Moment Methods for Rarefied Gases

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Outline

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Boltzmann equation

- **Distribution function $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$:**

$$(\text{No. of particles with position } \boldsymbol{x} \in X \text{ and velocity } \boldsymbol{\xi} \in V)$$
$$= \int_X \int_V f(\boldsymbol{x}, \boldsymbol{\xi}, t) \, \mathrm{d}\boldsymbol{\xi} \, \mathrm{d}\boldsymbol{x}$$

- **Boltzmann equation:**

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla_{\boldsymbol{x}} f = Q[f, f]$$

or

$$\frac{\partial f}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\boldsymbol{\xi} f) = Q[f, f]$$

  - Particles travelling at velocity $\boldsymbol{\xi}$ $\longrightarrow$ $\boldsymbol{\xi} \cdot \nabla_{\boldsymbol{x}}$
  - Binary collision between particles $\longrightarrow$ $Q[\cdot, \cdot]$

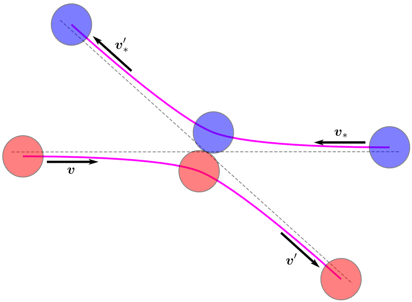
Collision operator

Binary collision operator:

$$Q[f,f](\boldsymbol{\xi}) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} \mathcal{B}(\boldsymbol{\xi}-\boldsymbol{\xi}_*,\boldsymbol{\sigma})[f(\boldsymbol{\xi}'_*)f(\boldsymbol{\xi}') - f(\boldsymbol{\xi}_*)f(\boldsymbol{\xi})]\,\mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}\boldsymbol{\xi}_*,$$

where

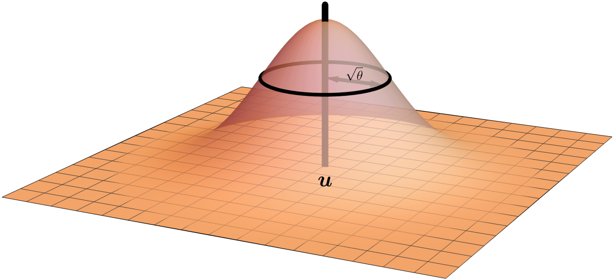
$$\boldsymbol{\xi}' = \frac{1}{2}(\boldsymbol{\xi}+\boldsymbol{\xi}_*) + \frac{1}{2}|\boldsymbol{\xi}-\boldsymbol{\xi}_*|\boldsymbol{\sigma}, \quad \boldsymbol{\xi}'_* = \frac{1}{2}(\boldsymbol{\xi}+\boldsymbol{\xi}_*) - \frac{1}{2}|\boldsymbol{\xi}-\boldsymbol{\xi}_*|\boldsymbol{\sigma}.$$



Equilibrium

Maxwellian:

$$\mathcal{M}(\boldsymbol{\xi}) = \frac{\rho}{m(2\pi\theta)^{3/2}} \exp\left(-\frac{|\boldsymbol{\xi} - \boldsymbol{u}|^2}{2\theta}\right)$$



$$\boxed{Q[\mathcal{M}, \mathcal{M}] = 0}$$

Linearization about the Maxwellian

Suppose the distribution function f is close to the Maxwellian $\mathcal{M}$:

$$f = \mathcal{M} + \varepsilon f'.$$

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Then

$$\begin{aligned}
Q[f,f] &= Q[\mathcal{M} + \varepsilon f', \mathcal{M} + \varepsilon f'] \\
&= Q[\mathcal{M},\mathcal{M}] + \varepsilon(Q[\mathcal{M}, f'] + Q[f', \mathcal{M}]) + \varepsilon^2 Q[f', f'] \\
&= 2Q[\mathcal{M},\mathcal{M}] + \varepsilon(Q[\mathcal{M}, f'] + Q[f', \mathcal{M}]) + \varepsilon^2 Q[f', f'] \\
&= Q[\mathcal{M}, f] + Q[f, \mathcal{M}] + \varepsilon^2 Q[f', f'] \\
&\approx Q[\mathcal{M}, f] + Q[f, \mathcal{M}].
\end{aligned}$$

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Then

$$\begin{aligned} Q[f,f] &= Q[\mathcal{M} + \varepsilon f', \mathcal{M} + \varepsilon f'] \\ &= Q[\mathcal{M},\mathcal{M}] + \varepsilon(Q[\mathcal{M},f'] + Q[f',\mathcal{M}]) + \varepsilon^2 Q[f',f'] \\ &= 2Q[\mathcal{M},\mathcal{M}] + \varepsilon(Q[\mathcal{M},f'] + Q[f',\mathcal{M}]) + \varepsilon^2 Q[f',f'] \\ &= Q[\mathcal{M},f] + Q[f,\mathcal{M}] + \varepsilon^2 Q[f',f'] \\ &\approx Q[\mathcal{M},f] + Q[f,\mathcal{M}]. \end{aligned}$$

Define

$$\mathcal{L}[f] = Q[\mathcal{M},f] + Q[f,\mathcal{M}].$$

Linearized collision operator

Linearized collision operator:

$$\mathcal{L}[f] = Q[\mathcal{M}, f] + Q[f, \mathcal{M}]$$

Choice of $\mathcal{M}$:

- Local Maxwellian:

$$\rho = \langle f \rangle, \qquad \boldsymbol{u} = \langle \boldsymbol{\xi} f \rangle / \rho, \qquad \theta = \frac{1}{3} \langle |\boldsymbol{\xi} - \boldsymbol{u}|^2 f \rangle / \rho$$

where

$$\langle \psi \rangle = \int_{\mathbb{R}^3} m \psi(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi}$$

- Global Maxwellian:

$$\rho = m, \quad \boldsymbol{u} = 0, \quad \theta = 1, \qquad \mathcal{M}(\boldsymbol{\xi}) = \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{|\boldsymbol{\xi}|^2}{2}\right)$$

Properties of the linearized collision operator

- **Conservation of mass, momentum, and energy:**

$$\langle \mathcal{L}[f] \rangle = 0, \quad \langle \boldsymbol{\xi} \mathcal{L}[f] \rangle = 0, \quad \langle |\boldsymbol{\xi}|^2 \mathcal{L}[f] \rangle = 0$$

- **Entropy dissipation:**

$$\langle \mathcal{L}[f] \log f \rangle \leqslant 0$$

- **Rotational invariance:** Let $f_R(\boldsymbol{\xi}) = f(\mathbf{R}\boldsymbol{\xi})$ for some orthogonal matrix $\mathbf{R}$. Then

$$\mathcal{L}[f_R](\boldsymbol{\xi}) = \mathcal{L}[f](\mathbf{R}\boldsymbol{\xi})$$

  if $\mathcal{M}$ is the Maxwellian with center at $\boldsymbol{u} = 0$.

- **Negative semi-definiteness:**

$$\left\langle \frac{f \mathcal{L}[f]}{\mathcal{M}} \right\rangle \leqslant 0$$

References

[1] H. Struchtrup, *Macroscopic Transport Equations for Rarefied Gas Flows*, Springer, (2005).

[2] C. Truesdell and R. G. Muncaster, *Fundamentals of Maxwell's Kinetic Theory of a Simple Monatomic Gas*, Academic Press, (1980).

[3] S. Chapman, *The Mathematical Theory of Non-Uniform Gases. Third Edition*, Cambridge University Press, (1990).

[4] I. Müller and T. Ruggeri, *Rational Extended Thermodynamics. Second Edition*, Springer, (1998).

Outline

Moments

- General definition of kth moments:

$$\langle p_k f \rangle = m \int_{\mathbb{R}^3} p_k(\boldsymbol{\xi}) f(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi}$$

  where $p_k(\boldsymbol{\xi})$ is a polynomial of degree k.

- **Examples:**
  - Density: $p_0(\boldsymbol{\xi}) = 1$
  - Momentum (density): $p_1(\boldsymbol{\xi}) = \boldsymbol{\xi}$
  - Energy (density): $p_2(\boldsymbol{\xi}) = |\boldsymbol{\xi}|^2/2$
  - Pressure: $p_2(\boldsymbol{\xi}) = |\boldsymbol{\xi} - \boldsymbol{u}|^2/3$
  - Pressure tensor: $p_2(\boldsymbol{\xi}) = (\boldsymbol{\xi} - \boldsymbol{u})(\boldsymbol{\xi} - \boldsymbol{u})^T$
  - Heat flux: $p_3(\boldsymbol{\xi}) = |\boldsymbol{\xi} - \boldsymbol{u}|^2(\boldsymbol{\xi} - \boldsymbol{u})/2$
  - ...

  These are the interesting quantities in the gas dynamics!

Why moment equations?

- The Boltzmann equation is hard to solve numerically:
  - High dimensionality
  - Complicated collision term
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- The Boltzmann equation is hard to solve numerically:
  - High dimensionality
  - Complicated collision term
  - Unbounded velocity domain
- We are usually not interested in the distribution function.
- It is known that the gas dynamics can be modeled by moments in certain regimes:
  - Euler equations
  - Navier-Stokes equations
  - ...

Three types of moments

Notations:

$$\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^T, \quad \xi = |\boldsymbol{\xi}|,$$
$$\boldsymbol{v} = \boldsymbol{\xi} - \boldsymbol{u}, \qquad v = |\boldsymbol{v}|.$$

- **Convective moments:** density, momentum, energy, ...

$$F_{i_1 i_2 \cdots i_n} = \langle \xi_{i_1} \cdots \xi_{i_n} f \rangle$$

- **Central moments:** density, pressure, heat flux, ...

$$\rho^n_{i_1 i_2 \cdots i_l} = \langle v^{2n} v_{i_1} \cdots v_{i_l} f \rangle$$

- **Trace-free moments:** stress tensor, heat flux, ...

$$\sigma^n_{i_1 i_2 \cdots i_l} = \rho^n_{\langle i_1 i_2 \cdots i_l \rangle} = \langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} f \rangle$$

Trace-free tensors

Given a tensor $T_{i_1 \cdots i_l}$, we use $T_{\langle i_1 \cdots i_l \rangle}$ to denote its symmetric and trace-free part.

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Example: If $l = 2$, the tensor T_{ij} is a matrix.

- Symmetrization:
$$T_{(ij)} = \frac{1}{2}(T_{ij} + T_{ji})$$
- Remove the trace part:
$$T_{\langle ij \rangle} = T_{(ij)} - \frac{1}{3} \sum_{k=1}^{3} T_{kk} \delta_{ij}$$

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In general, $T_{\langle i_1 \cdots i_l \rangle}$ is symmetric with respect to any two indices and satisfies
$$\sum_{i_j=1}^{3}\sum_{i_k=1}^{3} T_{\langle i_1 \cdots i_j \cdots i_k \cdots i_l \rangle}\delta_{i_j i_k} = 0$$

Harmonic polynomials

The polynomial

$$v_{\langle i_1} \cdots v_{i_l \rangle}$$

is defined by

$$\begin{aligned}
&v_{i_1} \cdots v_{i_l} \\
&- \alpha_1 \sum_{k_1=1}^{3} \big(\delta_{i_1 i_2} v_{i_3} v_{i_4} \cdots v_{i_l} v_{k_1} v_{k_1} + \delta_{i_1 i_3} v_{i_2} v_{i_4} \cdots v_{i_l} v_{k_1} v_{k_1} \\
&\qquad\qquad + \cdots + \delta_{i_{l-1} i_l} v_{i_1} v_{i_2} \cdots v_{i_{l-2}} v_{k_1} v_{k_1} \big) \\
&+ \alpha_2 \sum_{k_1=1}^{3} \sum_{k_2=1}^{3} \big(\delta_{i_1 i_2} \delta_{i_3 i_4} v_{i_5} \cdots v_{i_l} v_{k_1} v_{k_1} v_{k_2} v_{k_2} \\
&\qquad\qquad + \delta_{i_1 i_3} \delta_{i_2 i_4} v_{i_5} \cdots v_{i_l} v_{k_1} v_{k_1} v_{k_2} v_{k_2} \\
&\qquad\qquad + \cdots + \delta_{i_{n-3} i_l} \delta_{i_{l-2} i_{l-1}} v_{i_1} \cdots v_{i_{l-5}} v_{k_1} v_{k_1} v_{k_2} v_{k_2} \big) \\
&- \cdots\cdots\cdots\cdots
\end{aligned}$$

Harmonic polynomials

The coefficients $\alpha_1, \alpha_2, \cdots$ are chosen such that

$$\sum_{i_j=1}^{3}\sum_{i_k=1}^{3} v_{\langle i_1} \cdots v_{i_j} \cdots v_{i_k} \cdots v_{i_l\rangle}\delta_{i_j i_k} = 0$$

for any $1 \leqslant j < k \leqslant l$.

Example:

- If $l = 2$, then

$$v_{\langle i_1} v_{i_2\rangle} = v_{i_1} v_{i_2} - \alpha_1 \sum_{k_1=1}^{3} \delta_{i_1 i_2} v_{k_1} v_{k_1}$$

  such that

$$\sum_{i_1=1}^{3}\sum_{i_2=1}^{3} v_{\langle i_1} v_{i_2\rangle}\delta_{i_1 i_2} = 0 \quad \Longrightarrow \quad \alpha_1 = \frac{1}{3}.$$

Harmonic polynomials

When $l = 2$,

$$v_{\langle i_1}v_{i_2\rangle} = \begin{cases} v_1v_1 - \frac{1}{3}v^2, & i_1 = 1, \quad i_2 = 1, \\ v_1v_2, & i_1 = 1, \quad i_2 = 2, \\ v_1v_3, & i_1 = 1, \quad i_2 = 3, \\ v_2v_2 - \frac{1}{3}v^2, & i_1 = 2, \quad i_2 = 2, \\ v_2v_3, & i_1 = 2, \quad i_2 = 3, \\ v_3v_3 - \frac{1}{3}v^2, & i_1 = 3, \quad i_2 = 3. \end{cases}$$

Stress tensor:

$$\sigma_{ij} = \sigma_{ij}^0 = \langle v_{\langle i}v_{j\rangle} f \rangle$$

When $l = 3$,

$$v_{\langle i_1}v_{i_2}v_{i_3\rangle} = v_{i_1}v_{i_2}v_{i_3} - \frac{1}{5}v^2(v_{i_1}\delta_{i_2i_3} + v_{i_2}\delta_{i_1i_3} + v_{i_3}\delta_{i_1i_2})$$

Properties of harmonic polynomials

- Homogeneity:

$$v_{\langle i_1} \cdots v_{i_l \rangle}\big|_{\boldsymbol{v}=c\tilde{\boldsymbol{v}}} = c^l \tilde{v}_{\langle i_1} \cdots \tilde{v}_{i_l \rangle}$$

- Harmonic functions:

$$\left(\frac{\partial^2}{\partial v_1^2} + \frac{\partial^2}{\partial v_2^2} + \frac{\partial^2}{\partial v_3^2} \right) v_{\langle i_1} \cdots v_{i_l \rangle} = 0$$

- Orthogonality: If $l \neq k$, then

$$\int_{\mathbb{R}^3} {\color{red} v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle}} {\color{blue} v^{2m} v_{\langle j_1} \cdots v_{j_k \rangle}} \exp\left(-\frac{v^2}{2\theta} \right) \mathrm{d}\boldsymbol{v} = 0.$$

Orthogonal polynomials

Laguerre (Sonine) polynomials: $L_n^{(\alpha)}(x)$:

$$\int_0^{+\infty} L_m^{(\alpha)}(x) L_n^{(\alpha)}(x) x^\alpha \exp(-x)\,\mathrm{d}x = \frac{\Gamma(n+\alpha+1)}{n!}\delta_{mn}.$$

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Examples:

- $L_0^{(\alpha)}(x) = 1$
- $L_1^{(\alpha)}(x) = \alpha + 1 - x$
- $L_2^{(\alpha)}(x) = \frac{x^2}{2} - (\alpha+2)x + \frac{(\alpha+1)(\alpha+2)}{2}$

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If $m \neq n$ or $k \neq l$, then

$$\int_{\mathbb{R}^3} L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) v_{\langle i_1} \cdots v_{i_l\rangle} L_m^{(k+1/2)}\left(\frac{v^2}{2\theta}\right) v_{\langle j_1} \cdots v_{j_k\rangle} \exp\left(-\frac{v^2}{2\theta}\right)\mathrm{d}\boldsymbol{v} = 0.$$

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Orthogonal moments:

$$w_{i_1\cdots i_l}^n = \left\langle L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) v_{\langle i_1} \cdots v_{i_l\rangle} f \right\rangle$$

where $v_i = \xi_i - u_i$.

Review of four types of moments

- **Convective moments:**

$$F_{i_1 i_2 \cdots i_n} = \langle \xi_{i_1} \cdots \xi_{i_n} f \rangle$$

- **Central moments:**

$$\rho^n_{i_1 i_2 \cdots i_l} = \langle v^{2n} v_{i_1} \cdots v_{i_l} f \rangle$$

- **Trace-free moments:**

$$\sigma^n_{i_1 i_2 \cdots i_l} = \rho^n_{\langle i_1 i_2 \cdots i_l \rangle} = \langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} f \rangle$$

- **Orthogonal moments:**

$$w^n_{i_1 \cdots i_l} = \left\langle L_n^{(l+1/2)} \left(\frac{v^2}{2\theta} \right) v_{\langle i_1} \cdots v_{i_l \rangle} f \right\rangle$$

Outline

Summation convention

If the same index appears twice, a sum is taken over this index.

Examples:

- Given $\boldsymbol{v} = (v_1, v_2, v_3)^T$, $\boldsymbol{w} = (w_1, w_2, w_3)^T$, we have

$$\boldsymbol{v} \cdot \boldsymbol{w} = v_i w_i.$$

- The stress tensor σ_{ij} is trace-free:

$$\sigma_{kk} = \sigma_{11} + \sigma_{22} + \sigma_{33} = 0.$$

- The Laplacian operator can be written as

$$\Delta g = \frac{\partial^2 g}{\partial x_i \partial x_i}$$

- The directional derivative can be represented by

$$\boldsymbol{n} \cdot \nabla g = n_i \frac{\partial g}{\partial x_i}$$

Outline

Equations for convective moments

Convective moments:

$$F_{i_1 i_2 \cdots i_n} = \langle \xi_{i_1} \cdots \xi_{i_n} f \rangle$$

Boltzmann equation:

$$\frac{\partial f}{\partial t} + \xi_k \frac{\partial f}{\partial x_k} = Q[f,f]$$

$$\Downarrow$$

$$\frac{\partial}{\partial t} \langle \xi_{i_1} \cdots \xi_{i_n} f \rangle + \frac{\partial}{\partial x_k} \langle \xi_{i_1} \cdots \xi_{i_n} \xi_k f \rangle = \langle \xi_{i_1} \cdots \xi_{i_n} Q[f,f] \rangle$$

$$\Downarrow$$

$$\frac{\partial F_{i_1 \cdots i_n}}{\partial t} + \frac{\partial F_{i_1 \cdots i_n k}}{\partial x_k} = \mathcal{P}_{i_1 \cdots i_n}$$

- Simple balance laws
- Complicated collision terms

Moment closure

$$\boxed{\frac{\partial F_{i_1 \cdots i_n}}{\partial t} + \frac{\partial F_{i_1 \cdots i_n k}}{\partial x_k} = \mathcal{P}_{i_1 \cdots i_n}}$$

We cannot find a finite subsystem that is closed:

- The evolution of F depends on F_i.
- The evolution of F_i depends on F_{ij}.
- The evolution of F_{ij} depends on F_{ijk}.
- ...

We need to approximate $F_{i_1 \cdots i_n k}$ by

$$F_{i_1 \cdots i_n k} = F_{i_1 \cdots i_n k}(F, F_i, F_{i_1 i_2}, \cdots F_{i_1 \cdots i_n}).$$

Idea of moment closure

Question: Given $F, F_i, F_{i_1 i_2}, \cdots F_{i_1 \cdots i_n}$, how to guess the values of $F_{i_1 \cdots i_n k}$?

Two ideas:

- Asymptotic expansion (need to assume a small parameter)
- Find $f(\boldsymbol{\xi})$ satisfying

$$m \int_{\mathbb{R}^3} f(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi} = F,$$

$$m \int_{\mathbb{R}^3} \xi_i f(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi} = F_i,$$

$$\cdots \qquad \cdots \qquad \cdots \qquad \cdots$$

$$m \int_{\mathbb{R}^3} \xi_{i_1} \cdots \xi_{i_n} f(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi} = F_{i_1 \cdots i_n}.$$

Then set

$$F_{i_1 \cdots i_n k} = m \int_{\mathbb{R}^3} \xi_{i_1} \cdots \xi_{i_n} \xi_k f(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi}.$$

Method of maximum entropy

Thermodynamics point of view: Choose $f(\boldsymbol{\xi})$ that maximizes

$$\langle -f \log f \rangle$$

such that

$$\begin{aligned}
\langle f \rangle &= F, \\
\langle \xi_i f \rangle &= F_i, \\
\cdots \quad & \cdots \quad \cdots \\
\langle \xi_{i_1} \cdots \xi_{i_n} f \rangle &= F_{i_1 \cdots i_n}.
\end{aligned}$$

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Solution:

$$f(\boldsymbol{\xi}) = \exp\left(\sum_{k=0}^{n} a_{i_1 \cdots i_k} \xi_{i_1} \cdots \xi_{i_k} \right)$$

where the coefficients $a_{i_1 \cdots i_k}$ (symmetric tensors) are to be figured out by using the constraints.

Example: Gaussian approximation

For $n = 2$, the maximum entropy distribution function is

$$f(\boldsymbol{\xi}) = \exp(a + a_i \xi_i + a_{ij} \xi_i \xi_j)$$

or using another set of parameters ρ, u_i, θ_{ij}:

$$f(\boldsymbol{\xi}) = \frac{\rho}{(2\pi)^{3/2} m \sqrt{\det[\theta_{ij}]}} \exp\left(-\frac{1}{2}\theta^{ij}(\xi_i - u_i)(\xi_j - u_j)\right)$$

where θ^{ij} is the matrix inverse of θ_{ij}: $\theta_{ij}\theta^{jk} = \delta_{ik}$.

$$\begin{aligned}
\langle f \rangle &= \rho, \\
\langle \xi_i f \rangle &= \rho u_i, \\
\langle \xi_i \xi_j f \rangle &= \rho(\theta_{ij} + u_i u_j), \\
\langle \xi_i \xi_j \xi_k f \rangle &= \rho(u_i \theta_{jk} + u_j \theta_{ik} + u_k \theta_{ij} + u_i u_j u_k).
\end{aligned}$$

Example: Gaussian approximation

According to the moment constraints:

$$\rho = F, \qquad \rho u_i = F_i, \qquad \rho\theta_{ij} + \rho u_i u_j = F_{ij}$$

$$\Downarrow$$

$$\rho = F, \qquad u_i = \frac{F_i}{\rho}, \qquad \theta_{ij} = \frac{F_{ij}}{\rho} - \frac{F_i F_j}{\rho^2}$$

$$\Downarrow$$

$$\begin{aligned} F_{ijk} &= \rho(u_i\theta_{jk} + u_j\theta_{ik} + u_k\theta_{ij} + u_i u_j u_k) \\ &= \frac{F_i F_{jk} + F_j F_{ik} + F_k F_{ij}}{F} - \frac{2F_i F_j F_k}{F^2} \end{aligned}$$

Equations for F_{ij}:

$$\frac{\partial F_{ij}}{\partial t} + \frac{\partial}{\partial x_k}\left(\frac{F_i F_{jk} + F_j F_{ik} + F_k F_{ij}}{F} - \frac{2F_i F_j F_k}{F^2}\right) = \mathcal{P}_{ij}$$

Comments on the maximum entropy method

- It provides a systematic approach to derive a class of moment equations.
- The underlying distribution function is positive.
- The system is hyperbolic.
- The system is entropic.
- The Gaussian approximation does not include heat flux.
- The extension to $n > 2$ is hard: no explicit expressions.
- Computationally, it is expensive to find the closure for $n > 2$.
- The solution of the closure problem may not exist.
- The characteristic speed may go arbitrarily large.

Outline

Equations for trace-free moments I: Time derivative

Trace-free moments:

$$\sigma^n_{i_1 i_2 \cdots i_l} = \rho^n_{\langle i_1 i_2 \cdots i_l \rangle} = \langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} f \rangle$$

Properties:

$$\frac{\partial}{\partial t}(v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle}) = -\, l v^{2n} v_{\langle i_1} \cdots v_{i_{l-1}} \frac{\partial u_{i_l \rangle}}{\partial t} - 2n v^{2n-2} v_{\langle i_1} \cdots v_{i_l \rangle} v_j \frac{\partial u_j}{\partial t}$$

$$\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} v_j f \rangle = \sigma^n_{i_1 \cdots i_l j} + \frac{l}{2l+1} \sigma^{n+1}_{\langle i_1 \cdots i_{l-1}} \delta_{i_l \rangle j}$$

$$\Downarrow$$

$$\frac{\partial \sigma^n_{i_1 i_2 \cdots i_l}}{\partial t} = \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} \frac{\partial f}{\partial t} \right\rangle - \frac{l(2n+2l+1)}{2l+1} \sigma^n_{\langle i_1 \cdots i_{l-1}} \frac{\partial u_{i_l \rangle}}{\partial t} - 2n \sigma^{n-1}_{i_1 \cdots i_l j} \frac{\partial u_j}{\partial t}$$

Equations for trace-free moments II: Convective derivative

Similarly, we can derive that

$$u_k \frac{\partial \sigma^n_{i_1 i_2 \cdots i_l}}{\partial x_k} = \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} u_k \frac{\partial f}{\partial x_k} \right\rangle - \frac{l(2n+2l+1)}{2l+1} u_k \sigma^n_{\langle i_1 \cdots i_{l-1}} \frac{\partial u_{i_l \rangle}}{\partial x_k} - 2n u_k \sigma^{n-1}_{i_1 \cdots i_l j} \frac{\partial u_j}{\partial x_k}$$

Define material derivative:

$$\frac{\mathrm{D}}{\mathrm{D}t} = \frac{\partial}{\partial t} + u_k \frac{\partial}{\partial x_k}.$$

Then

$$\frac{\mathrm{D}\sigma^n_{i_1 i_2 \cdots i_l}}{\mathrm{D}x_k} = \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} \frac{\mathrm{D}f}{\mathrm{D}x_k} \right\rangle - \frac{l(2n+2l+1)}{2l+1} \sigma^n_{\langle i_1 \cdots i_{l-1}} \frac{\mathrm{D}u_{i_l \rangle}}{\mathrm{D}x_k} - 2n \sigma^{n-1}_{i_1 \cdots i_l j} \frac{\mathrm{D}u_j}{\mathrm{D}x_k}$$

Equations for trace-free moments III: Flux term

$$\frac{\partial}{\partial x_k}(v^{2n} v_k v_{\langle i_1} \cdots v_{i_l \rangle}) = -v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} \frac{\partial u_k}{\partial x_k}$$

$$- l v^{2n} v_k v_{\langle i_1} \cdots v_{i_{l-1}} \frac{\partial u_{i_l \rangle}}{\partial x_k} - 2n v^{2n-2} v_{\langle i_1} \cdots v_{i_l \rangle} v_k v_j \frac{\partial u_j}{\partial x_k}$$

$$\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} v_k v_j f \rangle = \sigma^n_{i_1 \cdots i_l jk} + \frac{l+1}{2l+3} \sigma^{n+1}_{\langle i_1 \cdots i_l} \delta_{k \rangle j}$$

$$+ \frac{l}{2l+1} \sigma^{n+1}_{j \langle i_1 \cdots i_{l-1}} \delta_{i_l \rangle k} + \frac{l(l-1)}{(2l+1)(2l-1)} \delta_{j \langle i_1} \sigma^{n+2}_{i_2 \cdots i_{n-1}} \delta_{i_n \rangle k}$$

$$\Downarrow$$

$$\frac{\partial}{\partial x_k} \langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} v_k f \rangle = \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} v_k \frac{\partial f}{\partial x_k} \right\rangle - \sigma^n_{i_1 \cdots i_l} \frac{\partial u_k}{\partial x_k}$$

$$- l \sigma^n_{k \langle i_1 \cdots i_{l-1}} \frac{\partial u_{i_l \rangle}}{\partial x_k} - \frac{l(l-1)}{(2l-1)(2l+1)} (2n+2l+1) \sigma^{n+1}_{\langle i_1 \cdots i_{l-2}} \frac{\partial u_{i_{l-1}}}{\partial x_{i_l \rangle}}$$

$$- 2n \sigma^{n-1}_{i_1 \cdots i_l jk} \frac{\partial u_j}{\partial x_k} - 2n \frac{l+1}{2l+3} \sigma^n_{\langle i_1 \cdots i_l} \frac{\partial u_{k \rangle}}{\partial x_k} - 2n \frac{l}{2l+1} \sigma^n_{j \langle i_1 \cdots i_{l-1}} \frac{\partial u_j}{\partial x_{i_l \rangle}}$$

Equations for trace-free moments

Moment equations:

$$\left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} \frac{\partial f}{\partial t} \right\rangle + \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} u_k \frac{\partial f}{\partial x_k} \right\rangle + \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} v_k \frac{\partial f}{\partial x_k} \right\rangle = \langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} Q[f,f] \rangle$$

Equations for trace-free moments

Moment equations:

$$\left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} \frac{\mathrm{D} f}{\mathrm{D} t} \right\rangle + \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} v_k \frac{\partial f}{\partial x_k} \right\rangle = \langle v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} Q[f, f] \rangle$$

Equations for trace-free moments

Moment equations:

$$\left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} \frac{\mathrm{D}f}{\mathrm{D}t} \right\rangle + \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} v_k \frac{\partial f}{\partial x_k} \right\rangle = \langle v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} Q[f,f] \rangle$$

$$\Downarrow$$

$$\frac{\mathrm{D}\sigma^n_{i_1 i_2 \cdots i_l}}{\mathrm{D}t} + \frac{l(2n+2l+1)}{2l+1} \sigma^n_{\langle i_1 \cdots i_{l-1}} \frac{\mathrm{D}u_{i_l\rangle}}{\mathrm{D}t} + 2n\sigma^{n-1}_{i_1 \cdots i_l j} \frac{\mathrm{D}u_j}{\mathrm{D}t}$$
$$+ \frac{\partial \sigma^n_{i_1 \cdots i_l k}}{\partial x_k} + \frac{l}{2l+1} \frac{\partial \sigma^{n+1}_{\langle i_1 \cdots i_{l-1}}}{\partial x_{i_l\rangle}} + \sigma^n_{i_1 \cdots i_l} \frac{\partial u_k}{\partial x_k} + l\sigma^n_{k\langle i_1 \cdots i_{l-1}} \frac{\partial u_{i_l\rangle}}{\partial x_k}$$
$$+ \frac{l(l-1)}{(2l-1)(2l+1)} (2n+2l+1) \sigma^{n+1}_{\langle i_1 \cdots i_{l-2}} \frac{\partial u_{i_{l-1}}}{\partial x_{i_l\rangle}} + 2n\sigma^{n-1}_{i_1 \cdots i_l jk} \frac{\partial u_j}{\partial x_k}$$
$$+ 2n \frac{l+1}{2l+3} \sigma^n_{\langle i_1 \cdots i_l} \frac{\partial u_{k\rangle}}{\partial x_k} + 2n \frac{l}{2l+1} \sigma^n_{j\langle i_1 \cdots i_{l-1}} \frac{\partial u_j}{\partial x_{i_l\rangle}} = \mathcal{Q}^n_{i_1 \cdots i_l}$$

Conservation laws

Note: $\sigma_i^0 = 0$

- Mass conservation ($\rho = \sigma^0$):

$$l = n = 0: \quad \frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho \frac{\partial u_k}{\partial x_k} = 0$$

- Momentum conservation ($\sigma_{ij} = \sigma_{ij}^0$, $\sigma^1 = 3p$):

$$l = 1,\ n = 0: \quad \rho \frac{\mathrm{D}u_i}{\mathrm{D}t} + \frac{\partial \sigma_{ik}}{\partial x_k} + \frac{\partial p}{\partial x_i} = 0$$

- Energy conservation ($\sigma_i^1 = 2q_i$):

$$l = 0,\ n = 1: \quad \frac{\mathrm{D}p}{\mathrm{D}t} + \frac{2}{3}\frac{\partial q_k}{\partial x_k} + \frac{5}{3}p\frac{\partial u_k}{\partial x_k} + \frac{2}{3}\sigma_{jk}\frac{\partial u_j}{\partial x_k} = 0.$$

Ideal gas: $p = \rho\theta$

Closure I: Euler equations

Moment closure:

$$\sigma_{ij} = 0, \qquad q_i = 0$$

Closure I: Euler equations

Moment closure:

$$\sigma_{ij} = 0, \qquad q_i = 0$$

Euler equations (convective form):

$$\begin{aligned} \frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial u_k}{\partial x_k} &= 0 \\ \rho\frac{\mathrm{D}u_i}{\mathrm{D}t} + \frac{\partial p}{\partial x_i} &= 0 \\ \frac{\mathrm{D}p}{\mathrm{D}t} + \frac{5}{3}p\frac{\partial u_k}{\partial x_k} &= 0 \end{aligned}$$

Closure I: Euler equations

Moment closure:

$$\sigma_{ij} = 0, \qquad q_i = 0$$

Euler equations (conservative form):

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_k)}{\partial x_k} &= 0 \\
\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_k)}{\partial x_k} + \frac{\partial(p\delta_{ik})}{\partial x_k} &= 0 \\
\frac{\partial(\rho u_i u_i + 3p)}{\partial t} + \frac{\partial[u_k(\rho u_i u_i + 5p)]}{\partial x_k} &= 0
\end{aligned}$$

Note:

$$F = \rho, \quad F_i = \rho u_i, \quad F_{ii} = \rho u_i u_i + 3p$$

Closure II: Gaussian closure

- Add equations for σ_{ij}:

$$\frac{\mathrm{D}\sigma_{ij}}{\mathrm{D}t} + \frac{\partial \sigma^0_{ijk}}{\partial x_k} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + \sigma_{ij}\frac{\partial u_k}{\partial x_k} + 2\sigma_{k\langle i}\frac{\partial u_{j\rangle}}{\partial x_k} + 2p\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} = \mathcal{Q}^0_{ij}$$

- **Moment closure:**

$$\sigma^0_{ijk} = 0, \qquad q_i = 0$$

- **10-moment equations:**

$$\begin{aligned}
\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial u_k}{\partial x_k} &= 0 \\
\rho\frac{\mathrm{D}u_i}{\mathrm{D}t} + \frac{\partial \sigma_{ik}}{\partial x_k} + \frac{\partial p}{\partial x_i} &= 0 \\
\frac{\mathrm{D}p}{\mathrm{D}t} + \frac{5}{3}p\frac{\partial u_k}{\partial x_k} + \frac{2}{3}\sigma_{jk}\frac{\partial u_j}{\partial x_k} &= 0 \\
\frac{\mathrm{D}\sigma_{ij}}{\mathrm{D}t} + \sigma_{ij}\frac{\partial u_k}{\partial x_k} + 2\sigma_{k\langle i}\frac{\partial u_{j\rangle}}{\partial x_k} + 2p\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} &= \mathcal{Q}^0_{ij}
\end{aligned}$$

Outline

More moments

We would like to include all the equations

$$\frac{\mathrm{D}\sigma^n_{i_1\cdots i_l}}{\mathrm{D}t} + \cdots = \mathcal{Q}^n_{i_1\cdots i_l}$$

for

$$l = 0, \cdots, L, \qquad n = 0, \cdots, N_l.$$

Examples:

- Euler equations:
$$L = 1, \quad N_0 = 1, \quad N_1 = 0$$
- Gaussian closure (10-moment system):
$$L = 2, \quad N_0 = 1, \quad N_1 = N_2 = 0$$
- 13-moment system:
$$L = 2, \quad N_0 = N_1 = 1, \quad N_2 = 0$$
- ...

Closure III: Grad's moment method

Given u_i and

$$\sigma^n_{i_1\cdots i_l}, \qquad l = 0, \cdots, L, \quad n = 0, \cdots, N_l,$$

we would like to find $f(\boldsymbol{\xi})$ satisfying

$$\langle v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} f \rangle = \sigma^n_{i_1\cdots i_l}, \qquad \forall l = 0, \cdots, L, \quad n = 0, \cdots, N_l.$$

A general approach:

$$f(\boldsymbol{\xi}) = \sum_{l=0}^{L} \sum_{n=0}^{N_l} a^n_{i_1\cdots i_l} v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} \cdot \frac{1}{(2\pi\theta)^{3/2}} \exp\left(-\frac{v^2}{2\theta}\right)$$

where $\theta = \dfrac{\sigma^1_0}{3\rho}$, and the coefficients $a^n_{i_1\cdots i_l}$ are symmetric tensors to be defined by the constraints.

Closure III: Grad's moment method

Recall: If $k \neq l$, then

$$\int_{\mathbb{R}^3} v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} v^{2m} v_{\langle j_1} \cdots v_{j_k\rangle} \exp\left(-\frac{v^2}{2\theta}\right) \mathrm{d}\boldsymbol{v} = 0$$

$$\Downarrow$$

If $l > L$, then $\left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} f \right\rangle = 0$ for any n

$$\Downarrow$$

$\sigma^n_{i_1 \cdots i_l} = 0$ if $l > L$

Closure III: Grad's moment method

Recall: If $k \neq l$, then

$$\int_{\mathbb{R}^3} v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} v^{2m} v_{\langle j_1} \cdots v_{j_k \rangle} \exp\left(-\frac{v^2}{2\theta}\right) \mathrm{d}\boldsymbol{v} = 0$$

$$\Downarrow$$

$$\text{If } l > L, \text{ then } \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} f \right\rangle = 0 \text{ for any } n$$

$$\Downarrow$$

$$\sigma^n_{i_1 \cdots i_l} = 0 \text{ if } l > L$$

It remains to find

$$\sigma^n_{i_1 \cdots i_l} = \left\langle v^{2n} v_{\langle i_1} \cdots v_{i_l \rangle} f \right\rangle$$

for $0 \leqslant l \leqslant L$ and $n > N_l$.

Closure III: Grad's moment method

Recall: If $m < n$ or $k < l$, then

$$\int_{\mathbb{R}^3} L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) v_{\langle i_1} \cdots v_{i_l\rangle} L_m^{(k+1/2)}\left(\frac{v^2}{2\theta}\right) v_{\langle j_1} \cdots v_{j_k\rangle} \exp\left(-\frac{v^2}{2\theta}\right) \mathrm{d}\boldsymbol{v} = 0$$

$$\Downarrow$$

$$\int_{\mathbb{R}^3} L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) v_{\langle i_1} \cdots v_{i_l\rangle} v^{2m} v_{\langle j_1} \cdots v_{j_k\rangle} \exp\left(-\frac{v^2}{2\theta}\right) \mathrm{d}\boldsymbol{v} = 0$$

$$\int_{\mathbb{R}^3} L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) v_{\langle i_1} \cdots v_{i_l\rangle} v^{2m} v_{\langle j_1} \cdots v_{j_l\rangle} \exp\left(-\frac{v^2}{2\theta}\right) \mathrm{d}\boldsymbol{v} = 0$$

$$\Downarrow$$

If $l > L$ or $n > N_l$, then $\left\langle L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) v_{\langle i_1} \cdots v_{i_l\rangle} f \right\rangle = 0$

Closure III: Grad's moment method

Explicit expression of Laguerre polynomials:

$$L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) = \sum_{m=0}^{n} \frac{(-1)^m}{m!} \binom{n+l+1/2}{n-m} \left(\frac{v^2}{2\theta}\right)^m$$

Closure III: Grad's moment method

Explicit expression of Laguerre polynomials:

$$L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) = \sum_{m=0}^{n} \frac{(-1)^m}{m!} \binom{n+l+1/2}{n-m} \left(\frac{v^2}{2\theta}\right)^m$$

For any $n > N_l$,

$$\sum_{m=0}^{n} \frac{(-1)^m}{m!} \binom{n+l+1/2}{n-m} \left(\frac{1}{2\theta}\right)^m \sigma_{i_1\cdots i_l}^m = 0$$

$$\Downarrow$$

$$\sigma_{i_1\cdots i_l}^n = \sum_{m=0}^{n-1} \frac{(-1)^{m-n+1} n!}{m!} \binom{n+l+1/2}{n-m} (2\theta)^{n-m} \sigma_{i_1\cdots i_l}^m$$

Closure III: Grad's moment method

Example: Grad's 13-moment equations:

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial u_k}{\partial x_k} = 0,$$

$$\rho\frac{\mathrm{D}u_i}{\mathrm{D}t} + \frac{\partial \sigma_{ik}}{\partial x_k} + \frac{\partial p}{\partial x_i} = 0,$$

$$\frac{\mathrm{D}p}{\mathrm{D}t} + \frac{2}{3}\frac{\partial q_k}{\partial x_k} + \frac{5}{3}p\frac{\partial u_k}{\partial x_k} + \frac{2}{3}\sigma_{jk}\frac{\partial u_j}{\partial x_k} = 0,$$

$$\frac{\mathrm{D}\sigma_{ij}}{\mathrm{D}t} + \frac{\partial \sigma^0_{ijk}}{\partial x_k} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + \sigma_{ij}\frac{\partial u_k}{\partial x_k} + 2\sigma_{k\langle i}\frac{\partial u_{j\rangle}}{\partial x_k} + 2p\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} = \mathcal{Q}^0_{ij},$$

$$\frac{\mathrm{D}q_i}{\mathrm{D}t} + \frac{5}{2}p\frac{\mathrm{D}u_i}{\mathrm{D}t} + \sigma_{ij}\frac{\mathrm{D}u_j}{\mathrm{D}t} + \frac{1}{2}\frac{\partial \sigma^1_{ik}}{\partial x_k} + \frac{1}{6}\frac{\partial \sigma^2}{\partial x_i} + q_i\frac{\partial u_k}{\partial x_k}$$
$$+ q_k\frac{\partial u_i}{\partial x_k} + \sigma^0_{ijk}\frac{\partial u_j}{\partial x_k} + \frac{4}{5}q_{\langle i}\frac{\partial u_{k\rangle}}{\partial x_k} + \frac{2}{3}q_k\frac{\partial u_k}{\partial x_i} = \frac{1}{2}\mathcal{Q}^1_i$$

Closure III: Grad's moment method

Moment closure for Grad's 13-moment equations:

$$L = 2, \quad N_0 = N_1 = 1, \quad N_2 = 0$$

- $\sigma^0_{ijk} = 0$
- Expression of σ^2:

$$\sigma^2 = \sum_{m=0}^{1} \frac{(-1)^{m-1} \cdot 2!}{m!} \binom{5/2}{2-m} (2\theta)^{2-m} \sigma^m$$
$$= 10\theta\sigma^1 - 15\rho\theta^2 = \frac{15p^2}{\rho}$$

- Expression of σ^1_{ij}:

$$\sigma^1_{ij} = \binom{7/2}{1} (2\theta)\sigma_{ij} = \frac{7p\sigma_{ij}}{\rho}$$

Collision terms

- **General collision term:** Since the collision term is quadratic, we have

$$\mathcal{Q}^n_{i_1\cdots i_l} = \sum_{r=0}^{+\infty}\sum_{n_1=0}^{+\infty}\sum_{n_2=0}^{+\infty}\sum_{k=0}^{l} \mathcal{Y}^{r,k,l}_{n,n_1,n_2} \frac{\sigma^{n_1}_{j_1\cdots j_r\langle i_1\cdots i_k}\sigma^{n_2}_{i_{k+1}\cdots i_l\rangle j_1\cdots j_r}}{\tau\rho\theta^{r+n_1+n_2-n}}$$

  where $\mathcal{Y}^{r,k,l}_{n,n_1,n_2}$ are constants.

- **A special case:**
  1. Maxwell molecules: $\mathcal{B}(\boldsymbol{\xi}-\boldsymbol{\xi}_*,\boldsymbol{\sigma}) = b\left(\frac{(\boldsymbol{\xi}-\boldsymbol{\xi}_*)\cdot\boldsymbol{\sigma}}{|\boldsymbol{\xi}-\boldsymbol{\xi}_*|}\right)$
  2. Linearized about the local Maxwellian

$$\left\langle L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) v_{\langle i_1}\cdots v_{i_l\rangle}\mathcal{L}[f]\right\rangle = -\frac{\alpha_{ln}}{\tau} w^n_{i_1\cdots i_l}$$

  The average relaxation time is usually chosen such that $\alpha_{20} = 1$.

Collision terms

- **General collision term:** Since the collision term is quadratic, we have

$$\mathcal{Q}^n_{i_1\cdots i_l} = \sum_{r=0}^{+\infty}\sum_{n_1=0}^{+\infty}\sum_{n_2=0}^{+\infty}\sum_{k=0}^{l} \mathcal{Y}^{r,k,l}_{n,n_1,n_2} \frac{\sigma^{n_1}_{j_1\cdots j_r\langle i_1\cdots i_k}\sigma^{n_2}_{i_{k+1}\cdots i_l\rangle j_1\cdots j_r}}{\tau\rho\theta^{r+n_1+n_2-n}}$$

  where $\mathcal{Y}^{r,k,l}_{n,n_1,n_2}$ are constants.

- **A special case:**
  1. Maxwell molecules: $\mathcal{B}(\boldsymbol{\xi}-\boldsymbol{\xi}_*,\boldsymbol{\sigma}) = b\left(\frac{(\boldsymbol{\xi}-\boldsymbol{\xi}_*)\cdot\boldsymbol{\sigma}}{|\boldsymbol{\xi}-\boldsymbol{\xi}_*|}\right)$
  2. Linearized about the local Maxwellian

$$\mathcal{Q}^n_{i_1\cdots i_l} = -\frac{1}{\tau}\sum_{m=0}^{n}\mathcal{C}_{mn}\theta^{n-m}\sigma^m_{i_1\cdots i_l}$$

Outline

Outline

General idea

- Consider the long time, large scale behavior of the Boltzmann equation:

$$t' = \varepsilon t, \qquad \boldsymbol{x}' = \varepsilon \boldsymbol{x}$$
$$\Downarrow$$
$$\frac{\partial f}{\partial t'} + \xi_k \frac{\partial f}{\partial x'_k} = \frac{1}{\varepsilon} Q[f, f]$$

Omit primes:

$$\frac{\partial f}{\partial t} + \xi_k \frac{\partial f}{\partial x_k} = \frac{1}{\varepsilon} Q[f, f]$$

- Write down moment equations:

$$\frac{\mathrm{D}\sigma^n_{i_1 \cdots i_l}}{\mathrm{D}t} + \cdots = \frac{1}{\varepsilon} \mathcal{Q}^n_{i_1 \cdots i_l}$$

General idea

- Select a set of moments to include:

$$\sigma^n_{i_1\cdots i_l}, \qquad l = 0, 1, \cdots, L, \quad n = 0, 1, \cdots, N_l. \qquad (*)$$

- Asymptotic expansion for the moments:

$$\sigma^n_{i_1\cdots i_l} = \sigma^{n|0}_{i_1\cdots i_l} + \varepsilon\sigma^{n|1}_{i_1\cdots i_l} + \varepsilon^2\sigma^{n|2}_{i_1\cdots i_l} + \cdots$$

  For the moments in (*), only leading-order term exists!

$$\sigma^n_{i_1\cdots i_l} = \varepsilon^k\sigma^{n|k}_{i_1\cdots i_l}, \qquad l = 0, 1, \cdots, L, \quad n = 0, 1, \cdots, N_l.$$

- Use the asymptotic expansion of moment equations to express other moments using the moments in (*).

Simplification of the problem

For simplicity, we only consider

- Maxwell molecules:

$$\mathcal{B}(\boldsymbol{\xi} - \boldsymbol{\xi}_*, \boldsymbol{\sigma}) = b\left(\frac{(\boldsymbol{\xi} - \boldsymbol{\xi}_*) \cdot \boldsymbol{\sigma}}{|\boldsymbol{\xi} - \boldsymbol{\xi}_*|}\right)$$

- Orthogonal moments:

$$u_i, \quad \theta, \quad \text{and} \quad w^n_{i_1 \cdots i_l} = \left\langle L_n^{(l+1/2)}\left(\frac{v^2}{2\theta}\right) f \right\rangle$$

Note: $w_i^0 = w^1 \equiv 0$

- Linearized equations about a global Maxwellian:

$$f(\boldsymbol{x}, \boldsymbol{\xi}, t) = \mathcal{M}(\boldsymbol{\xi}) + \epsilon \hat{f}(\boldsymbol{x}, \boldsymbol{\xi}, t)$$

The methodology introduced below can also be applied to the nonlinear case!

Linearization

- For the global Maxwellian

$$\mathcal{M}(\boldsymbol{\xi}) = \frac{\bar{\rho}}{m(2\pi\bar{\theta})^{3/2}} \exp\left(-\frac{\xi^2}{2\bar{\theta}}\right),$$

the orthogonal moments are

$$\bar{w}^0 = \bar{\rho}, \qquad \bar{u}_i = 0, \qquad \bar{w}^n_{i_1\cdots i_l} = 0 \text{ if } l+n>0$$

- Assume that

$$\rho = \bar{\rho}(1+\epsilon\hat{\rho}), \quad u_i = \epsilon\bar{\theta}^{1/2}\hat{u}_i, \quad \theta = \bar{\theta}(1+\epsilon\hat{\theta}),$$
$$w^n_{i_1\cdots i_l} = \epsilon\bar{\rho}\bar{\theta}^{l/2+n}\hat{w}^n_{i_1\cdots i_l} \text{ if } l+n>1$$

- Insert into the moment equations and drop $O(\epsilon^2)$ and higher-order terms.

Linear moment equations

For simplicity, the hats "$\hat{}$" are omitted below.

- **Linear conservation laws:**

$$\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} = 0,$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w^0_{ik}}{\partial x_k} = 0,$$

$$\frac{\partial \theta}{\partial t} - \frac{2}{3}\frac{\partial w^1_k}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} = 0.$$

Note: $w^0_{ik} = \sigma_{ik}$, $q_k = -w^1_k$.

- **Equations for stress and heat flux:**

$$\frac{\partial w^0_{ij}}{\partial t} - \frac{4}{5}\frac{\partial w^1_{\langle i}}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial w^0_{ijk}}{\partial x_k} = -\frac{\alpha_{20}}{\varepsilon} w^0_{ij},$$

$$\frac{\partial w^1_i}{\partial t} - \frac{5}{2}\frac{\partial \theta}{\partial x_i} - \frac{\partial w^0_{ik}}{\partial x_k} + \frac{\partial w^1_{ik}}{\partial x_k} - \frac{4}{3}\frac{\partial w^2}{\partial x_i} = -\frac{\alpha_{11}}{\varepsilon} w^1_i.$$

Outline

Linearized Euler equations

We would like to have five moments (ρ, u_i, θ) in the system:

$$\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} = 0,$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w_{ik}^0}{\partial x_k} = 0,$$

$$\frac{\partial \theta}{\partial t} - \frac{2}{3}\frac{\partial w_k^1}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} = 0.$$

Linearized Euler equations

We would like to have five moments (ρ, u_i, θ) in the system:

$$\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} = 0,$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w_{ik}^0}{\partial x_k} = 0,$$

$$\frac{\partial \theta}{\partial t} - \frac{2}{3}\frac{\partial w_k^1}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} = 0.$$

Assume

$$w_{ij}^0 = w_{ij}^{0|0} + \varepsilon w_{ij}^{0|1} + \varepsilon^2 w_{ij}^{0|2} + \cdots$$

Insert the above expansion into

$$\frac{\partial w_{ij}^0}{\partial t} - \frac{4}{5}\frac{\partial w_{\langle i}^1}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial w_{ijk}^0}{\partial x_k} = -\frac{\alpha_{20}}{\varepsilon} w_{ij}^0,$$

and balance the $O(\varepsilon^{-1})$ terms on both sides $\Longrightarrow$ $w_{ij}^{0|0} = 0$.

Linearized Euler equations

We would like to have five moments (ρ, u_i, θ) in the system:

$$\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} = 0,$$
$$\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w_{ik}^0}{\partial x_k} = 0,$$
$$\frac{\partial \theta}{\partial t} - \frac{2}{3}\frac{\partial w_k^1}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} = 0.$$

Assume

$$w_{ij}^0 = w_{ij}^{0|0} + \varepsilon w_{ij}^{0|1} + \varepsilon^2 w_{ij}^{0|2} + \cdots$$

Insert the above expansion into

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and balance the $O(\varepsilon^{-1})$ terms on both sides $\Longrightarrow w_{ij}^{0|0} = 0$.

Similarly, $w_k^{1|0} = 0$.

Linearized Euler equations

We would like to have five moments (ρ, u_i, θ) in the system:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} &= 0, \\
\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} \qquad &= 0, \\
\frac{\partial \theta}{\partial t} \qquad + \frac{2}{3}\frac{\partial u_k}{\partial x_k} &= 0.
\end{aligned}$$

Assume

$$w_{ij}^0 = w_{ij}^{0|0} + \varepsilon w_{ij}^{0|1} + \varepsilon^2 w_{ij}^{0|2} + \cdots$$

Insert the above expansion into

$$\frac{\partial w_{ij}^0}{\partial t} - \frac{4}{5}\frac{\partial w_{\langle i}^1}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial w_{ijk}^0}{\partial x_k} = -\frac{\alpha_{20}}{\varepsilon} w_{ij}^0,$$

and balance the $O(\varepsilon^{-1})$ terms on both sides $\Longrightarrow w_{ij}^{0|0} = 0$.

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Linearized Navier-Stokes-Fourier equations

- $w_{ij}^{0} = \varepsilon w_{ij}^{0|1} + \varepsilon^2 w_{ij}^{0|2} + \cdots$
  $w_{k}^{1} = \varepsilon w_{k}^{1|1} + \varepsilon^2 w_{k}^{1|2} + \cdots$
  $w_{ijk}^{0} = \varepsilon w_{ijk}^{0|1} + \varepsilon^2 w_{ijk}^{0|2} + \cdots$

Linearized Navier-Stokes-Fourier equations

- $w^0_{ij} = \varepsilon w^{0|1}_{ij} + \varepsilon^2 w^{0|2}_{ij} + \cdots$
  $w^1_k = \varepsilon w^{1|1}_k + \varepsilon^2 w^{1|2}_k + \cdots$
  $w^0_{ijk} = \varepsilon w^{0|1}_{ijk} + \varepsilon^2 w^{0|2}_{ijk} + \cdots$
- Equations for w^0_{ij}:

$$\frac{\partial w^0_{ij}}{\partial t} - \frac{4}{5}\frac{\partial w^1_{\langle i}}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial w^0_{ijk}}{\partial x_k} = -\frac{\alpha_{20}}{\varepsilon} w^0_{ij},$$

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- Equations for w^0_{ij}:

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- $O(1)$ terms:

$$2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} = -\alpha_{20} w^{0|1}_{ij}$$

Linearized Navier-Stokes-Fourier equations

- $w_{ij}^0 = \varepsilon w_{ij}^{0|1} + \varepsilon^2 w_{ij}^{0|2} + \cdots$
  $w_k^1 = \varepsilon w_k^{1|1} + \varepsilon^2 w_k^{1|2} + \cdots$
  $w_{ijk}^0 = \varepsilon w_{ijk}^{0|1} + \varepsilon^2 w_{ijk}^{0|2} + \cdots$
- Equations for w_{ij}^0:

$$\frac{\partial w_{ij}^0}{\partial t} - \frac{4}{5}\frac{\partial w_{\langle i}^1}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial w_{ijk}^0}{\partial x_k} = -\frac{\alpha_{20}}{\varepsilon} w_{ij}^0,$$

- $O(1)$ terms:

$$2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} = -\alpha_{20} w_{ij}^{0|1}$$

- Closure:

$$w_{ij}^0 \approx \varepsilon w_{ij}^{0|1} = -\frac{2\varepsilon}{\alpha_{20}}\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}$$

Linearized Navier-Stokes-Fourier equations

- Closure for stress tensor (Navier-Stokes law):

$$w_{ij}^{0} = -\frac{2\varepsilon}{\alpha_{20}} \frac{\partial u_{\langle i}}{\partial x_{j\rangle}}$$

Linearized Navier-Stokes-Fourier equations

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$$w^0_{ij} = -\frac{2\varepsilon}{\alpha_{20}} \frac{\partial u_{\langle i}}{\partial x_{j\rangle}}$$

- Closure for heat flux (Fourier law):

$$w^1_k = \frac{5\varepsilon}{2\alpha_{11}} \frac{\partial \theta}{\partial x_k}$$

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- Closure for heat flux (Fourier law):

$$w_k^1 = \frac{5\varepsilon}{2\alpha_{11}} \frac{\partial \theta}{\partial x_k}$$

- Moment equations:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} &= 0, \\ \frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w_{ik}^0}{\partial x_k} &= 0, \\ \frac{\partial \theta}{\partial t} - \frac{2}{3}\frac{\partial w_k^1}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} &= 0. \end{aligned}$$

Linearized Navier-Stokes-Fourier equations

- Closure for stress tensor (Navier-Stokes law):

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$$w_k^1 = \frac{5\varepsilon}{2\alpha_{11}} \frac{\partial \theta}{\partial x_k}$$

- Moment equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} = 0,$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} - \frac{2\varepsilon}{\alpha_{20}} \frac{\partial^2 u_{\langle i}}{\partial x_{k\rangle} \partial x_k} = 0,$$

$$\frac{\partial \theta}{\partial t} - \frac{5\varepsilon}{3\alpha_{11}} \frac{\partial^2 \theta}{\partial x_k \partial x_k} + \frac{2}{3} \frac{\partial u_k}{\partial x_k} = 0.$$

13-moment equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} &= 0, \\
\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w_{ik}^0}{\partial x_k} &= 0, \\
\frac{\partial \theta}{\partial t} - \frac{2}{3}\frac{\partial w_k^1}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} &= 0. \\
\frac{\partial w_{ij}^0}{\partial t} - \frac{4}{5}\frac{\partial w_{\langle i}^1}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial w_{ijk}^0}{\partial x_k} &= -\frac{\alpha_{20}}{\varepsilon} w_{ij}^0, \\
\frac{\partial w_i^1}{\partial t} - \frac{5}{2}\frac{\partial \theta}{\partial x_i} - \frac{\partial w_{ik}^0}{\partial x_k} + \frac{\partial w_{ik}^1}{\partial x_k} - \frac{4}{3}\frac{\partial w^2}{\partial x_i} &= -\frac{\alpha_{11}}{\varepsilon} w_i^1.
\end{aligned}
$$

General moment equations

$$\frac{\partial w^n_{i_1\cdots i_l}}{\partial t} + \frac{\partial w^n_{i_1\cdots i_l k}}{\partial x_k} - \frac{\partial w^{n-1}_{i_1\cdots i_l k}}{\partial x_k} + \frac{l(2n+2l+1)}{2l+1}\frac{\partial w^n_{\langle i_1\cdots i_{l-1}}}{\partial x_{i_l\rangle}} - \frac{2l(n+1)}{2l+1}\frac{\partial w^{n+1}_{\langle i_1\cdots i_{l-1}}}{\partial x_{i_l\rangle}} = -\frac{\alpha_{ln}}{\varepsilon} w^n_{i_1\cdots i_l}$$

General moment equations

$$\frac{\partial w^n_{i_1\cdots i_l}}{\partial t} + \frac{\partial w^n_{i_1\cdots i_l k}}{\partial x_k} - \frac{\partial w^{n-1}_{i_1\cdots i_l k}}{\partial x_k} + \frac{l(2n+2l+1)}{2l+1}\frac{\partial w^n_{\langle i_1\cdots i_{l-1}}}{\partial x_{i_l\rangle}} - \frac{2l(n+1)}{2l+1}\frac{\partial w^{n+1}_{\langle i_1\cdots i_{l-1}}}{\partial x_{i_l\rangle}} = -\frac{\alpha_{ln}}{\varepsilon} w^n_{i_1\cdots i_l}$$

Equations needed for the closure:

$$\frac{\partial w^0_{ijk}}{\partial t} + \frac{\partial w^0_{ijkl}}{\partial x_l} + 3\frac{\partial w^0_{\langle ij}}{\partial x_{k\rangle}} - \frac{6}{7}\frac{\partial w^1_{\langle ij}}{\partial x_{k\rangle}} = -\frac{\alpha_{30}}{\varepsilon} w^0_{ijk},$$

$$\frac{\partial w^1_{ij}}{\partial t} + \frac{\partial w^1_{ijk}}{\partial x_k} - \frac{\partial w^0_{ijk}}{\partial x_k} + \frac{14}{5}\frac{\partial w^1_{\langle i}}{\partial x_{j\rangle}} - \frac{8}{5}\frac{\partial w^2_{\langle i}}{\partial x_{j\rangle}} = -\frac{\alpha_{21}}{\varepsilon} w^1_{ij},$$

$$\frac{\partial w^2}{\partial t} + \frac{\partial w^2_k}{\partial x_k} - \frac{\partial w^1_k}{\partial x_k} = -\frac{\alpha_{02}}{\varepsilon} w^2.$$

General moment equations

$$
\frac{\partial w^n_{i_1\cdots i_l}}{\partial t} + \frac{\partial w^n_{i_1\cdots i_l k}}{\partial x_k} - \frac{\partial w^{n-1}_{i_1\cdots i_l k}}{\partial x_k}
+ \frac{l(2n+2l+1)}{2l+1}\frac{\partial w^n_{\langle i_1\cdots i_{l-1}}}{\partial x_{i_l\rangle}} - \frac{2l(n+1)}{2l+1}\frac{\partial w^{n+1}_{\langle i_1\cdots i_{l-1}}}{\partial x_{i_l\rangle}} = -\frac{\alpha_{ln}}{\varepsilon} w^n_{i_1\cdots i_l}
$$

Equations needed for the closure:

$$
\frac{\partial w^0_{ijk}}{\partial t} + \frac{\partial w^0_{ijkl}}{\partial x_l} + 3\frac{\partial w^0_{\langle ij}}{\partial x_{k\rangle}} - \frac{6}{7}\frac{\partial w^1_{\langle ij}}{\partial x_{k\rangle}} = -\frac{\alpha_{30}}{\varepsilon} w^0_{ijk},
$$

$$
\frac{\partial w^1_{ij}}{\partial t} + \frac{\partial w^1_{ijk}}{\partial x_k} - \frac{\partial w^0_{ijk}}{\partial x_k} + \frac{14}{5}\frac{\partial w^1_{\langle i}}{\partial x_{j\rangle}} - \frac{8}{5}\frac{\partial w^2_{\langle i}}{\partial x_{j\rangle}} = -\frac{\alpha_{21}}{\varepsilon} w^1_{ij},
$$

$$
\frac{\partial w^2}{\partial t} + \frac{\partial w^2_k}{\partial x_k} - \frac{\partial w^1_k}{\partial x_k} = -\frac{\alpha_{02}}{\varepsilon} w^2.
$$

$$
\Rightarrow w^{0|1}_{ijk} = w^{1|1}_{ij} = w^{2|1} = 0
$$

Grad's 13-moment equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} &= 0, \\
\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w_{ik}^0}{\partial x_k} &= 0, \\
\frac{\partial \theta}{\partial t} - \frac{2}{3}\frac{\partial w_k^1}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} &= 0. \\
\frac{\partial w_{ij}^0}{\partial t} - \frac{4}{5}\frac{\partial w_{\langle i}^1}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial {\color{red} w_{ijk}^0}}{\partial x_k} &= -\frac{\alpha_{20}}{\varepsilon} w_{ij}^0, \\
\frac{\partial w_i^1}{\partial t} - \frac{5}{2}\frac{\partial \theta}{\partial x_i} - \frac{\partial w_{ik}^0}{\partial x_k} + \frac{\partial {\color{red} w_{ik}^1}}{\partial x_k} - \frac{4}{3}\frac{\partial {\color{red} w^2}}{\partial x_i} &= -\frac{\alpha_{11}}{\varepsilon} w_i^1.
\end{aligned}
$$

Grad's 13-moment equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} &= 0, \\
\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w_{ik}^0}{\partial x_k} &= 0, \\
\frac{\partial \theta}{\partial t} - \frac{2}{3}\frac{\partial w_k^1}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} &= 0. \\
\frac{\partial w_{ij}^0}{\partial t} - \frac{4}{5}\frac{\partial w_{\langle i}^1}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} &= -\frac{\alpha_{20}}{\varepsilon} w_{ij}^0, \\
\frac{\partial w_i^1}{\partial t} - \frac{5}{2}\frac{\partial \theta}{\partial x_i} - \frac{\partial w_{ik}^0}{\partial x_k} &= -\frac{\alpha_{11}}{\varepsilon} w_i^1.
\end{aligned}
$$

Burnett equations

- Includes five moments: ρ, u_i, θ.
- w_{ij}^0 and w_k^1 approximated up to second order.

Burnett equations

- Includes five moments: ρ, u_i, θ.
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$$\frac{\partial w_{ij}^0}{\partial t} - \frac{4}{5}\frac{\partial w_{\langle i}^1}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial w_{ijk}^0}{\partial x_k} = -\frac{\alpha_{20}}{\varepsilon} w_{ij}^0$$

$O(\varepsilon)$ terms:

$$-\frac{2}{\alpha_{20}}\frac{\partial}{\partial t}\left(\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}\right) - \frac{2}{\alpha_{11}}\frac{\partial^2 \theta}{\partial x_{\langle i}\partial x_{j\rangle}} = -\alpha_{20} w_{ij}^{0|2}$$

Therefore

$$w_{ij}^{0|2} = \frac{2}{\alpha_{20}^2}\frac{\partial}{\partial t}\left(\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}\right) + \frac{2}{\alpha_{20}\alpha_{11}}\frac{\partial^2 \theta}{\partial x_{\langle i}\partial x_{j\rangle}}$$

Burnett equations

Since

$$\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w_{ik}^0}{\partial x_k} = 0,$$

we have

$$\frac{\partial u_i}{\partial t} = -\frac{\partial \theta}{\partial x_i} - \frac{\partial \rho}{\partial x_i} + O(\varepsilon).$$

Therefore

$$\begin{aligned} w_{ij}^{0|2} &= \frac{2}{\alpha_{20}^2} \frac{\partial}{\partial t} \left(\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} \right) + \frac{2}{\alpha_{20}\alpha_{11}} \frac{\partial^2 \theta}{\partial x_{\langle i} \partial x_{j\rangle}} \\ &= -\frac{2}{\alpha_{20}^2} \frac{\partial^2 \rho}{\partial x_{\langle i} \partial x_{j\rangle}} + \frac{2}{\alpha_{20}} \left(\frac{1}{\alpha_{11}} - \frac{1}{\alpha_{20}} \right) \frac{\partial^2 \theta}{\partial x_{\langle i} \partial x_{j\rangle}} + O(\varepsilon) \end{aligned}$$

Closure:

$$\begin{aligned} w_{ij}^0 &= \varepsilon w_{ij}^{0|1} + \varepsilon^2 w_{ij}^{0|2} \\ &= -\frac{2\varepsilon}{\alpha_{20}} \frac{\partial u_{\langle i}}{\partial x_{j\rangle}} - \frac{2\varepsilon^2}{\alpha_{20}^2} \frac{\partial^2 \rho}{\partial x_{\langle i} \partial x_{j\rangle}} + \frac{2\varepsilon^2}{\alpha_{20}} \left(\frac{1}{\alpha_{11}} - \frac{1}{\alpha_{20}} \right) \frac{\partial^2 \theta}{\partial x_{\langle i} \partial x_{j\rangle}} \end{aligned}$$

Burnett equations

- Closure for stress tensor:

$$w_{ij}^0 = -\frac{2\varepsilon}{\alpha_{20}} \frac{\partial u_{\langle i}}{\partial x_{j\rangle}} - \frac{2\varepsilon^2}{\alpha_{20}^2} \frac{\partial^2 \rho}{\partial x_{\langle i} \partial x_{j\rangle}} + \frac{2\varepsilon^2}{\alpha_{20}} \left(\frac{1}{\alpha_{11}} - \frac{1}{\alpha_{20}} \right) \frac{\partial^2 \theta}{\partial x_{\langle i} \partial x_{j\rangle}}$$

- Closure for heat flux:

$$\begin{aligned} w_i^1 &= \frac{5\varepsilon}{2\alpha_{11}} \frac{\partial \theta}{\partial x_i} + \frac{5\varepsilon^2}{3\alpha_{11}^2} \frac{\partial^2 u_k}{\partial x_i \partial x_k} - \frac{2\varepsilon^2}{\alpha_{11}\alpha_{20}} \frac{\partial^2 u_{\langle i}}{\partial x_{k\rangle} \partial x_k} \\ &= \frac{5\varepsilon}{2\alpha_{11}} \frac{\partial \theta}{\partial x_i} - \frac{\varepsilon^2}{\alpha_{11}\alpha_{20}} \frac{\partial^2 u_i}{\partial x_k \partial x_k} \\ &\quad + \frac{\varepsilon^2}{3\alpha_{11}} \left(\frac{5}{\alpha_{11}} - \frac{1}{\alpha_{20}} \right) \frac{\partial^2 u_k}{\partial x_i \partial x_k} \end{aligned}$$

- Plugging into the conservation laws yields Burnett equations.

Regularized 13-moment equations

- Includes 13 moments: ρ, u_i, θ, w_{ij}^0, w_i^1.
- w_{ijk}^0, w_{ij}^1 and w^2 approximated up to second order.

Regularized 13-moment equations

- Includes 13 moments: ρ, u_i, θ, w^0_{ij}, w^1_i.
- w^0_{ijk}, w^1_{ij} and w^2 approximated up to second order.

$$\frac{\partial w^0_{ijk}}{\partial t} + \frac{\partial w^0_{ijkl}}{\partial x_l} + 4\frac{\partial w^0_{\langle ij}}{\partial x_{k\rangle}} - \frac{6}{7}\frac{\partial w^1_{\langle ij}}{\partial x_{k\rangle}} = -\frac{\alpha_{30}}{\varepsilon} w^0_{ijk}$$

$O(\varepsilon)$ terms:

$$4\frac{\partial w^{0|1}_{\langle ij}}{\partial x_{k\rangle}} = -\alpha_{30} w^{0|2}_{ijk}$$

Closure:

$$w^0_{ijk} = \varepsilon^2 w^{0|2}_{ijk} = -\frac{4\varepsilon}{\alpha_{30}}\frac{\partial w^0_{\langle ij}}{\partial x_{k\rangle}}$$

Regularized 13-moment equations

- Closure for w^0_{ijk}:

$$w^0_{ijk} = -\frac{3\varepsilon}{\alpha_{30}} \frac{\partial w^0_{\langle ij}}{\partial x_{k\rangle}}$$

- Closure for w^1_{ij}:

$$w^1_{ij} = -\frac{14\varepsilon}{5\alpha_{21}} \frac{\partial w^1_{\langle i}}{\partial x_{j\rangle}}$$

- Closure for w^2:

$$w^2 = \frac{\varepsilon}{\alpha_{02}} \frac{\partial w^1_k}{\partial x_k}$$

Regularized 13-moment equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} = 0,$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial w_{ik}^0}{\partial x_k} = 0,$$

$$\frac{\partial \theta}{\partial t} - \frac{2}{3}\frac{\partial w_k^1}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} = 0.$$

$$\frac{\partial w_{ij}^0}{\partial t} - \frac{4}{5}\frac{\partial w_{\langle i}^1}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} - \frac{3\varepsilon}{\alpha_{30}}\frac{\partial^2 w_{\langle ij}^0}{\partial x_{k\rangle}\partial x_k} = -\frac{\alpha_{20}}{\varepsilon} w_{ij}^0,$$

$$\frac{\partial w_i^1}{\partial t} - \frac{5}{2}\frac{\partial \theta}{\partial x_i} - \frac{\partial w_{ik}^0}{\partial x_k} - \frac{14\varepsilon}{5\alpha_{21}}\frac{\partial w_{\langle i}^1}{\partial x_{k\rangle}\partial x_k} - \frac{4\varepsilon}{3\alpha_{02}}\frac{\partial^2 w_k^1}{\partial x_i \partial x_k} = -\frac{\alpha_{11}}{\varepsilon} w_i^1.$$

Outline

1. Review of the Boltzmann equation

2. Moments of the distribution function

3. Moment equations
   - Moment equations based on convective moments
   - Moment equations based on trace-free moments
   - Grad's moment method

4. Order of magnitude approach
   - General approach
   - Derivation of linear moment equations
   - Summary

5. Assessment of moment systems
   - Well-posedness of the moment equations
   - Realizability and order of accuracy
   - Benchmark tests and others

List of moment systems

Moment system	No. of moments	Order of unclosed moments	Max. order of derivatives
Euler	5	0	1
Navier-Stokes	5	1	2
Burnett	5	2	3
G13	13	1	1
R13	13	2	2
...	...	...	...

List of moment systems

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...	...	...	...

Which is a “good” moment system?

Outline

How to define a "good" moment system?

- **PDE perspective:**
  - Existence and uniqueness
  - Stability
- **Physical perspective:**
  - Positivity and realizability
  - Asymptotic order of accuracy
- **Benchmark tests:**
  - Shock structure
  - Boundary value problems (Couette/Poseuille flow, ...)
  - Lid-driven cavity flow
  - ...

One-dimensional settings

For simplicity, we assume

- For any moment ψ,

$$\frac{\partial \psi}{\partial x_2} = \frac{\partial \psi}{\partial x_3} = 0$$

- The distribution function is axisymmetric about the ξ_1 axis: For any moment $F_{i_1 i_2 \cdots i_l}$ or $\sigma^n_{i_1 i_2 \cdots i_l}$ or $w^n_{i_1 i_2 \cdots i_l}$, suppose

$$i_1 = \cdots = i_{k_1} = 1, \quad i_{k_1+1} = \cdots = i_{k_2} = 2,$$
$$i_{k_2+1} = \cdots = i_l = 3.$$

It holds that

1. The moment is zero if $k_2 - k_1$ is odd.
2. The moment is zero if $l - k_2$ is odd.
3. If both $k_2 - k_1$ and $l - k_2$ are even, the moment is the same for all possible k_2.

One-dimensional equations

5-moment equations: Only three variables left (ρ, $u = u_1$, θ)

Linear Euler/Navier-Stokes-Fourier/Burnett equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial x} = 0$$

$$\frac{\partial u}{\partial t} + \frac{\partial \theta}{\partial x} + \frac{\partial \rho}{\partial x} = \frac{4}{3\alpha_{20}} \left[\frac{\partial^2 u}{\partial x^2} + \frac{1}{\alpha_{20}} \frac{\partial^3 \rho}{\partial x^3} - \left(\frac{1}{\alpha_{11}} - \frac{1}{\alpha_{20}} \right) \frac{\partial^3 \theta}{\partial x^3} \right]$$

$$\frac{\partial \theta}{\partial t} + \frac{2}{3} \frac{\partial u}{\partial x} = \frac{5}{3\alpha_{11}} \frac{\partial^2 \theta}{\partial x^2} + \frac{2}{9\alpha_{11}} \left(\frac{5}{\alpha_{11}} - \frac{4}{\alpha_{20}} \right) \frac{\partial^3 u}{\partial x^3}$$

For Maxwell molecules, after proper nondimensionalization,

$$\alpha_{20} = 1, \qquad \alpha_{11} = \frac{2}{3}.$$

One-dimensional equations

13-moment equations: Only five variables left (ρ, u, θ, $\sigma = w_{11}^0$, $q = -w_1^1$)

Linear Grad's/regularized 13-moment equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial x} = 0$$

$$\frac{\partial u}{\partial t} + \frac{\partial \theta}{\partial x} + \frac{\partial \rho}{\partial x} + \frac{\partial \sigma}{\partial x} = 0$$

$$\frac{\partial \theta}{\partial t} + \frac{2}{3}\frac{\partial u}{\partial x} + \frac{2}{3}\frac{\partial q}{\partial x} = 0$$

$$\frac{\partial \sigma}{\partial t} + \frac{8}{15}\frac{\partial q}{\partial x} + \frac{4}{3}\frac{\partial u}{\partial x} = -\alpha_{20}\sigma + \frac{9}{5\alpha_{30}}\frac{\partial^2 \sigma}{\partial x^2}$$

$$\frac{\partial q}{\partial t} + \frac{5}{2}\frac{\partial \theta}{\partial x} + \frac{\partial \sigma}{\partial x} = -\alpha_{11} q + \left(\frac{28}{15\alpha_{21}} + \frac{4}{3\alpha_{02}}\right)\frac{\partial^2 q}{\partial x^2}$$

For Maxwell molecules, $\alpha_{30} = 3/2$, $\alpha_{02} = 2/3$, $\alpha_{21} = 7/6$.

Outline

Linear stability

In general, consider the linear system

$$\frac{\partial \boldsymbol{w}}{\partial t} + \mathbf{A}^{(0)}\boldsymbol{w} + \mathbf{A}^{(1)}\frac{\partial \boldsymbol{w}}{\partial x} + \mathbf{A}^{(2)}\frac{\partial^2 \boldsymbol{w}}{\partial x^2} + \cdots = 0.$$

- Plane wave solution:

$$\boldsymbol{w}(x,t) = \boldsymbol{w}_0 \exp(\mathrm{i}(\Omega t - kx))$$

$$\Longrightarrow [\mathrm{i}\Omega\mathbf{I} + \mathbf{A}^{(0)} - \mathrm{i}k\mathbf{A}^{(1)} - k^2\mathbf{A}^{(2)} + \cdots]\boldsymbol{w}_0 = 0$$

$$\Longrightarrow \det[\mathrm{i}\Omega\mathbf{I} + \mathbf{A}^{(0)} - \mathrm{i}k\mathbf{A}^{(1)} - k^2\mathbf{A}^{(2)} + \cdots] = 0$$

- For any $k \in \mathbb{R}$, we need

$$\operatorname{Im}\Omega \geqslant 0$$

to ensure stability.

Example

Euler equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial x} = 0$$
$$\frac{\partial u}{\partial t} + \frac{\partial \theta}{\partial x} + \frac{\partial \rho}{\partial x} = 0$$
$$\frac{\partial \theta}{\partial t} + \frac{2}{3}\frac{\partial u}{\partial x} = 0$$

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- $\boldsymbol{w} = \begin{pmatrix} \rho \\ u \\ \theta \end{pmatrix}, \quad \mathbf{A}^{(1)} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 2/3 & 0 \end{pmatrix}$

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- $\det(\mathrm{i}\Omega\mathbf{I} - \mathrm{i}k\mathbf{A}^{(1)}) = \det \begin{pmatrix} \mathrm{i}\Omega & -\mathrm{i}k & 0 \\ -\mathrm{i}k & \mathrm{i}\Omega & -\mathrm{i}k \\ 0 & -\frac{2}{3}\mathrm{i}k & \mathrm{i}\Omega \end{pmatrix}$

$$= \mathrm{i}\Omega\left(\frac{5}{3}k^2 - \Omega^2\right)$$

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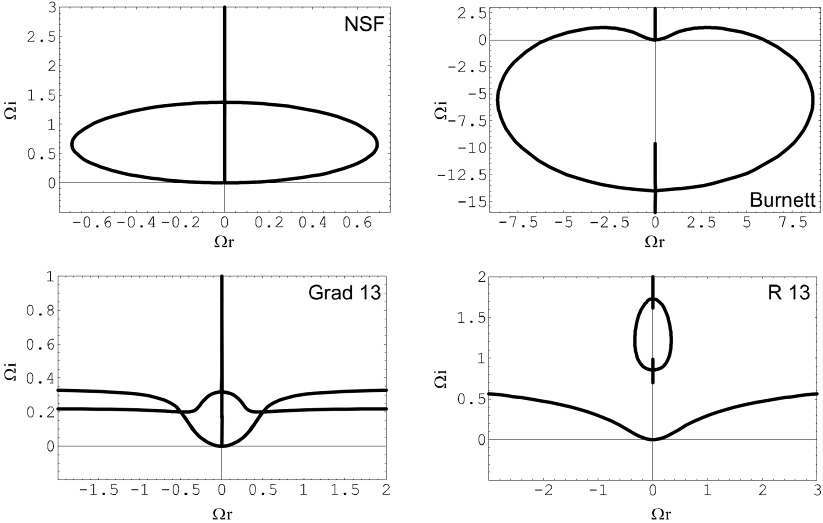
- $\det(\mathrm{i}\Omega\mathbf{I} - \mathrm{i}k\mathbf{A}^{(1)}) \Longrightarrow \Omega = 0, \ \pm\sqrt{5/3}k$ Linearly stable!

Other moment equations

Fig. from [Struchtrup, *Macroscopic Transport Equations for Rarefied Gas Flows*, 2005]:



Burnett equations are unstable!

Hyperbolicity of nonlinear first-order equations

Grad's moment equations (nonlinear) have the form

$$\frac{\partial \boldsymbol{w}}{\partial t} + \mathbf{A}(\boldsymbol{w}) \frac{\partial \boldsymbol{w}}{\partial x} = \boldsymbol{S}(\boldsymbol{w}) \qquad (*)$$

1D Euler equations:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x} &= 0, \\ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \frac{\theta}{\rho} \frac{\partial \rho}{\partial x} + \rho \frac{\partial \theta}{\partial x} &= 0, \\ \frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial x} + \frac{2}{3} \theta \frac{\partial u}{\partial x} &= 0. \end{aligned}$$

The system (*) is hyperbolic if $\mathbf{A}(\boldsymbol{w})$ is diagonalizable with real eigenvalues.

The hyperbolicity is crucial for the existence of the solution!

Hyperbolicity of Euler equations

For Euler equations,

$$\mathbf{A}(\boldsymbol{w}) = \begin{pmatrix} u & \rho & 0 \\ \theta/\rho & u & \rho \\ 0 & \frac{2}{3}\theta & u \end{pmatrix}$$

The eigenvalues are

$$\lambda_1 = u, \qquad \lambda_2 = u - \sqrt{\frac{5}{3}\theta}, \qquad \lambda_3 = u + \sqrt{\frac{5}{3}\theta}.$$

$\Longrightarrow$ $\mathbf{A}(\boldsymbol{w})$ is real diagonalizable if $\theta > 0$

Hyperbolicity of Grad's 13-moment equations

One-dimensional Grad's 13-moment equations:

$$\boldsymbol{w} = (\rho, u, \theta, \sigma, q)^T,$$

$$\mathbf{A}(\boldsymbol{w}) = \begin{pmatrix} u & \rho & 0 & 0 & 0 \\ \theta/\rho & u & 1 & -1/\rho & 0 \\ 0 & \frac{2}{3}(\theta + \sigma/\rho) & u & 0 & \frac{2}{3}\rho^{-1} \\ 0 & \frac{1}{3}(7\sigma + 4\rho\theta) & 0 & u & \frac{8}{15} \\ -\theta\sigma/\rho & \frac{16}{5}q & \frac{5}{2}(\sigma + \rho\theta) & \sigma/\rho - \theta & u \end{pmatrix}$$

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Let $\hat{\lambda} = (\lambda - u)/\sqrt{\theta}$, $\hat{\sigma} = \sigma/(\rho\theta)$, $\hat{q} = q/(\rho\theta^{3/2})$. Then

$$\det(\lambda \mathbf{I} - \mathbf{A}(\boldsymbol{w})) = 0$$

$$\Downarrow$$

$$\hat{\lambda}\left[\hat{\lambda}^4 - \frac{2}{15}(39 + 31\hat{\sigma})\hat{\lambda}^2 - \frac{96}{25}\hat{q}\hat{\lambda} + \left(3 + 6\hat{\sigma} + \frac{21\hat{\sigma}^2}{5}\right)\right] = 0$$

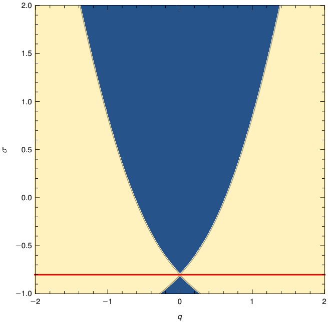
Hyperbolicity of Grad's 13-moment equations

In general, the equation

$$\hat{\lambda}^4 + c\hat{\lambda}^2 + d\hat{\lambda} + e = 0$$

has four distinct real solutions if and only if $c < 0$,
$P := 4e - c^2 < 0$, and

$$D := 16c^4e - 4c^3d^2 - 128c^2e^2 + 144cd^2e - 27d^4 + 256e^3 > 0.$$



Hyperbolicity of Grad's 13-moment equations

1D Grad's 13-moment system is hyperbolic only around equilibrium ($\sigma = q = 0$)!

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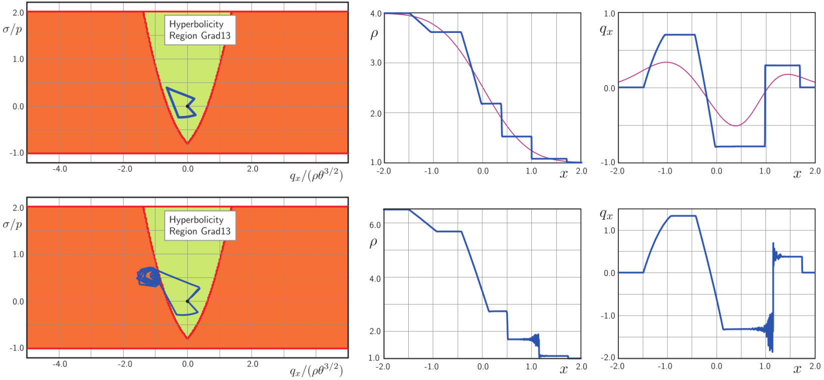
Figure from [Torrilhon, CiCP (2010)]:



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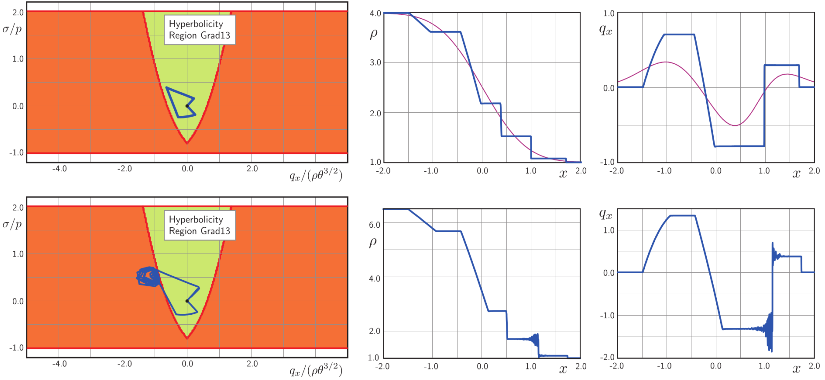

For the 3D Grad's 13-moment system, even the neighborhood of the equilibrium is not hyperbolic! [Cai, Fan & Li, KRM (2014)]

Possible fixes

Fixes for Burnett equations:

- Augmented Burnett equations [Zhong, AIAA (1991)]
- Hyperbolic Burnett equations [Bobylev, JSP (2006)]
- Generalized Burnett equations [Bobylev, JSP (2008)]
- Stable Burnett equations [Singh et al., PRE (2017)]

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Fixes for Grad's 13-moment equations:

- Modified 13-moment system (larger hyperbolicity region) [Cai et al., KRM (2014)]
- Hyperbolic 13-moment system [Cai et al., SIAM J. Appl. Math. (2015)]

Outline

Realizable moments

The set of moments

$$\{\sigma^n_{i_1\cdots i_l} \mid (l,n) \in \mathcal{I}, \quad i_1, \cdots, i_l = 1,2,3\}$$

is realizable if there exists $f \in L^1(\mathbb{R}^+)$ such that

$$\langle v_{\langle i_1} \cdots v_{i_l\rangle} f \rangle = \sigma^n_{i_1\cdots i_l}, \qquad \forall (l,n) \in \mathcal{I}, \quad i_1, \cdots, i_l = 1,2,3.$$

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$$\{\text{Moments in the system}\} \cup \{\text{Moments used for closure}\}$$

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Grad's moment equations are generally not realizable since

$$f(\boldsymbol{\xi}) = \sum_{l=0}^{L} \sum_{n=0}^{N_l} a^n_{i_1\cdots i_l} v^{2n} v_{\langle i_1} \cdots v_{i_l\rangle} \cdot \frac{1}{(2\pi\theta)^{3/2}} \exp\left(-\frac{v^2}{2\theta}\right)$$

is generally non-positive.

Realizable moment equations

- Maximum entropy closure [Levermore, JSP (1996)]:

$$f(\boldsymbol{\xi}) = \exp\left(\sum_{k=0}^{n} a_{i_1\cdots i_k}\xi_{i_1}\cdots\xi_{i_k}\right)$$

  is always positive.

- Pearson-Type-IV closure [Torrilhon, CiCP (2000)]:

$$f(\boldsymbol{\xi}) = \frac{1}{K\det\mathbf{A}}\frac{\exp(-\nu\arctan(\boldsymbol{n}^T\mathbf{A}^{-1}(\boldsymbol{\xi}-\boldsymbol{\lambda})))}{(1+(\boldsymbol{\xi}-\boldsymbol{\lambda})^T\mathbf{A}^{-2}(\boldsymbol{\xi}-\boldsymbol{\lambda}))^m}$$

- Quadrature-based moment methods [Fox, JCP (2008)]:

$$f(\boldsymbol{\xi}) = \sum_i f_i\delta(\boldsymbol{\xi}-\boldsymbol{\xi}_i)$$

Order of accuracy

We say a moment theory is of λth-order accuracy, if both σ_{ij} and q_i are approximated up to order $O(\varepsilon^\lambda)$.

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Linear 5-moment equations:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial u_k}{\partial x_k} &= 0, \\
\frac{\partial u_i}{\partial t} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \rho}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} &= 0, \\
\frac{\partial \theta}{\partial t} + \frac{2}{3}\frac{\partial q_k}{\partial x_k} + \frac{2}{3}\frac{\partial u_k}{\partial x_k} &= 0.
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- Euler equations (0th order): $\sigma_{ij} = q_i = 0$
- Navier-Stokes-Fourier equations (1st order):

$$\sigma_{ij} = -\frac{2\varepsilon}{\alpha_{20}} \frac{\partial u_{\langle i}}{\partial x_{j\rangle}}, \qquad q_i = -\frac{5\varepsilon}{2\alpha_{11}} \frac{\partial \theta}{\partial x_i}$$

- Burnett equations (2nd order)

Order of accuracy for 13-moment equations

Linear Grad's 13-moment equations:

$$\frac{\partial \sigma_{ij}}{\partial t} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} = -\frac{\alpha_{20}}{\varepsilon}\sigma_{ij}, \quad \frac{\partial q_i}{\partial t} + \frac{5}{2}\frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = -\frac{\alpha_{11}}{\varepsilon} q_i$$

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$$\Downarrow$$

$$\sigma_{ij} = -\frac{\varepsilon}{\alpha_{20}}\left(\frac{\partial \sigma_{ij}}{\partial t} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}\right)$$

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$$\Downarrow$$

$$\sigma_{ij} = -\frac{\varepsilon}{\alpha_{20}}\left[-\frac{2\varepsilon}{\alpha_{20}}\frac{\partial}{\partial t}\left(\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}\right) - \frac{2\varepsilon}{\alpha_{11}}\frac{\partial^2 \theta}{\partial x_{\langle i}\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}\right] + O(\varepsilon^3)$$

$$q_i = -\frac{\varepsilon}{\alpha_{11}}\left[-\frac{5\varepsilon}{2\alpha_{11}}\frac{\partial}{\partial t}\left(\frac{\partial \theta}{\partial x_i}\right) - \frac{2\varepsilon}{\alpha_{20}}\frac{\partial^2 u_{\langle i}}{\partial x_{k\rangle}\partial x_k} + \frac{5}{2}\frac{\partial \theta}{\partial x_i}\right] + O(\varepsilon^3)$$

Order of accuracy for 13-moment equations

Linear Grad's 13-moment equations: (2nd order)

$$\frac{\partial \sigma_{ij}}{\partial t} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}} = -\frac{\alpha_{20}}{\varepsilon}\sigma_{ij}, \quad \frac{\partial q_i}{\partial t} + \frac{5}{2}\frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = -\frac{\alpha_{11}}{\varepsilon} q_i$$

$$\Downarrow$$

$$\sigma_{ij} = -\frac{\varepsilon}{\alpha_{20}}\left(\frac{\partial \sigma_{ij}}{\partial t} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}\right)$$

$$q_i = -\frac{\varepsilon}{\alpha_{11}}\left(\frac{\partial q_i}{\partial t} + \frac{5}{2}\frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k}\right)$$

$$\Downarrow$$

$$\sigma_{ij} = -\frac{\varepsilon}{\alpha_{20}}\left[-\frac{2\varepsilon}{\alpha_{20}}\frac{\partial}{\partial t}\left(\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}\right) - \frac{2\varepsilon}{\alpha_{11}}\frac{\partial^2 \theta}{\partial x_{\langle i}\partial x_{j\rangle}} + 2\frac{\partial u_{\langle i}}{\partial x_{j\rangle}}\right] + O(\varepsilon^3)$$

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Outline

One-dimensional shock structure problem

One-dimensional Euler equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} = 0$$

$$\frac{\partial(\rho u^2 + 3p)}{\partial t} + \frac{\partial[u(\rho u^2 + 5p)]}{\partial x} = 0$$

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Rankine-Hugoniot condition:

$$\rho_l u_l - \rho_r u_r = s(\rho_l - \rho_r)$$

$$(\rho_l u_l^2 + p_l) - (\rho_r u_r^2 + p_r) = s(\rho_l u_l - \rho_r u_r)$$

$$u_l(\rho_l u_l^2 + 5p_l) - u_r(\rho_r u_r^2 + 5p_r) = s[(\rho_l u_l^2 + 3p_l) - (\rho_r u_r^2 + 3p_r)]$$

- s: shock speed
- ψ_l: quantities to the left of the discontinuity
- ψ_r: quantities to the right of the discontinuity

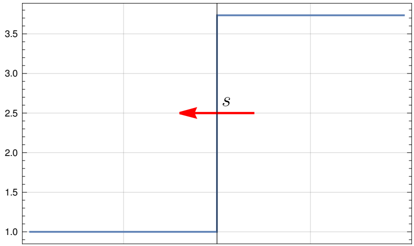
One-dimensional shock structure problem

A moving shock solution for Euler equations:

$$\rho_l = 1, \quad u_l = 0, \quad p_l = 1,$$

$$\rho_r = \frac{4Ma^2}{Ma^2+3}, \quad u_r = \frac{\sqrt{15}}{4}\frac{1-Ma^2}{Ma}, \quad p_r = \frac{5Ma^2-1}{4}.$$

- Ma: Mach number $(= s/c)$
- s: shock speed
- c: speed of sound in front of the shock wave $\left(= \sqrt{\dfrac{5p_l}{3\rho_l}}\right)$

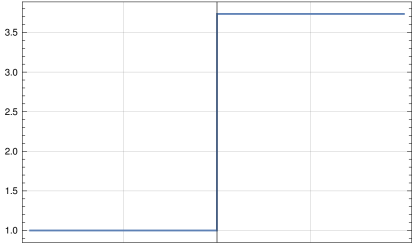


One-dimensional shock structure problem

A steady shock solution for Euler equations:

$$\rho_l = 1, \quad u_l = \sqrt{\frac{5}{3}} Ma, \quad p_l = 1,$$

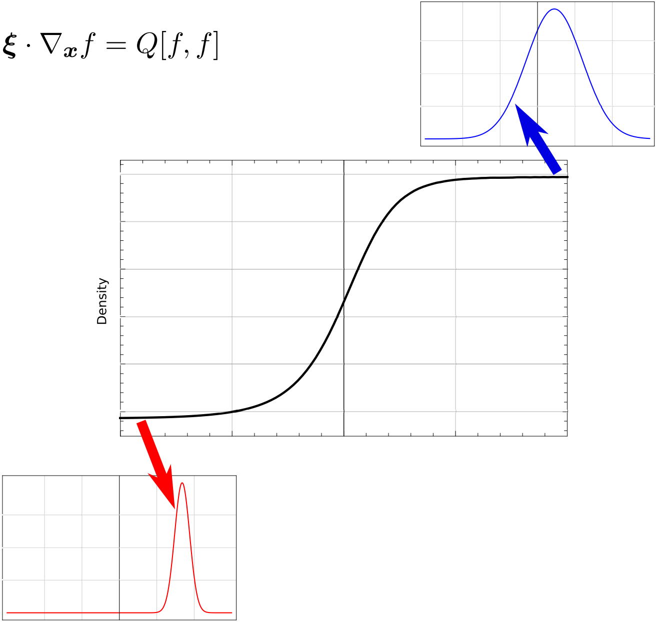
$$\rho_r = \frac{4Ma^2}{Ma^2+3}, \quad u_r = \sqrt{\frac{5}{3}} \frac{Ma^2+3}{4Ma}, \quad p_r = \frac{5Ma^2-1}{4}.$$



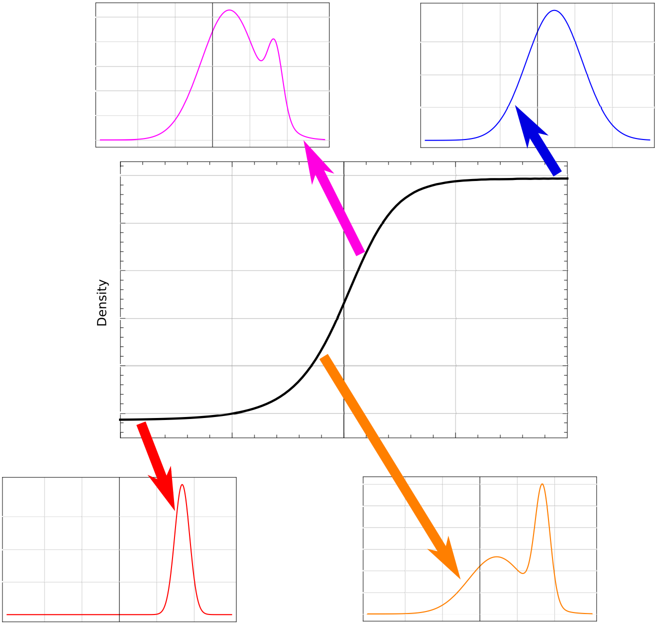
$$\frac{\partial(\rho u)}{\partial x} = \frac{\partial(\rho u^2 + p)}{\partial x} = \frac{\partial[u(\rho u^2 + 5p)]}{\partial x} = 0$$

Steady shock solution for Boltzmann equation:

$$\boldsymbol{\xi} \cdot \nabla_{\boldsymbol{x}} f = Q[f, f]$$



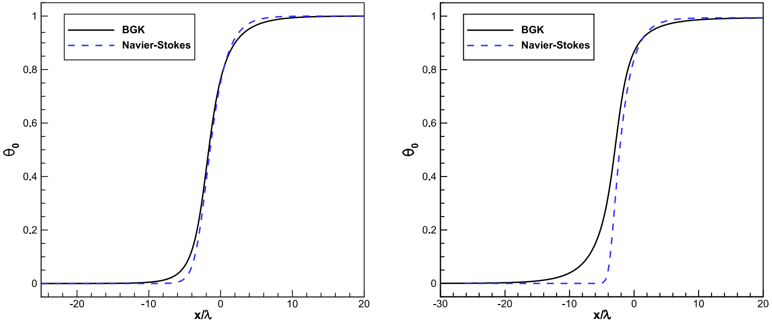
Mott-Smith bimodal theory



Shock structure for moment systems

Navier-Stokes-Fourier equations (temperature profiles):

Figure from [McDonald & Torrilhon, JCP (2013)]:

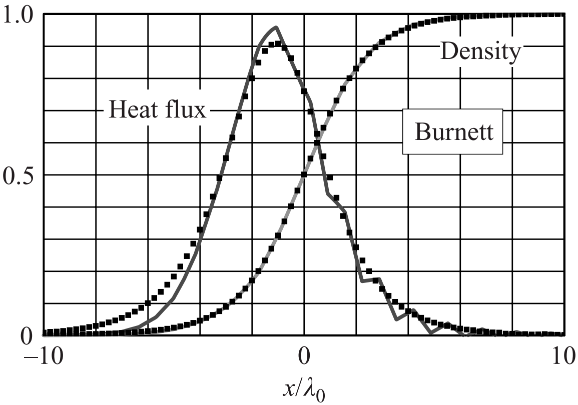


$Ma = 2.0$ $Ma = 4.0$

Shock structure for moment systems

Burnett equations (Mach number 2.0):

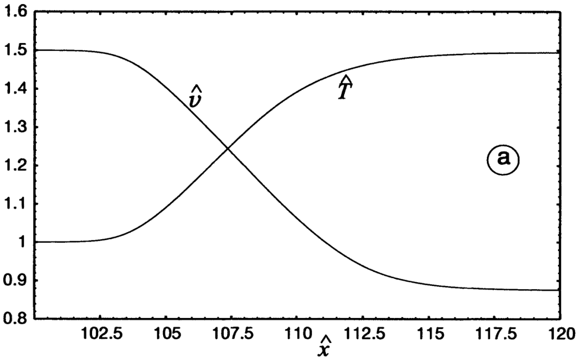
Figure from [Torrilhon & Struchtrup, JFM (2004)]:



Shock structure for moment systems

Grad's 13-moment equations:

Figure from [Müller & Ruggeri, *Rational Extended Thermodynamics* (1998)]:

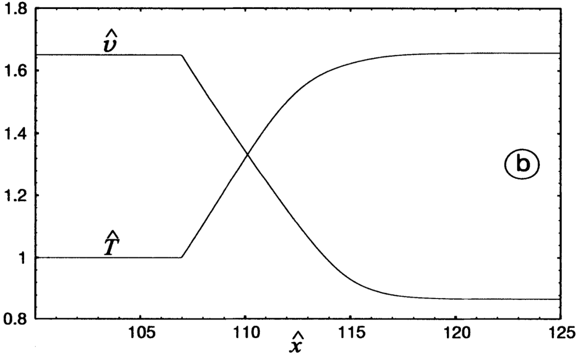


$Ma = 1.5$

Shock structure for moment systems

Grad's 13-moment equations:

Figure from [Müller & Ruggeri, *Rational Extended Thermodynamics* (1998)]:

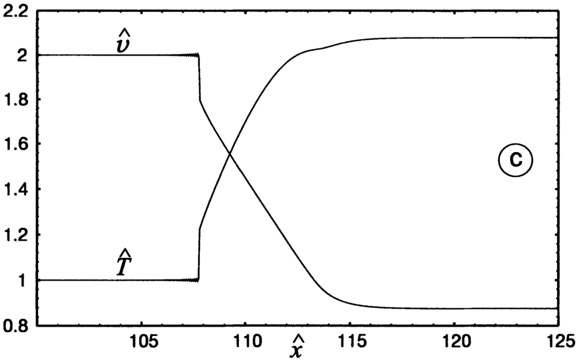


$Ma = 1.65$

Shock structure for moment systems

Grad's 13-moment equations:

Figure from [Müller & Ruggeri, *Rational Extended Thermodynamics* (1998)]:

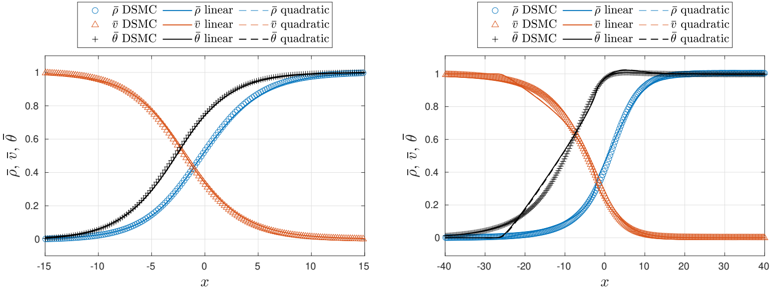


$Ma = 2.0$

Shock structure for moment systems

Regularized 13-moment equations:

Figure from [Cai & Wang, JFM (2020)]:

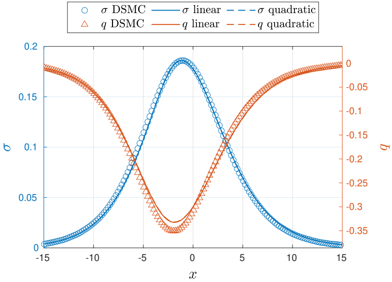


$Ma = 1.55$ $\qquad$ $Ma = 9.0$

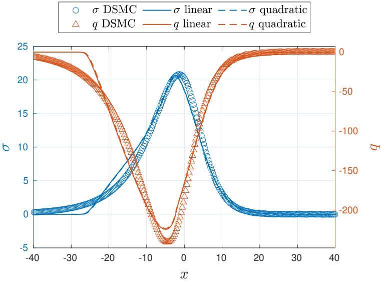
Shock structure for moment systems

Regularized 13-moment equations:

Figure from [Cai & Wang, JFM (2020)]:



$Ma = 1.55$



$Ma = 9.0$

More topics

Topics not covered:

- Problems in the maximum entropy closure:
  - Non-convex domain of admissible solutions
  - large characteristic speeds
- Wall boundary conditions:
  - Failure of asymptotic expansion near the wall
  - Discontinuous distribution functions for moment methods
- Convergence theory of moment methods
  - Convergence of linear Grad's moment methods
  - Divergence for the nonlinear Grad's moment methods
- Novel methods for the moment closure
  - Quadrature-based moment methods [R. Fox et al.]
  - Entropic quadrature closure [Böhmer & Torrilhon, JCP (2020)]
  - Machine learning based approach
- and many more...

Thank you for your attention!

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