Topic: Modeling and Numerical Simulation for Rarefied Gases

Lecture 4: Model Reduction in the Gas Kinetic Theory

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Outline

1. Model reduction for the Broadwell model
   - Zeroth-order approximation
   - First-order approximation
2. Model reduction for the Boltzmann equation
3. A brief introduction to moment methods
4. Summary

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Review of the Broadwell model

Broadwell model:

$$\partial_t u + \partial_x u = \sigma(wz - uv), \qquad \partial_t v - \partial_x v = \sigma(wz - uv),$$
$$\partial_t w + \partial_y w = \sigma(uv - wz), \qquad \partial_t z - \partial_y z = \sigma(uv - wz).$$

Review of the Broadwell model

Broadwell model:

$$\frac{\partial u}{\partial t}+\frac{\partial u}{\partial x}=\sigma m\left(\frac{(m+p+q)(m+p-q)}{4m}-u\right),$$
$$\frac{\partial v}{\partial t}-\frac{\partial v}{\partial x}=\sigma m\left(\frac{(m-p+q)(m-p-q)}{4m}-v\right),$$
$$\frac{\partial w}{\partial t}+\frac{\partial w}{\partial y}=\sigma m\left(\frac{(m+p+q)(m-p+q)}{4m}-w\right),$$
$$\frac{\partial z}{\partial t}-\frac{\partial z}{\partial y}=\sigma m\left(\frac{(m+p-q)(m-p-q)}{4m}-z\right),$$

where $m=u+v+w+z$, $p=u-v$, and $q=w-z$.

General idea to simplify the model

When ϵ is small,

$$u \approx \frac{(m+p+q)(m+p-q)}{4m}, \quad v \approx \frac{(m-p+q)(m-p-q)}{4m},$$
$$w \approx \frac{(m+p+q)(m-p+q)}{4m}, \quad z \approx \frac{(m+p-q)(m-p-q)}{4m}.$$

Can we build a model for m, p and q?

Broadwell equations in new variables

Let

$$p = u - v, \quad q = w - z,$$
$$m = u + v + w + z, \quad s = u + v - w - z.$$

Then

$$\begin{pmatrix} p \\ q \\ m \\ s \end{pmatrix} = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \end{pmatrix} \begin{pmatrix} u \\ v \\ w \\ z \end{pmatrix}$$

Broadwell equations in new variables

$$\frac{\partial m}{\partial t} + \frac{\partial p}{\partial x} + \frac{\partial q}{\partial y} = 0, \quad \text{(mass conservation)}$$

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x}\left(\frac{m+s}{2}\right) = 0, \quad \text{(horizontal momentum conservation)}$$

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial y}\left(\frac{m-s}{2}\right) = 0, \quad \text{(vertical momentum conservation)}$$

$$\frac{\partial s}{\partial t} + \frac{\partial p}{\partial x} - \frac{\partial q}{\partial y} = \frac{m}{\epsilon}\left(\frac{p^2-q^2}{m} - s\right).$$

Zeroth-order approximation

When ϵ is small,

$$s \approx \frac{p^2 - q^2}{m}.$$

The conservation laws can be approximated by

$$\begin{aligned}
&\frac{\partial m}{\partial t} + \frac{\partial p}{\partial x} + \frac{\partial q}{\partial y} = 0, \\
&\frac{\partial p}{\partial t} + \frac{\partial}{\partial x}\left(\frac{m^2 + p^2 - q^2}{2m}\right) = 0, \\
&\frac{\partial q}{\partial t} + \frac{\partial}{\partial y}\left(\frac{m^2 - p^2 + q^2}{2m}\right) = 0.
\end{aligned}$$

An alternative derivation

- **Equation of p:**

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

Approximation:

$$\begin{aligned} & u+v \\ \approx & \frac{(m+p+q)(m+p-q)}{4m} + \frac{(m-p+q)(m-p-q)}{4m} \\ = & \frac{m^2+p^2-q^2}{2m} \end{aligned}$$

- **Equation of q** can be derived similarly.

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Asymptotic expansion

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \sigma m \left(\frac{(m+p+q)(m+p-q)}{4m} - u \right)$$

$$\Downarrow$$

$$u = \frac{(m+p+q)(m+p-q)}{4m} + O\left(\frac{1}{\sigma}\right)$$

Asymptotic expansion

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \sigma m \left(\frac{(m+p+q)(m+p-q)}{4m} - u \right)$$

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$$u = \frac{(m+p+q)(m+p-q)}{4m} + O\left(\frac{1}{\sigma}\right)$$

Asymptotic expansion:

$$u = \frac{(m+p+q)(m+p-q)}{4m} + \frac{1}{\sigma} u_1 + \frac{1}{\sigma^2} u_2 + \cdots$$

Asymptotic expansion

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \sigma m \left(\frac{(m+p+q)(m+p-q)}{4m} - u \right)$$

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$$u = \frac{(m+p+q)(m+p-q)}{4m} + O\left(\frac{1}{\sigma}\right)$$

Asymptotic expansion:

$$u = \frac{(m+p+q)(m+p-q)}{4m} + \frac{1}{\sigma} u_1 + \frac{1}{\sigma^2} u_2 + \cdots$$

$$v = \frac{(m-p+q)(m-p-q)}{4m} + \frac{1}{\sigma} v_1 + \frac{1}{\sigma^2} v_2 + \cdots$$

Asymptotic expansion

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \sigma m \left(\frac{(m+p+q)(m+p-q)}{4m} - u \right)$$

$$\Downarrow$$

$$u = \frac{(m+p+q)(m+p-q)}{4m} + O\left(\frac{1}{\sigma}\right)$$

Asymptotic expansion:

$$w = \frac{(m+p+q)(m-p+q)}{4m} + \frac{1}{\sigma} w_1 + \frac{1}{\sigma^2} w_2 + \cdots$$

$$z = \frac{(m+p-q)(m-p-q)}{4m} + \frac{1}{\sigma} z_1 + \frac{1}{\sigma^2} z_2 + \cdots$$

Balancing terms of the same order

Let

$$u_0 = \frac{(m+p+q)(m+p-q)}{4m}.$$

Then

$$\partial_t u + \partial_x u = \sigma m(u_0 - u)$$

$$\Downarrow$$

$$\frac{\partial}{\partial t}\left(u_0 + \frac{1}{\sigma}u_1 + \cdots\right) + \frac{\partial}{\partial x}\left(u_0 + \frac{1}{\sigma}u_1 + \cdots\right) = -m\left(u_1 + \frac{1}{\sigma}u_2 + \cdots\right)$$

Balancing terms of the same order

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$$u_0 = \frac{(m+p+q)(m+p-q)}{4m}.$$

Then

$$\partial_t u + \partial_x u = \sigma m(u_0 - u)$$

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Approximation: $u_1 = -(\partial_t u_0 + \partial_x u_0)/m + O(1/\sigma)$

First-order approximation

Since

$$\frac{\partial m}{\partial t} = -\left(\frac{\partial p}{\partial x} + \frac{\partial q}{\partial y}\right),$$
$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{m^2 + p^2 - q^2}{2m}\right) + O\left(\frac{1}{\sigma}\right),$$
$$\frac{\partial q}{\partial t} = -\frac{\partial}{\partial y}\left(\frac{m^2 - p^2 + q^2}{2m}\right) + O\left(\frac{1}{\sigma}\right),$$

we obtain

$$\frac{\partial}{\partial t}u_0 = -\frac{m+p}{2m}\frac{\partial}{\partial x}\left(\frac{m^2 + p^2 - q^2}{2m}\right) + \frac{q}{2m}\frac{\partial}{\partial y}\left(\frac{m^2 - p^2 + q^2}{2m}\right)$$
$$-\frac{m^2 - p^2 + q^2}{4m^2}\left(\frac{\partial p}{\partial x} + \frac{\partial q}{\partial y}\right) + O\left(\frac{1}{\sigma}\right).$$

First-order approximation

Approximation of u_1:

$$
\begin{aligned}
u_1 &= -\frac{1}{m}\left(\frac{\partial u_0}{\partial t} + \frac{\partial u_0}{\partial x}\right) + O\left(\frac{1}{\sigma}\right) \\
&= \frac{p}{2m^2}\frac{\partial}{\partial x}\left(\frac{m^2+p^2-q^2}{2m}\right) - \frac{q}{2m^2}\frac{\partial}{\partial y}\left(\frac{m^2-p^2+q^2}{2m}\right) \\
&\quad - \frac{m^2+p^2-q^2}{4m^3}\frac{\partial p}{\partial x} + \frac{m^2-p^2+q^2}{4m^3}\frac{\partial q}{\partial y} + O\left(\frac{1}{\sigma}\right).
\end{aligned}
$$

First-order approximation

Approximation of u_1:

$$u_1 = -\frac{1}{m}\left(\frac{\partial u_0}{\partial t} + \frac{\partial u_0}{\partial x}\right) + O\left(\frac{1}{\sigma}\right)$$
$$= \frac{p}{2m^2}\frac{\partial}{\partial x}\left(\frac{m^2+p^2-q^2}{2m}\right) - \frac{q}{2m^2}\frac{\partial}{\partial y}\left(\frac{m^2-p^2+q^2}{2m}\right)$$
$$- \frac{m^2+p^2-q^2}{4m^3}\frac{\partial p}{\partial x} + \frac{m^2-p^2+q^2}{4m^3}\frac{\partial q}{\partial y} + O\left(\frac{1}{\sigma}\right).$$

Similarly, we can also get

$$v_1 = \frac{p}{2m^2}\frac{\partial}{\partial x}\left(\frac{m^2+p^2-q^2}{2m}\right) - \frac{q}{2m^2}\frac{\partial}{\partial y}\left(\frac{m^2-p^2+q^2}{2m}\right)$$
$$- \frac{m^2+p^2-q^2}{4m^3}\frac{\partial p}{\partial x} + \frac{m^2-p^2+q^2}{4m^3}\frac{\partial q}{\partial y} + O\left(\frac{1}{\sigma}\right).$$

First-order approximation

$$
\begin{aligned}
& u + v \\
\approx\ & u_0 + v_0 + \frac{1}{\sigma}(u_1 + v_1) + O\left(\frac{1}{\sigma^2}\right) \\
\approx\ & \frac{m^2 + p^2 - q^2}{2m} \\
& + \frac{1}{\sigma}\left[\frac{p}{m^2}\frac{\partial}{\partial x}\left(\frac{m^2 + p^2 - q^2}{2m}\right) - \frac{q}{m^2}\frac{\partial}{\partial y}\left(\frac{m^2 - p^2 + q^2}{2m}\right)\right. \\
& \left. - \frac{m^2 + p^2 - q^2}{2m^3}\frac{\partial p}{\partial x} + \frac{m^2 - p^2 + q^2}{2m^3}\frac{\partial q}{\partial y}\right].
\end{aligned}
$$

First-order equation for p

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = \sigma(wz - uv), \quad \frac{\partial v}{\partial t} - \frac{\partial v}{\partial x} = \sigma(wz - uv)$$

$$\Downarrow$$

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

$$\Downarrow$$

$$\frac{\partial p}{\partial t} + \frac{\partial}{\partial x}\frac{m^2 + p^2 - q^2}{2m} + \frac{1}{\sigma}\frac{\partial}{\partial x}\left[\frac{p}{m^2}\frac{\partial}{\partial x}\left(\frac{m^2 + p^2 - q^2}{2m}\right) - \frac{q}{m^2}\frac{\partial}{\partial y}\left(\frac{m^2 - p^2 + q^2}{2m}\right) - \frac{m^2 + p^2 - q^2}{2m^3}\frac{\partial p}{\partial x} + \frac{m^2 - p^2 + q^2}{2m^3}\frac{\partial q}{\partial y}\right] = 0$$

First-order equation for q

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial y}\frac{m^2 - p^2 + q^2}{2m} - \frac{1}{\sigma}\frac{\partial}{\partial y}\left[\frac{p}{m^2}\frac{\partial}{\partial x}\left(\frac{m^2 + p^2 - q^2}{2m}\right) + \frac{q}{m^2}\frac{\partial}{\partial y}\left(\frac{m^2 - p^2 + q^2}{2m}\right) - \frac{m^2 + p^2 - q^2}{2m^3}\frac{\partial p}{\partial x} + \frac{m^2 - p^2 + q^2}{2m^3}\frac{\partial q}{\partial y}\right] = 0$$

Final equations

Final equations: Let

$$g = \frac{m^2 + p^2 - q^2}{2m}, \qquad h = \frac{m^2 - p^2 + q^2}{2m}.$$

Then the first-order equations are

$$\frac{\partial m}{\partial t} + \frac{\partial p}{\partial x} + \frac{\partial q}{\partial y} = 0,$$

$$\frac{\partial p}{\partial t} + \frac{\partial g}{\partial x} + \frac{1}{\sigma}\frac{\partial}{\partial x}\left(\frac{p}{m^2}\frac{\partial g}{\partial x} - \frac{q}{m^2}\frac{\partial h}{\partial y} - \frac{g}{m^2}\frac{\partial p}{\partial x} + \frac{h}{m^2}\frac{\partial q}{\partial y}\right) = 0,$$

$$\frac{\partial q}{\partial t} + \frac{\partial h}{\partial y} - \frac{1}{\sigma}\frac{\partial}{\partial y}\left(\frac{p}{m^2}\frac{\partial g}{\partial x} - \frac{q}{m^2}\frac{\partial h}{\partial y} - \frac{g}{m^2}\frac{\partial p}{\partial x} + \frac{h}{m^2}\frac{\partial q}{\partial y}\right) = 0.$$

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Boltzmann equation and conservative moments

Boltzmann equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = \frac{1}{\epsilon} Q[f, f],$$

where

$$Q[f, f](\boldsymbol{x}, \boldsymbol{v}, t) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} B\left(|\boldsymbol{v} - \boldsymbol{v}_*|, \frac{(\boldsymbol{v} - \boldsymbol{v}_*) \cdot \boldsymbol{\omega}}{|\boldsymbol{v} - \boldsymbol{v}_*|} \right) \left[f(\boldsymbol{v}') f(\boldsymbol{v}'_*) - f(\boldsymbol{v}) f(\boldsymbol{v}_*) \right] \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\boldsymbol{v}_*.$$

Boltzmann equation and conservative moments

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$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = \frac{1}{\epsilon} Q[f, f],$$

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Conservative moments:

- Density: $\rho = m\langle f \rangle$
- Momentum density: $\rho \boldsymbol{u} = m\langle \boldsymbol{v} f \rangle$
- Energy density: $E = \frac{1}{2} m \langle |\boldsymbol{v}|^2 f \rangle$

Here $\langle \cdot \rangle$ stands for the integration w.r.t. $\boldsymbol{v}$.

Conservation laws

Using

$$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \boldsymbol{v} \\ \frac{1}{2}|\boldsymbol{v}|^2 \end{pmatrix} Q[f,f]\,\mathrm{d}\boldsymbol{v} = 0,$$

we obtain the conservation laws:

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho \\ \rho\boldsymbol{u} \\ E \end{pmatrix} + \nabla_{\boldsymbol{x}} \cdot \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \boldsymbol{v} \\ \frac{1}{2}|\boldsymbol{v}|^2 \end{pmatrix} m\boldsymbol{v} f(\boldsymbol{x},\boldsymbol{v},t)\,\mathrm{d}\boldsymbol{v} = 0.$$

Can we get a closed system for ρ, $\rho\boldsymbol{u}$, and E that approximates the Boltzmann equation?

Equilibrium and asymptotic expansion

Equilibrium:

$$\mathcal{M}(\boldsymbol{x},\boldsymbol{v},t)=\frac{\rho(\boldsymbol{x},t)}{m[2\pi k_B T(\boldsymbol{x},t)/m]^{3/2}}\exp\left(-\frac{m|\boldsymbol{v}-\boldsymbol{u}(\boldsymbol{x},t)|^2}{2k_B T(\boldsymbol{x},t)}\right)$$

Asymptotic expansion:

$$f=f_0+\epsilon f_1+\epsilon^2 f_2+\cdots.$$

Then

$$\frac{\partial f_0}{\partial t}+\epsilon\frac{\partial f_1}{\partial t}+\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_0+\epsilon\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f_1+\cdots=\frac{1}{\epsilon}Q[f_0,f_0]$$
$$+(Q[f_0,f_1]+Q[f_1,f_0])+\epsilon(Q[f_0,f_2]+Q[f_1,f_1]+Q[f_2,f_0])+\cdots.$$

Chapman-Enskog expansion

$O(1/\epsilon)$ terms:

$$Q[f_0, f_0] = 0 \;\Rightarrow\; f_0 \text{ is a Maxwellian (isotropic Gaussian).}$$

With the extra assumption that

$$f_0 = \mathcal{M},$$

the asymptotic expansion

$$f = \mathcal{M} + \epsilon f_1 + \epsilon^2 f_2 + \cdots$$

is called the Chapman-Enskog expansion.

Zeroth-order approximation: Euler equations

Plugging the expression of f_0 into the conservation laws, we obtain the Euler equations:

$$\frac{\partial \rho}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u}) = 0,$$
$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + p \boldsymbol{I}) = 0,$$
$$\frac{\partial E}{\partial t} + \nabla_{\boldsymbol{x}} \cdot [\boldsymbol{u}(E + p)] = 0,$$

where

$$p = \frac{2}{3}\left(E - \frac{1}{2}\rho |\boldsymbol{u}|^2\right).$$

First-order approximation

The first-order term f_1 can be solved from

$$\frac{\partial f_0}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f_0 = Q[f_0, f_1] + Q[f_1, f_0] + O(\epsilon).$$

The first-order approximation of the Boltzmann equation is the Navier-Stokes-Fourier equations:

$$\begin{aligned}
&\partial_t \rho + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u}) = 0, \\
&\partial_t (\rho \boldsymbol{u}) + \nabla_{\boldsymbol{x}} \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + p\mathbf{I} - \boldsymbol{\Sigma}) = 0, \\
&\partial_t E + \nabla_{\boldsymbol{x}} \cdot [\boldsymbol{u}(E+p) - \boldsymbol{\Sigma}\boldsymbol{u} + \boldsymbol{q}] = 0,
\end{aligned}$$

where

$$\boldsymbol{\Sigma} = \mu \left[(\nabla \boldsymbol{u}) + (\nabla \boldsymbol{u})^T - \frac{2}{3} (\nabla \cdot \boldsymbol{u}) \boldsymbol{I} \right], \quad \boldsymbol{q} = -\kappa \nabla T.$$

The values of μ and κ depend on the collision kernel.

Navier-Stokes and Fourier laws

Navier-Stokes law:

$$\boldsymbol{\Sigma} = \mu \left[(\nabla \boldsymbol{u}) + (\nabla \boldsymbol{u})^T - \frac{2}{3}(\nabla \cdot \boldsymbol{u})\boldsymbol{I} \right],$$

which indicates how the stress tensor $\boldsymbol{\Sigma}$ is related to the velocity gradient $\nabla \boldsymbol{u}$.

Fourier law:

$$\boldsymbol{q} = -\kappa \nabla \theta,$$

which indicates that the heat flux $\boldsymbol{q}$ is proportional to the negative temperature gradient $-\nabla \theta$.

Navier-Stokes and Fourier laws

Navier-Stokes law:

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The Navier-Stokes-Fourier equations are usually considered accurate when the Knudsen number is less than 0.01.

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Moments

Moments:

$$F_{i_1 i_2 \cdots i_n} = m \int_{\mathbb{R}^3} v_{i_1} v_{i_2} \cdots v_{i_n} f(\boldsymbol{x}, \boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{v},$$

where $i_1, i_2, \ldots, i_n \in \{1, 2, 3\}$.

Examples:

- $n = 0$: $F = \rho$ (Number density)
- $n = 1$: $F_i = \rho u_i$ (Momentum density)
- $n = 2$: $\dfrac{F_{11} + F_{22} + F_{33}}{2} = E$ (Energy density)

Moment equations

Moment equations:

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

$$\Downarrow$$

$$\frac{\partial}{\partial t}\langle v_{i_1} \cdots v_{i_n} f \rangle + \sum_{k=1}^{3} \frac{\partial}{\partial x_k}\langle v_{i_1} \cdots v_{i_n} v_k f \rangle = \langle v_{i_1} \cdots v_{i_n} Q[f, f] \rangle$$

$$\Downarrow$$

$$\frac{\partial F_{i_1 i_2 \cdots i_n}}{\partial t} + \sum_{k=1}^{3} \frac{\partial F_{i_1 i_2 \cdots i_n k}}{\partial x_k} = \mathcal{P}_{i_1 i_2 \cdots i_n}$$

The equations yield a system of infinitely many equations!

Closure problem

Closure problem: For a given n, express $F_{i_1 i_2 \cdots i_{n+1}}$ in terms of $F_{i_1 i_2 \cdots i_m}$ with $m \leq n$.

Closure by reconstruction: Given $F_{i_1 i_2 \cdots i_\ell}$ with $\ell \leq n$, reconstruct a distribution function $\tilde{f}$ such that

$$F_{i_1 i_2 \cdots i_\ell} = m \int_{\mathbb{R}^3} v_{i_1} v_{i_2} \cdots v_{i_\ell} \tilde{f}(\boldsymbol{x}, \boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{v}, \quad \ell = 0, 1, \ldots, n,$$

and then compute

$$F_{i_1 i_2 \cdots i_{n+1}} = m \int_{\mathbb{R}^3} v_{i_1} v_{i_2} \cdots v_{i_{n+1}} \tilde{f}(\boldsymbol{x}, \boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{v}.$$

Maximum entropy closure

Maximum entropy closure: Given $F_{i_1 i_2 \cdots i_\ell}$ with $\ell \leq n$, solve the following optimization problem:

$$\min_{\tilde{f}} \int_{\mathbb{R}^3} \tilde{f}(\boldsymbol{x}, \boldsymbol{v}, t) \log \tilde{f}(\boldsymbol{x}, \boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{v},$$

$$\text{s.t. } F_{i_1 i_2 \cdots i_\ell} = m \int_{\mathbb{R}^3} v_{i_1} v_{i_2} \cdots v_{i_\ell} \tilde{f}(\boldsymbol{x}, \boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{v},$$

$$\ell = 0, 1, \ldots, n.$$

Maximum entropy closure

Maximum entropy closure: Given $F_{i_1 i_2 \cdots i_\ell}$ with $\ell \leq n$, solve the following optimization problem:

$$\min_{\tilde{f}} \int_{\mathbb{R}^3} \tilde{f}(\boldsymbol{x}, \boldsymbol{v}, t) \log \tilde{f}(\boldsymbol{x}, \boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{v},$$

$$\text{s.t. } F_{i_1 i_2 \cdots i_\ell} = m \int_{\mathbb{R}^3} v_{i_1} v_{i_2} \cdots v_{i_\ell} \tilde{f}(\boldsymbol{x}, \boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{v},$$

$$\ell = 0, 1, \ldots, n.$$

Solution:

$$\tilde{f}(\boldsymbol{x}, \boldsymbol{v}, t) = \exp\left(\sum_{\ell=0}^{n} \sum_{i_1, \ldots, i_\ell = 1}^{3} \lambda_{i_1 i_2 \cdots i_\ell}(\boldsymbol{x}, t) v_{i_1} v_{i_2} \cdots v_{i_\ell} \right),$$

where $\lambda_{i_1 i_2 \cdots i_\ell}(\boldsymbol{x}, t)$ are Lagrange multipliers determined by the constraints.

Example: Gaussian approximation

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

$$f(\boldsymbol{v}) = \exp(a + a_i v_i + a_{ij} v_i v_j)$$

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

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

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

$$\begin{aligned}
m\langle f \rangle &= \rho, \\
m\langle \boldsymbol{v}_i f \rangle &= \rho u_i, \\
m\langle \boldsymbol{v}_i \boldsymbol{v}_j f \rangle &= \rho(\theta_{ij} + u_i u_j), \\
m\langle \boldsymbol{v}_i \boldsymbol{v}_j \boldsymbol{v}_k f \rangle &= \rho(u_i\theta_{jk} + u_j\theta_{ik} + u_k\theta_{ij} + u_i u_j u_k).
\end{aligned}$$

Example: Gaussian approximation

Moment closure:

$$F_{ijk} = \frac{F_{ij}F_k + F_{ik}F_j + F_{jk}F_i}{F} - \frac{2F_iF_jF_k}{F^2}.$$

Moment equations:

$$\frac{\partial F}{\partial t} + \sum_{k=1}^{3} \frac{\partial F_k}{\partial x_k} = 0,$$

$$\frac{\partial F_i}{\partial t} + \sum_{k=1}^{3} \frac{\partial F_{ik}}{\partial x_k} = 0,$$

$$\frac{\partial F_{ij}}{\partial t} + \sum_{k=1}^{3} \frac{\partial}{\partial x_k} \left(\frac{F_{ij}F_k + F_{ik}F_j + F_{jk}F_i}{F} - \frac{2F_iF_jF_k}{F^2} \right) = \mathcal{P}_{ij}.$$

A list of moment methods

Unfortunately, explicit formulas for the maximum entropy closure are only available for $n \leq 2$.

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Other moment methods:

- **Grad's moment method**
  $f = (\text{polynomial}) \times \mathcal{M}$
- **Quadrature-based moment methods**
  $f = (\text{sum of Dirac delta functions})$
- **Regularized moment methods**
  Close the system by asymptotic analysis
- **GENERIC framework**
  Find the closure with thermodynamical admissibility.
- ...

Outline

1. Model reduction for the Broadwell model
2. Model reduction for the Boltzmann equation
3. A brief introduction to moment methods
4. Summary

Summary

Model reduction by Chapman-Enskog expansion:

- Zeroth-order approximation: Euler equations
- First-order approximation: Navier-Stokes-Fourier equations

Model reduction by moment methods:

- Moment closure problem
- Method of maximum entropy