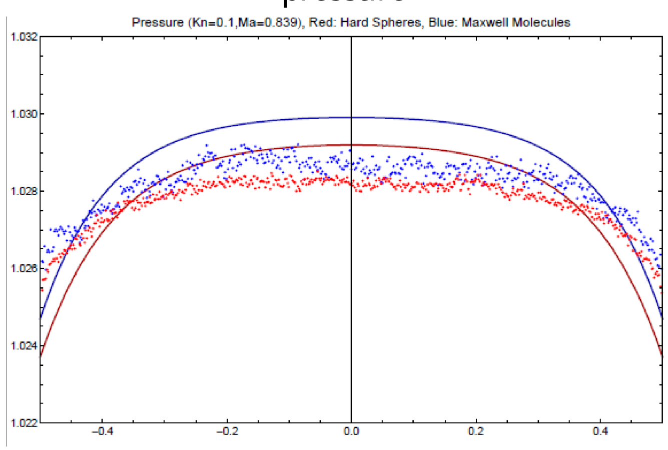
normal stress

$$\sigma_{yy}\left(y\right) = -\frac{2 + 2a^{(2,1)} + a^{(2,6)}}{3a^{(2,0)}}\,\mathrm{Kn}^2\, C_0^2 - \frac{2a^{(2,7)}}{3a^{(2,0)}}\,\mathrm{Kn}^2\, C_0^4\, y^2 + C_3\cosh\left(\sqrt{\frac{15a^{(1,0)}a^{(2,0)}}{9a^{(2,3)} + 15a^{(2,4)} + 10a^{(2,2)}(a^{(1,2)} - a^{(1,1)})}}\frac{y}{\mathrm{Kn}}\right)$$

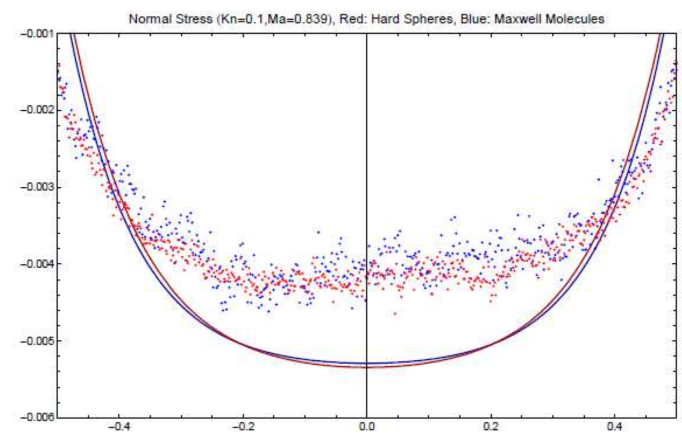
temperature



pressure



normal stress



constants of integration C_α from BC

R13 distribution function

Recall Grad distribution used for closure

$$f_G = f_{|E}\left[1 - \frac{1}{k}\lambda_B\varphi_B\right] = f_{|E}\left[1 - \frac{1}{k}\left\{\mathcal{A}^{-1}_{BA}\left(u_A - u_{A|E}\right)\right\}\varphi_B\right]$$

Order of Magnitude: constructs moments with clear Kn order

zeroth order: $\rho, \;\; v_i, \;\; \theta$

first order $\sigma_{ij} \;\; , \;\; q_i$

second order m_{ijk}

$$w_i^a = u_i^{a-1} - \frac{\kappa_a}{\kappa_1}2q_i \;\; (a = 2, 3)$$

$$w_{ij}^a = u_{ij}^{a-1} - \frac{\mu_a}{\mu_0}\sigma_{ij} \;\; (a = 2, 3)$$

at least 3rd order

$$\tilde{z}^c = \tilde{w}^c - \tfrac{\zeta_c}{\zeta_1}\tilde{w}^1 \qquad (c = 2, \ldots, N)$$

$$\tilde{z}_i^b = \tilde{w}_i^b - \frac{\eta_b\vartheta_3 - \eta_3\vartheta_b}{\eta_2\vartheta_3 - \eta_3\vartheta_2}\tilde{w}_i^2 - \frac{\eta_2\vartheta_b - \eta_b\vartheta_2}{\eta_2\vartheta_3 - \eta_3\vartheta_2}\tilde{w}_i^3 \qquad (b = 4, \ldots, N)$$

$$\tilde{z}_{ij}^b = \tilde{w}_{ij}^b - \frac{\phi_b\varphi_3 - \phi_3\varphi_b}{\phi_2\varphi_3 - \phi_3\varphi_2}\tilde{w}_{ij}^2 - \frac{\phi_2\varphi_b - \phi_b\varphi_2}{\phi_2\varphi_3 - \phi_3\varphi_2}\tilde{w}_{ij}^3 \qquad (b = 4, \ldots, N)$$

$$\tilde{z}_{ijk}^b = \tilde{u}_{ijk}^b - \frac{\xi_b}{\xi_1}m_{ijk}$$

R13 distribution function

leading orders for second order variables

$$\tilde{w}^b = -\zeta_b \varepsilon \frac{\partial q_k}{\partial x_k}$$

$$\tilde{w}_i^b = -\vartheta_b \varepsilon \frac{\partial \sigma_{ik}}{\partial x_k} - \eta_b \left[q_i + \frac{5\varepsilon}{2\,\mathrm{Pr}} \frac{\partial \theta}{\partial x_i} \right]$$

$$\tilde{w}_{ij}^b = -\varphi_b \varepsilon \frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \phi_b \left[\sigma_{ij} + 2\varepsilon \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right]$$

$$\tilde{u}_{ijk}^b = -\xi_b \varepsilon \frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}}$$

phase density to 2nd order gives R13 closure

$$f = \frac{\rho}{m} \frac{\exp\left(-\frac{\xi^2}{2}\right)}{\sqrt{2\pi\theta}^3} \Big[1 + A_\mu \xi_{\langle i}\xi_{j\rangle} \sigma_{ij} + A_\kappa \xi_i q_i$$
$$- A_\zeta \left(\varepsilon \frac{\partial q_k}{\partial x_k} \right) - A_\varphi \xi_{\langle i}\xi_{j\rangle} \left(\varepsilon \frac{\partial q_{\langle i}}{\partial x_{j\rangle}} \right) - A_\xi \xi_{\langle i}\xi_j \xi_{k\rangle} \left(\varepsilon \frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} \right)$$
$$-A_\vartheta \xi_i \left(\varepsilon \frac{\partial \sigma_{ik}}{\partial x_k} \right) - A_\eta \xi_i \left(q_i + \varepsilon \frac{\kappa_1}{2} \frac{\partial \theta}{\partial x_i} \right) - A_\phi \xi_{\langle i}\xi_{j\rangle} \left(\sigma_{ij} + \varepsilon \mu_1 \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right) \Big]$$
$$+ \mathcal{O}\left(\varepsilon^3\right)$$

R13 distribution function (non-eq manifold!!!)

$$f = \frac{\rho}{m}\frac{\exp\left(-\frac{\xi^2}{2}\right)}{\sqrt{2\pi\theta}^3}\left[1 + A_\mu \xi_{\langle i}\xi_{j\rangle}\sigma_{ij} + A_\kappa \xi_i q_i - A_\zeta\left(\varepsilon\frac{\partial q_k}{\partial x_k}\right) - A_\varphi \xi_{\langle i}\xi_{j\rangle}\left(\varepsilon\frac{\partial q_{\langle i}}{\partial x_{j\rangle}}\right) - A_\xi \xi_{\langle i}\xi_j\xi_{k\rangle}\left(\varepsilon\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}}\right)\right.$$
$$\left. - A_\vartheta \xi_i\left(\varepsilon\frac{\partial \sigma_{ik}}{\partial x_k}\right) - A_\eta \xi_i\left(q_i + \varepsilon\frac{\kappa_1}{2}\frac{\partial\theta}{\partial x_i}\right) - A_\phi \xi_{\langle i}\xi_{j\rangle}\left(\sigma_{ij} + \varepsilon\mu_1\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right)\right]$$

Maxwell molecules: Sonine polynomials

$$A_\mu = \frac{1}{2}\ ,\quad A_\kappa = -1 + \frac{\xi^2}{5}\ ,\quad A_\zeta = \frac{3}{2} - \xi^2 + \frac{\xi^4}{10}$$
$$A_\varphi = -\frac{6}{5} + \frac{6}{35}\xi^2\ ,\quad A_\xi = \frac{1}{3}\ ,\quad A_\vartheta = A_\eta = A_\phi = 0$$

hard spheres (3×3 matrices, round-off)**:**

$$A_\mu = 0.644446 - 0.0259338\,\xi^2 + 0.00058875\,\xi^4$$
$$A_\kappa = -1.21624 + 0.296686\,\xi^2 - 0.00909016\,\xi^4 + 0.000161778\,\xi^6$$
$$A_\zeta = 1.7532 - 1.35824\,\xi^2 + 0.200694\,\xi^4 - 0.00770945\,\xi^6 + 0.000127611\,\xi^8$$
$$A_\varphi = -1.59174 + 0.292273\,\xi^2 - 0.007209\,\xi^4$$
$$A_\xi = 0.594947 - 0.0412998\,\xi^2 + 0.0009871\,\xi^4$$
$$A_\vartheta = -0.0419332 + 0.0222017\,\xi^2 - 0.00274908\,\xi^4 + 0.0000861661\,\xi^6$$
$$A_\eta = 0.154386 - 0.0711059\,\xi^2 + 0.0070829\,\xi^4 - 0.000148437\,\xi^6$$
$$A_\phi = -0.138697 + 0.0265345\,\xi^2 - 0.000746734\,\xi^4$$

The trouble with the 2nd law

Boltzmann equation guarantees 2nd law

$$\frac{\partial \eta}{\partial t} + \frac{\partial \phi_k}{\partial x_k} = \Sigma \geq 0$$

with

$$\eta = -k \int f \ln \frac{f}{y} d\mathbf{c} \quad , \quad \phi_k = -k \int c_k f \ln \frac{f}{y} d\mathbf{c} \quad , \quad \Sigma = -k \int \mathcal{S} \ln \frac{f}{y} d\mathbf{c}$$

moment system, and Grad distribution f_G are only approximations

particular problems:

$$f_G = f_{|E} \left[1 - \frac{1}{k} \lambda_B \varphi_B \right] \quad \text{with} \quad \varphi_B = c_{i_1} c_{i_2} \cdots c_{i_n}$$

- f_G may become negative for large c_i (somewhat suppressed by Maxwellian $f_{|E}$)
- $\Longrightarrow \ln \frac{f_G}{y}$ does not exist for large c_i
- series expansion for $\ln \left[1 - \frac{1}{k} \lambda_B \varphi_B \right]$ requires $\left| \frac{1}{k} \lambda_B \varphi_B \right| < 1$, hence problematic

$\Longrightarrow$ **2nd law not guaranteed**

however: good quality of results indicates good *approximation* for 2nd law. Large values of moments will lead to problems (similar to radius of hyperbolicity in ET)

Summary: (Rational) Extended Thermodynamics

what you may like

- equations of balance law form
- 2nd law guaranteed
- symmetric hyperbolic eqs with convex extension $\Longrightarrow$ well-posed
- finite speeds of propagation
- good solutions for solvable problems (with enough variables, no boundaries)

what you may not like

- full structure only for a handful of small systems (e.g., Euler, 10 moments)
- difficult to fill with life without underlying microscopic model
- no *a priori* statement on number of variables $\Longrightarrow$ trial & error
- no theory for boundary conditions
- workable approximations with larger number of moments lose structure
  ($\Longrightarrow$ equivalent Grad moment method)
- finite speeds of propagation

Summary: Moment Method with Order of Magnitude Method

what you may like

- straightforward but cumbersome approximation of Boltzmann equation
- number of variables and their equations *a priori* linked to Kn
  $\Longrightarrow$ **only keep what's necessary**
- includes boundary conditions
- good agreement to Boltzmann solutions (with boundaries, Kn limited)
- regularization terms remove hyperbolicity $\Longrightarrow$ smooth shocks

what you may not like

- no entropy/2nd law for non-linear case
- reliance on Grad closure $\Longrightarrow$ negative phase density for large c
- no balance law structure for non-Maxwellian molecules
- regularization terms remove hyperbolicity $\Longrightarrow$ infinite speeds
- Knudsen layers don't obey bulk scaling laws

Summary: Moment Method with Order of Magnitude Method

what we would like

- **alternative closures:** positive f, easy to integrate,
- **link to 2nd law:** at least clear statement about approximation
- **more insight into resolution of Knudsen layers**

The case for moment equations and Extended Thermodynamics

- **Microscopic theory: Boltzmann Equation**
  - **microscopic variable: distribution function** $f(x_i, t, c_i)$ (7 independent variables!)
  - **Direct Numerical Solutions are accurate, but numerically expensive**
  - **Direct Simulation Monte Carlo is powerful (molecules, reactions), but expensive**

- **Macroscopic transport equations**
  - **Approximation to Boltzmann** $\Rightarrow$ **limited range of validity** $\mathbf{Kn}^n \ll \mathbf{1}$
  - **collective behavior described by finite number** N **of macroscopic variables, e.g.**
    $\rho(x_i, t)$ – density, $v_i(x_i, t)$ – velocity, $T(x_i, t)$ – temperature
    $\sigma_{ij}(x_i, t)$ – stress, $q_i(x_i, t)$ – heat flux , . . .
  - **fast deterministic solutions**
  - **explicit equations, analytic solutions give deeper insight into processes**

Proper moment equations capture the essence:

Accurate and efficient models for Micro and Vacuum flows

- **Analytic solutions**
  - simple geometry, 1-D / 2-D
  - great for understanding of basic rarefaction phenomena

- **Numeric solutions (CFD)**
  - 2-D / 3-D / transient
  - give deep insight into complex flow processes
  - allow simulation for design optimization

- **R13 equations for monatomic gases: continuing**
- **Extension to polyatomic gases, mixtures: in progress**
- **Heat transfer in the phonon gas: in progress**

IF we cannot have both, what do we value higher:

- **accuracy in approximation?**
- **thermodynamic/mathematical structure?**