Topic: Modeling and Numerical Simulation for Rarefied Gases

Lecture 1: Boltzmann equation

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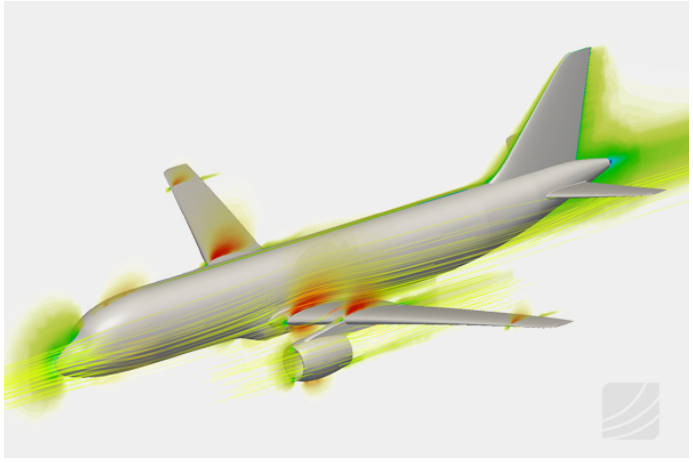
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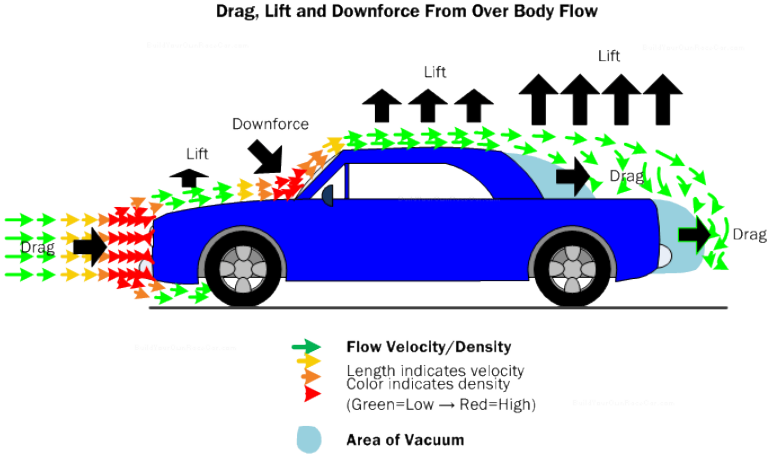
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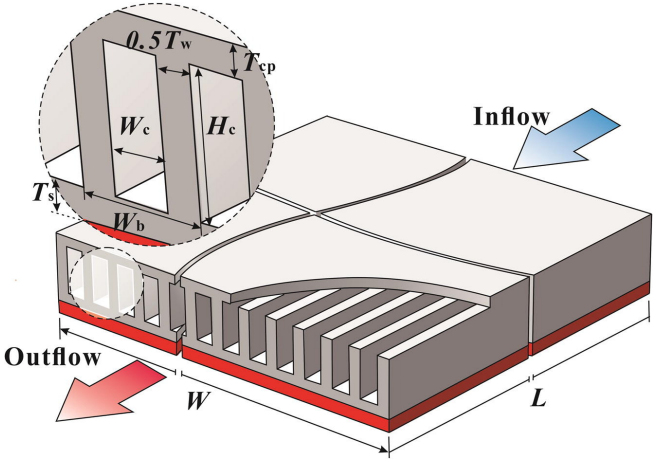
1 Introduction to rarefied gas dynamics
2 A 2D Broadwell model
3 From Broadwell model to Boltzmann equation
4 Fourier transform of the Boltzmann collision operator
5 Summary

Gas dynamics









Rarefied gas dynamics

Two scenarios for rarefied gas dynamics:

- Low density, usual characteristic scale (space vehicles)
- Usual density, small characteristic scale (micro-electro-mechanical-systems)

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$$\frac{\langle \text{Average distance between gas molecules} \rangle}{\langle \text{Characteristic length} \rangle}$$

Rarefied gas dynamics

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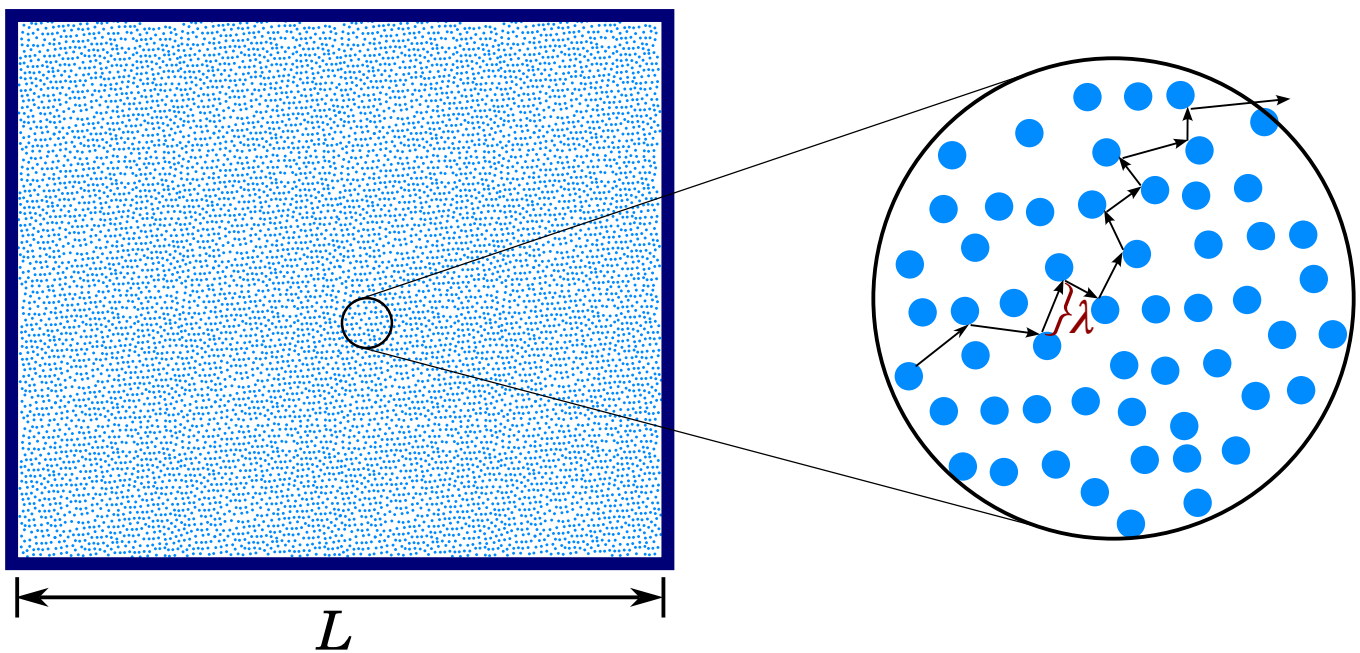
- Low density, usual characteristic scale (space vehicles)
- Usual density, small characteristic scale (micro-electro-mechanical-systems)

Characterization of rarefaction:

$$\frac{\text{Mean free path}}{\langle \cancel{\text{Average distance between gas molecules}} \rangle} \Big/ \langle \text{Characteristic length} \rangle$$

Mean free path

The mean free path of the gas is the average distance the gas molecule travels between two successive collisions.



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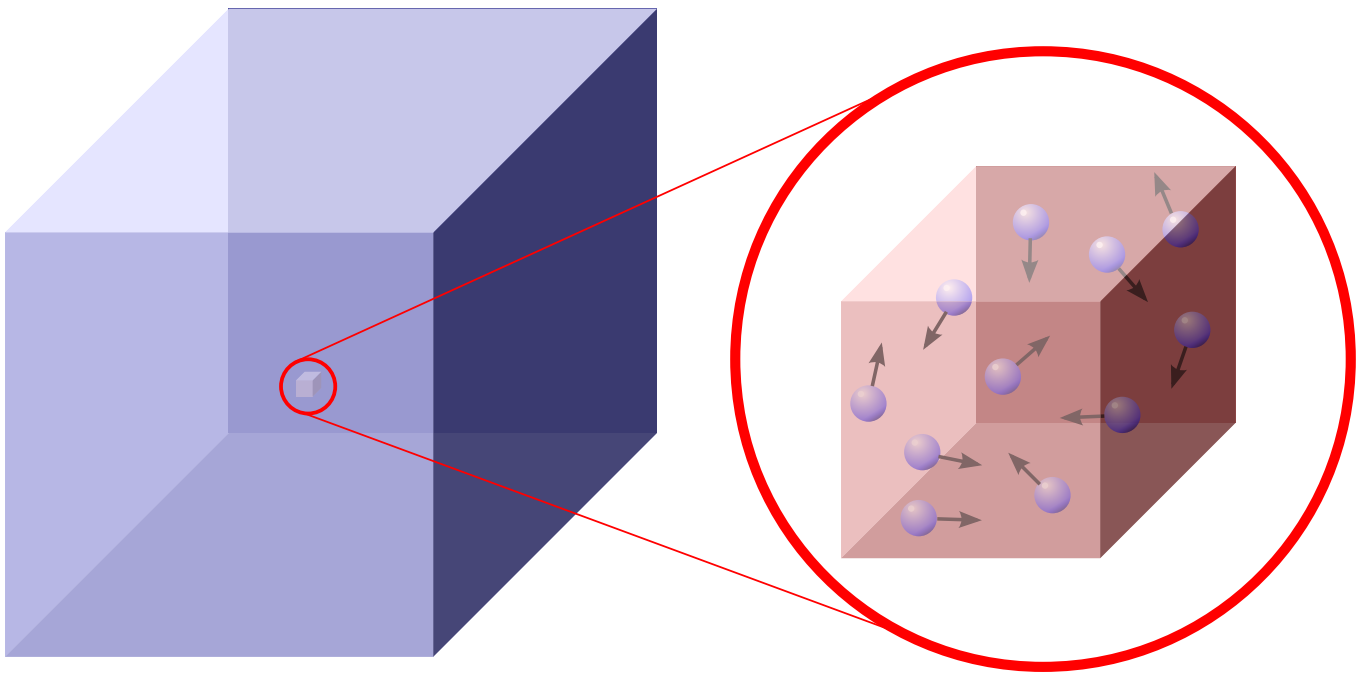
Mean free path of atmosphere:

- Sea level: 0.07μm
- Altitude 70km: 1mm
- Altitude 85km: 1cm
- Altitude 100km: 16cm
- Altitude 300km: 20km

Description of the gas flow

Continuum hypothesis:

The gas flow completely fills the space it occupies.



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Physical quantities describing the gas:

- Density (ρ): mass per unit volume
- Velocity ($\boldsymbol{u}$): local motion of the gas
- Temperature (T): internal energy per mass

$$(\text{Mass in a volume } \Omega) = \int_{\Omega} \rho(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$$

Continuum breakdown

Models based on the continuum hypotheses are no longer accurate for rarefied gas flows:

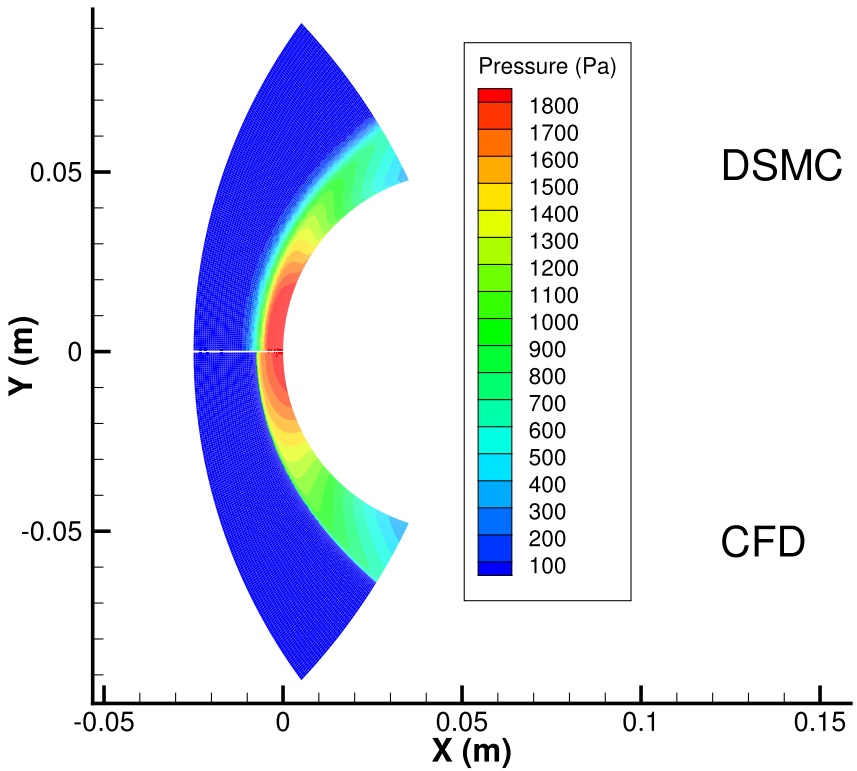
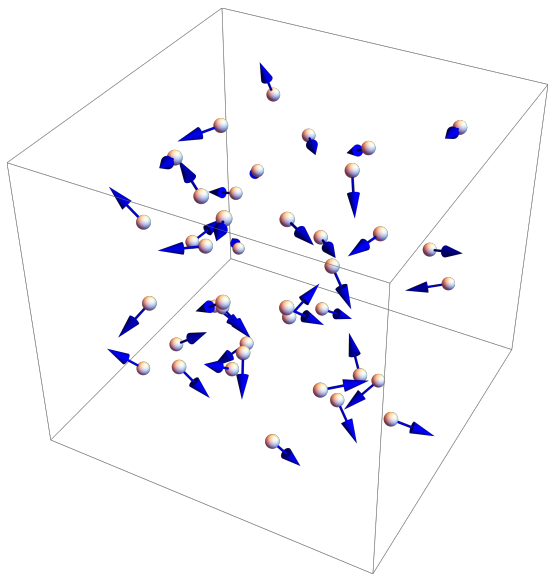


Figure from [D. Cinquegrana et al., Aerosp. Sci. Technol., 88, pp. 258–272]

Using a particle system to describe the gas flow

Systems with a large number of particles:

- Each particle has a position and a velocity.
- Particles travel at their own velocities.
- The particles can interact with each other.



Molecular dynamics

Equations of motion: for all $k = 1, \cdots, N$,

$$\frac{\mathrm{d}\boldsymbol{x}_k}{\mathrm{d}t} = \boldsymbol{v}_k,$$
$$\frac{\mathrm{d}\boldsymbol{v}_k}{\mathrm{d}t} = \frac{1}{m} F_k(\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N).$$

The number of molecules N can be huge:

$$N = \frac{V}{\sqrt{2}\pi d^2 \lambda}.$$

For the argon gas, $d \approx 4.17 \times 10^{-10}$m.

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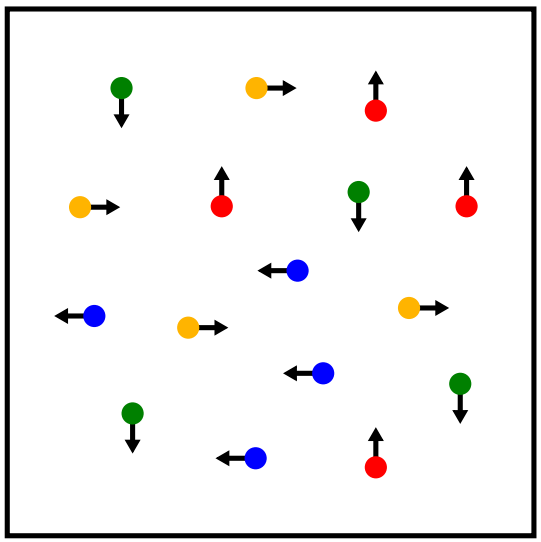
5 Summary

A two-dimensional four-velocity model

Assume that

- We live in a 2D space.
- Particles have only four velocities:

$$(1,0)^T, \quad (-1,0)^T,$$
$$(0,1)^T, \quad (0,-1)^T.$$

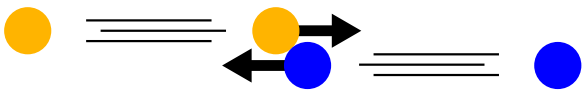


- Only two types of collisions can take place:

$$\{(1,0)^T,(-1,0)^T\} \longrightarrow \{(0,1)^T,(0,-1)^T\},$$
$$\{(0,1)^T,(0,-1)^T\} \longrightarrow \{(1,0)^T,(-1,0)^T\}.$$

Interaction between particles

Before collision:



After collision:



Before collision:



After collision:



Distribution functions

Define

- $u(\boldsymbol{x}, t)$: number density of particles w/ velocity $(1, 0)^T$:

$$(\#\text{ of particles with velocity } (1,0)^T \text{ in } \Omega \text{ at time } t) = \int_\Omega u(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x}.$$

- $v(\boldsymbol{x}, t)$: number density of particles w/ velocity $(-1, 0)^T$.
- $w(\boldsymbol{x}, t)$: number density of particles w/ velocity $(0, 1)^T$.
- $z(\boldsymbol{x}, t)$: number density of particles w/ velocity $(0, -1)^T$.

These functions are called distribution functions.

Collision-only dynamics

Assumptions:

- The system is spatially homogeneous, i.e. u, v, w, z are independent of x.
- Particles interact only through collisions (short-range interactions).

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Collision-only dynamics:

$$
\begin{aligned}
u(\boldsymbol{x}, t + \mathrm{d}t)\,\mathrm{d}\boldsymbol{x} &= u(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} + \mathcal{S}_u^+ - \mathcal{S}_u^-, \\
v(\boldsymbol{x}, t + \mathrm{d}t)\,\mathrm{d}\boldsymbol{x} &= v(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} + \mathcal{S}_v^+ - \mathcal{S}_v^-, \\
w(\boldsymbol{x}, t + \mathrm{d}t)\,\mathrm{d}\boldsymbol{x} &= w(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} + \mathcal{S}_w^+ - \mathcal{S}_w^-, \\
z(\boldsymbol{x}, t + \mathrm{d}t)\,\mathrm{d}\boldsymbol{x} &= z(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} + \mathcal{S}_z^+ - \mathcal{S}_z^-.
\end{aligned}
$$

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$$u(\boldsymbol{x}, t + \mathrm{d}t)\,\mathrm{d}\boldsymbol{x} = u(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} + \mathcal{S}_u^+ - \mathcal{S}_u^-,$$

- $\mathcal{S}_u^+$: number of collisions that generate particles with velocity $(1, 0)^T$.
- $\mathcal{S}_u^-$: number of collisions that consume particles with velocity $(1, 0)^T$.

Count the collisions

$$\boxed{u(\boldsymbol{x}, t + \mathrm{d}t)\,\mathrm{d}\boldsymbol{x} = u(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} + \mathcal{S}_u^+ - \mathcal{S}_u^-}$$

Loss term:

$\mathcal{S}_u^-$ = (the number of binary collisions
that consume particles with velocity $(1, 0)^T$ at $\boldsymbol{x}$)

Questions:

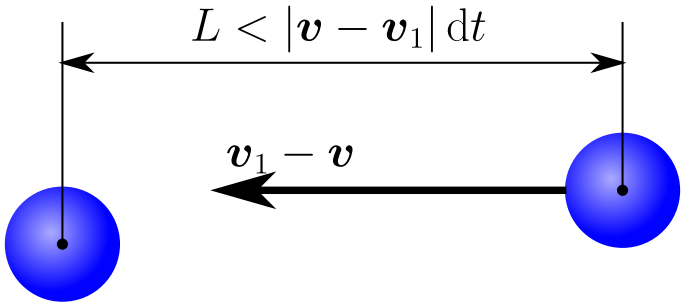
1. Given a particle with velocity $(1, 0)^T$, from t to $t + \mathrm{d}t$, how many particles with velocity $(-1, 0)^T$ will collide with this particle?
2. How many particles are there with velocity $(1, 0)^T$ at $\boldsymbol{x}$?

Count the collisions

Q1: How many particles with velocity $\boldsymbol{v}_1 = (-1, 0)^T$ will collide with the particle with velocity $\boldsymbol{v} = (1, 0)^T$?

Frame of reference: The particle with velocity $\boldsymbol{v} = (1, 0)^T$.

Illustration:



Answer:

$$\int_{-d}^{d} \int_{0}^{|\boldsymbol{v}-\boldsymbol{v}_1|\,\mathrm{d}t} v(\boldsymbol{x}, t)\,\mathrm{d}L\,\mathrm{d}b,$$

where d is the diameter of the particle.

Count the collisions

Q2: How many particles are there with velocity $(1,0)^T$ at $\boldsymbol{x}$?

Answer:

$$u(\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{x}.$$

Count the collisions

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Answer:

$$u(\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{x}.$$

Number of collisions: The total number of collisions $\{(1,0)^T,(-1,0)^T\} \longrightarrow \{(0,1)^T,(0,-1)^T\}$ is

$$\begin{aligned}\mathcal{S}_u^- &= \left(\int_{-d}^{d}\int_0^{|\boldsymbol{v}-\boldsymbol{v}_1|\,\mathrm{d}t} v(\boldsymbol{x},t)\,\mathrm{d}L\,\mathrm{d}b\right) u(\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{x}\\ &= 4d\,v(\boldsymbol{x},t)u(\boldsymbol{x},t)\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x}.\end{aligned}$$

Loss terms

Other loss terms can be calculated similarly:

$$\begin{aligned}
\mathcal{S}_u^- &= 4d\, v(\boldsymbol{x},t)u(\boldsymbol{x},t)\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x},\\
\mathcal{S}_v^- &= 4d\, u(\boldsymbol{x},t)v(\boldsymbol{x},t)\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x},\\
\mathcal{S}_w^- &= 4d\, z(\boldsymbol{x},t)w(\boldsymbol{x},t)\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x},\\
\mathcal{S}_z^- &= 4d\, w(\boldsymbol{x},t)z(\boldsymbol{x},t)\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x}.
\end{aligned}$$

Gain term

$$\boxed{u(\boldsymbol{x}, t + \mathrm{d}t)\,\mathrm{d}\boldsymbol{x} = u(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} + \mathcal{S}_u^+ - \mathcal{S}_u^-}$$

Gain term:

$\mathcal{S}_u^+ =$ (the number of binary collisions
that generate particles with velocity $(1,0)^T$ at $\boldsymbol{x}$)

The type of collision that generates the velocity $(1,0)^T$ is $\{(0,1)^T, (0,-1)^T\} \longrightarrow \{(1,0)^T, (-1,0)^T\}$. Therefore,

$$\begin{aligned}
&\mathcal{S}_u^+ \\
&= (\#\text{ of collisions } \{(0,1)^T, (0,-1)^T\} \to \{(1,0)^T, (-1,0)^T\}) \\
&= \mathcal{S}_w^- \text{ (or } \mathcal{S}_z^-) = 4d\, w(\boldsymbol{x}, t) z(\boldsymbol{x}, t)\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x}.
\end{aligned}$$

Collision-only equations

Equation of u:

$$u(\boldsymbol{x}, t + \mathrm{d}t)\,\mathrm{d}\boldsymbol{x} = u(\boldsymbol{x}, t)\,\mathrm{d}\boldsymbol{x} + \underbrace{4d\,w(\boldsymbol{x}, t)z(\boldsymbol{x}, t)\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x}}_{\mathcal{S}_u^+} - \underbrace{4d\,v(\boldsymbol{x}, t)u(\boldsymbol{x}, t)\,\mathrm{d}t\,\mathrm{d}\boldsymbol{x}}_{\mathcal{S}_u^-}.$$

$$\Downarrow$$

$$\frac{\partial u}{\partial t} = 4d\,(wz - uv).$$

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$$\frac{\partial u}{\partial t} = 4d\,(wz - uv).$$

The complete system of collision-only equations is

$$\frac{\partial u}{\partial t} = 4d\,(wz - uv), \qquad \frac{\partial v}{\partial t} = 4d\,(wz - uv),$$

$$\frac{\partial w}{\partial t} = 4d\,(uv - wz), \qquad \frac{\partial z}{\partial t} = 4d\,(uv - wz).$$

Properties of the collision-only equations

- **Mass conservation:**

$$\frac{\partial}{\partial t}(u+v+w+z)=0.$$

- **Momentum conservation:**

$$\frac{\partial}{\partial t}(u-v)=0, \quad \frac{\partial}{\partial t}(w-z)=0.$$

- **Energy conservation (identical to mass conservation):**

$$\frac{\partial}{\partial t}(u+v+w+z)=0.$$

Properties of the collision-only equations

- **Equilibrium:** as $t \to \infty$,

$$
\begin{aligned}
u &\to \frac{[u(0)+w(0)][u(0)+z(0)]}{u(0)+v(0)+w(0)+z(0)},\\
v &\to \frac{[v(0)+w(0)][v(0)+z(0)]}{u(0)+v(0)+w(0)+z(0)},\\
w &\to \frac{[w(0)+u(0)][w(0)+v(0)]}{u(0)+v(0)+w(0)+z(0)},\\
z &\to \frac{[z(0)+u(0)][z(0)+v(0)]}{u(0)+v(0)+w(0)+z(0)}.
\end{aligned}
$$

- **H-theorem:** let $H(t) = u\ln u + v\ln v + w\ln w + z\ln z$. Then $H'(t) \le 0$, and the equality holds if and only if the system is at equilibrium.

Transport-only equations

Assumption: The particles do not interact with each other. They just travel at their own velocities.

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$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \qquad \frac{\partial v}{\partial t} - \frac{\partial v}{\partial x} = 0,$$
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The exact solution is

$$u(x_1, x_2, t) = u(x_1 - t, x_2, 0), \quad v(x_1, x_2, t) = v(x_1 + t, x_2, 0),$$
$$w(x_1, x_2, t) = w(x_1, x_2 - t, 0), \quad z(x_1, x_2, t) = z(x_1, x_2 + t, 0).$$

Two-dimensional Broadwell model

For simplicity, we let $\sigma = 4d$. Then the complete equations including both transport and collision are

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

This model is called the **Broadwell model**.

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Example:

- Domain: $\Omega = (0,1) \times (0,1)$.
- Boundary conditions:

$$u(0,y) = u_b(y), \quad v(1,y) = v_b(y),$$
$$w(x,0) = w_b(x), \quad z(x,1) = z_b(x).$$

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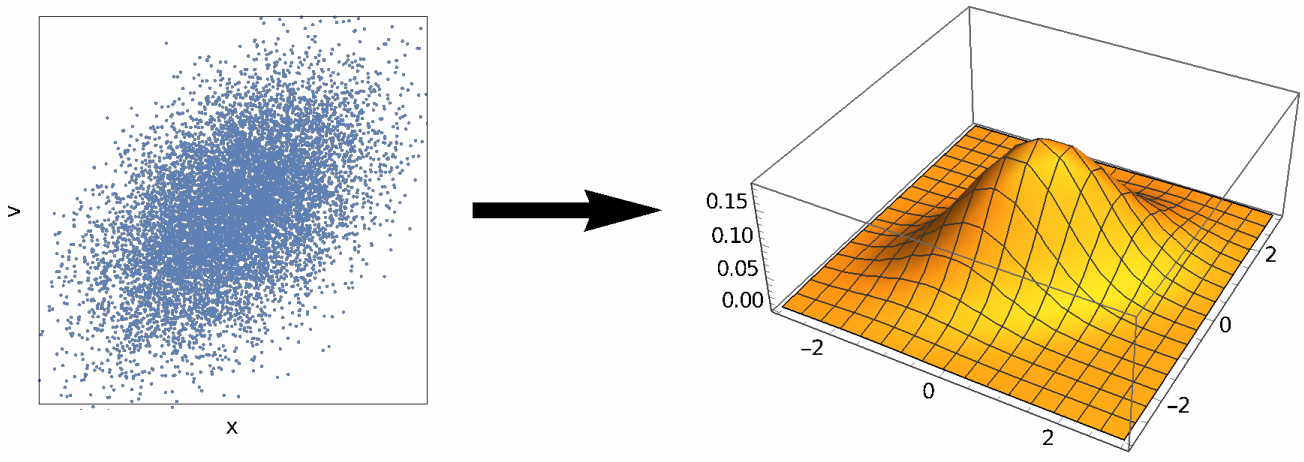
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Distribution function

Distribution function: $f(\boldsymbol{x}, \boldsymbol{v}, t)$



Given $\Omega \in \mathbb{R}^3$ and $\Sigma \in \mathbb{R}^3$, the quantity

$$\int_{\Omega} \int_{\Sigma} f(\boldsymbol{x}, \boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{v} \, \mathrm{d}\boldsymbol{x}$$

is the number of particles locating in Ω with velocity in Σ at time t.

Collision-only dynamics

Assumptions:

- The system is spatially homogeneous, i.e. f is independent of x.
- Only binary interactions take place.
- Particles interact by "collision" (short-range interaction).
- Molecular chaos: the values of f for different velocities are independent.

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Collision-only dynamics:

$$f(\boldsymbol{x}, \boldsymbol{v}, t + \mathrm{d}t)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v} = f(\boldsymbol{x}, \boldsymbol{v}, t)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{v} + \mathcal{S}^+ - \mathcal{S}^-.$$

- $\mathcal{S}^+$: Some particles get velocity $\boldsymbol{v}$ during the collision
- $\mathcal{S}^-$: Some particles with velocity $\boldsymbol{v}$ change the velocity during the collision

Broadwell model vs Boltzmann equation

Broadwell model:

- Only particles with velocity $-\boldsymbol{v}$ can collide with the particle with velocity $\boldsymbol{v}$.

Boltzmann equation:

- Particles with any velocity $\boldsymbol{v}_1$ can collide with the particle with velocity $\boldsymbol{v}$.

Broadwell model vs Boltzmann equation

Broadwell model:

- Only particles with velocity $-\boldsymbol{v}$ can collide with the particle with velocity $\boldsymbol{v}$.
- The collision of two particles with velocity $\boldsymbol{v}$ and $-\boldsymbol{v}$ always generates two particles with velocity $\boldsymbol{v}^{\perp}$ and $-\boldsymbol{v}^{\perp}$.

Boltzmann equation:

- Particles with any velocity $\boldsymbol{v}_1$ can collide with the particle with velocity $\boldsymbol{v}$.
- The collision of two particles with velocity $\boldsymbol{v}$ and $\boldsymbol{v}_1$ can generate any velocity $\boldsymbol{v}'$ and $\boldsymbol{v}_1'$ that satisfy

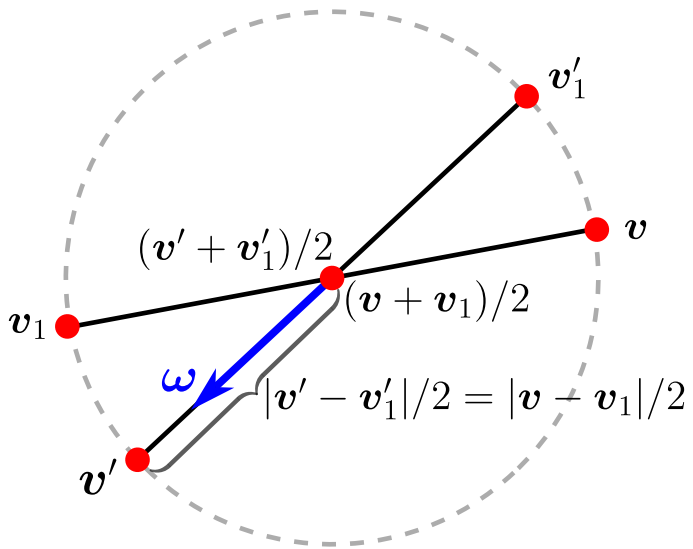
$$\boldsymbol{v}+\boldsymbol{v}_1=\boldsymbol{v}'+\boldsymbol{v}_1', \quad \text{(momentum conservation)}$$

$$|\boldsymbol{v}|^2+|\boldsymbol{v}_1|^2=|\boldsymbol{v}'|^2+|\boldsymbol{v}_1'|^2. \quad \text{(energy conservation)}$$

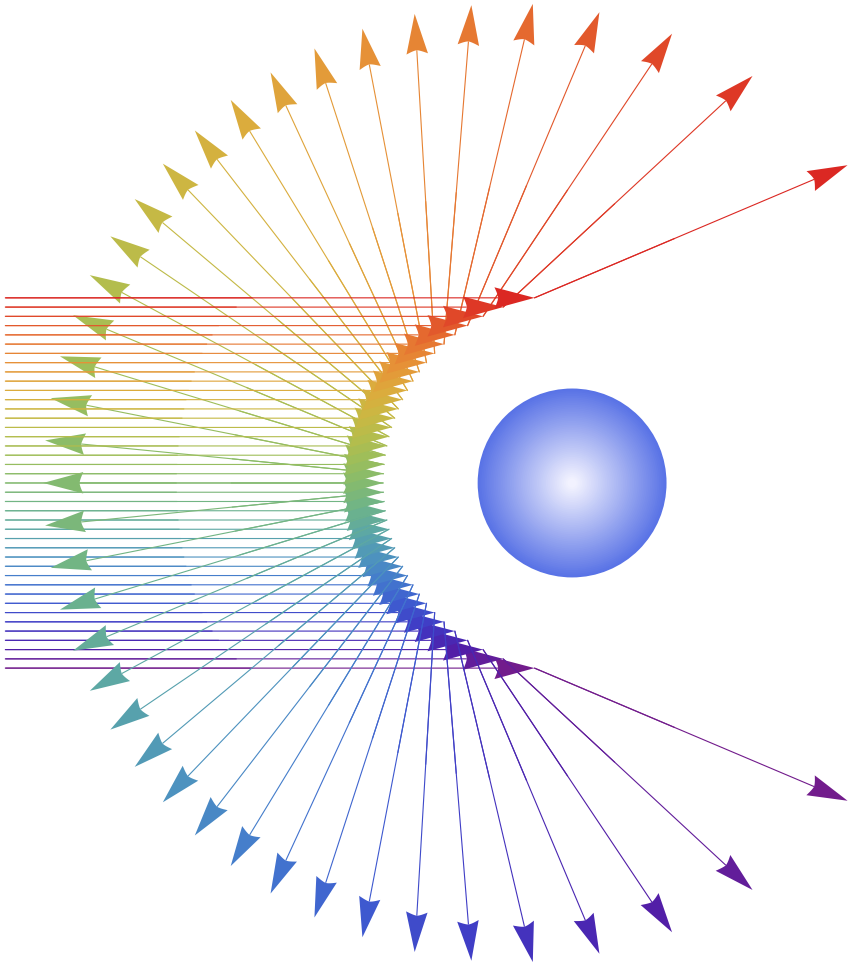
Binary collision

In a binary collision $(\boldsymbol{v}, \boldsymbol{v}_1) \longrightarrow (\boldsymbol{v}', \boldsymbol{v}_1')$, there exists a unit vector $\boldsymbol{\omega}$ such that

$$\boldsymbol{v}' = \frac{\boldsymbol{v}+\boldsymbol{v}_1}{2} + \frac{|\boldsymbol{v}-\boldsymbol{v}_1|}{2}\boldsymbol{\omega}, \quad \boldsymbol{v}_1' = \frac{\boldsymbol{v}+\boldsymbol{v}_1}{2} - \frac{|\boldsymbol{v}-\boldsymbol{v}_1|}{2}\boldsymbol{\omega}.$$



Binary collision



Collision-only Boltzmann equation

$$\frac{\partial f(\boldsymbol{x},\boldsymbol{v},t)}{\partial t} = \underbrace{\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B\left(|\boldsymbol{v}-\boldsymbol{v}_1|, \frac{(\boldsymbol{v}-\boldsymbol{v}_1)\cdot\boldsymbol{\omega}}{|\boldsymbol{v}-\boldsymbol{v}_1|}\right) f(\boldsymbol{x},\boldsymbol{v}',t) f(\boldsymbol{x},\boldsymbol{v}_1',t)\,\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}\boldsymbol{v}_1}_{\text{gain term}}$$
$$- \underbrace{\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B\left(|\boldsymbol{v}-\boldsymbol{v}_1|, \frac{(\boldsymbol{v}-\boldsymbol{v}_1)\cdot\boldsymbol{\omega}}{|\boldsymbol{v}-\boldsymbol{v}_1|}\right) f(\boldsymbol{x},\boldsymbol{v},t) f(\boldsymbol{x},\boldsymbol{v}_1,t)\,\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}\boldsymbol{v}_1}_{\text{loss term}},$$

where

$$\boldsymbol{v}' = \frac{\boldsymbol{v}+\boldsymbol{v}_1}{2} + \frac{|\boldsymbol{v}-\boldsymbol{v}_1|}{2}\boldsymbol{\omega}, \quad \boldsymbol{v}_1' = \frac{\boldsymbol{v}+\boldsymbol{v}_1}{2} - \frac{|\boldsymbol{v}-\boldsymbol{v}_1|}{2}\boldsymbol{\omega},$$

and $B(\cdot,\cdot)$ is the collision kernel, which depends on the type of interaction between particles.

Properties of the collision-only Boltzmann equation

- **Mass conservation:** (m is the mass of a particle)

$$\frac{\partial}{\partial t}\rho(\boldsymbol{x},t) = \frac{\partial}{\partial t}\int_{\mathbb{R}^3} mf(\boldsymbol{x},\boldsymbol{v},t)\,\mathrm{d}\boldsymbol{v} = 0.$$

- **Momentum conservation:**

$$\frac{\partial}{\partial t}[\rho(\boldsymbol{x},t)\boldsymbol{u}(\boldsymbol{x},t)] = \frac{\partial}{\partial t}\int_{\mathbb{R}^3} m\boldsymbol{v}f(\boldsymbol{x},\boldsymbol{v},t)\,\mathrm{d}\boldsymbol{v} = 0.$$

- **Energy conservation:** (k_B is the Boltzmann constant)

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho(\boldsymbol{x},t)|\boldsymbol{u}(\boldsymbol{x},t)|^2 + \frac{3k_B}{2m}\rho(\boldsymbol{x},t)T(\boldsymbol{x},t)\right)$$
$$= \frac{\partial}{\partial t}\int_{\mathbb{R}^3}\frac{1}{2}m|\boldsymbol{v}|^2 f(\boldsymbol{x},\boldsymbol{v},t)\,\mathrm{d}\boldsymbol{v} = 0.$$

Properties of the collision-only Boltzmann equation

- **Equilibrium:** as $t \to \infty$, $f(\boldsymbol{x}, \boldsymbol{v}, t)$ converges to the Maxwellian distribution

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

  where $\rho(\boldsymbol{x})$, $\boldsymbol{u}(\boldsymbol{x})$, and $T(\boldsymbol{x})$ are the density, velocity, and temperature of the gas at $\boldsymbol{x}$, which are independent of t and can be computed from the initial distribution.

- **H-theorem:** let

$$H(\boldsymbol{x}, t) = \int_{\mathbb{R}^3} f(\boldsymbol{x}, \boldsymbol{v}, t) \ln f(\boldsymbol{x}, \boldsymbol{v}, t) \, \mathrm{d}\boldsymbol{v}.$$

  Then $\partial_t H(\boldsymbol{x}, t) \leq 0$, and the equality holds if and only if the system is at equilibrium.

Transport-only Boltzmann equation

Assumption: The particles do not interact with each other. They just travel at their own velocities.

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Exact solution:

$$f(\boldsymbol{x}, \boldsymbol{v}, t) = f(\boldsymbol{x} - \boldsymbol{v}t, \boldsymbol{v}, 0).$$

Complete Boltzmann equation

Boltzmann equation:

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

where $Q(f, f)$ is the collision operator, given by

$$Q(f,f) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} B\left(|\boldsymbol{v} - \boldsymbol{v}_1|, \frac{(\boldsymbol{v} - \boldsymbol{v}_1) \cdot \boldsymbol{\omega}}{|\boldsymbol{v} - \boldsymbol{v}_1|} \right) \times \left(f(\boldsymbol{x}, \boldsymbol{v}', t) f(\boldsymbol{x}, \boldsymbol{v}_1', t) - f(\boldsymbol{x}, \boldsymbol{v}, t) f(\boldsymbol{x}, \boldsymbol{v}_1, t) \right) \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\boldsymbol{v}_1$$

with

$$\boldsymbol{v}' = \frac{\boldsymbol{v} + \boldsymbol{v}_1}{2} + \frac{|\boldsymbol{v} - \boldsymbol{v}_1|}{2} \boldsymbol{\omega}, \quad \boldsymbol{v}_1' = \frac{\boldsymbol{v} + \boldsymbol{v}_1}{2} - \frac{|\boldsymbol{v} - \boldsymbol{v}_1|}{2} \boldsymbol{\omega}.$$

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Fourier transform

Given a function $f(\boldsymbol{v})$, its Fourier transform is defined as

$$\hat{f}(\boldsymbol{\xi}) = \int_{\mathbb{R}^3} f(\boldsymbol{v}) \mathrm{e}^{-\mathrm{i}\boldsymbol{v}\cdot\boldsymbol{\xi}} \, \mathrm{d}\boldsymbol{v}.$$

Also, $f(\boldsymbol{v})$ can be recovered from $\hat{f}(\boldsymbol{\xi})$ by the inverse Fourier transform:

$$f(\boldsymbol{v}) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \hat{f}(\boldsymbol{\xi}) \mathrm{e}^{\mathrm{i}\boldsymbol{v}\cdot\boldsymbol{\xi}} \, \mathrm{d}\boldsymbol{\xi}.$$

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Theorem

Let $h(\boldsymbol{v}) = f(\boldsymbol{v})g(\boldsymbol{v})$. Then the Fourier transform of h is

$$\hat{h}(\boldsymbol{\xi}) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \hat{f}(\boldsymbol{\xi} - \boldsymbol{\zeta}) \hat{g}(\boldsymbol{\zeta}) \, \mathrm{d}\boldsymbol{\zeta}.$$

Fourier transform of the collision operator

Collision operator: given a distribution function $f(\boldsymbol{v})$,

$$Q(f,f)(\boldsymbol{v}) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B\left(|\boldsymbol{v}-\boldsymbol{v}_1|, \frac{(\boldsymbol{v}-\boldsymbol{v}_1)\cdot\boldsymbol{\omega}}{|\boldsymbol{v}-\boldsymbol{v}_1|}\right) \times \left[f(\boldsymbol{v}')f(\boldsymbol{v}_1') - f(\boldsymbol{v})f(\boldsymbol{v}_1)\right] \mathrm{d}\boldsymbol{\omega}\,\mathrm{d}\boldsymbol{v}_1.$$

Fourier transform of $Q(f,f)$:

$$\widehat{Q(f,f)}(\boldsymbol{\xi}) = \frac{1}{(2\pi)^3}\int_{\mathbb{R}^3}\left[K(\boldsymbol{\xi}-\boldsymbol{\zeta},\boldsymbol{\zeta}) - K(-\boldsymbol{\zeta},\boldsymbol{\zeta})\right]\hat{f}(\boldsymbol{\xi}-\boldsymbol{\zeta})\hat{f}(\boldsymbol{\zeta})\,\mathrm{d}\boldsymbol{\zeta},$$

where

$$K(\boldsymbol{\eta},\boldsymbol{\zeta}) = \int_{\mathbb{R}^3}\int_{\mathbb{S}^2} B\left(|\boldsymbol{g}|, \frac{\boldsymbol{g}\cdot\boldsymbol{\omega}}{|\boldsymbol{g}|}\right) \mathrm{e}^{-\frac{\mathrm{i}}{2}(\boldsymbol{\eta}-\boldsymbol{\zeta})\cdot\boldsymbol{g}} \mathrm{e}^{-\frac{\mathrm{i}}{2}|\boldsymbol{g}|(\boldsymbol{\eta}+\boldsymbol{\zeta})\cdot\boldsymbol{\omega}}\,\mathrm{d}\boldsymbol{\omega}\,\mathrm{d}\boldsymbol{g}.$$

An alternative form

It also holds that

$$\widehat{Q(f,f)}(\boldsymbol{\xi}) = \frac{1}{(2\pi)^3}\int_0^{+\infty}\int_{\mathbb{S}^2} K_+(g,\boldsymbol{\sigma},\boldsymbol{\xi})I(g,\boldsymbol{\sigma},\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}g - \frac{1}{2\pi^2}\int_{\mathbb{R}^3} K_-(\boldsymbol{\zeta})\hat{f}(\boldsymbol{\xi}-\boldsymbol{\zeta})\hat{f}(\boldsymbol{\zeta})\,\mathrm{d}\boldsymbol{\zeta},$$

where

$$K_+(g,\boldsymbol{\sigma},\boldsymbol{\xi}) = \int_{\mathbb{S}^2} g^2 B(g,\boldsymbol{\omega}\cdot\boldsymbol{\sigma})\mathrm{e}^{-\frac{\mathrm{i}}{2}g\boldsymbol{\xi}\cdot\boldsymbol{\omega}}\,\mathrm{d}\boldsymbol{\omega},$$

$$K_-(\boldsymbol{\zeta}) = \int_0^{+\infty}\int_{\mathbb{S}^2} \frac{g}{|\boldsymbol{\zeta}|}B(g,\boldsymbol{\omega}\cdot\boldsymbol{\sigma})\sin\left(g|\boldsymbol{\zeta}|\right)\,\mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}g,$$

$$I(g,\boldsymbol{\sigma},\boldsymbol{\xi}) = \int_{\mathbb{R}^3} \hat{f}(\boldsymbol{\xi}-\boldsymbol{\zeta})\mathrm{e}^{\mathrm{i}g\boldsymbol{\sigma}\cdot(\boldsymbol{\xi}-\boldsymbol{\zeta})/2}\cdot\hat{f}(\boldsymbol{\zeta})\mathrm{e}^{-\mathrm{i}g\boldsymbol{\sigma}\cdot\boldsymbol{\zeta}/2}\,\mathrm{d}\boldsymbol{\zeta}.$$

In the next lecture

These two forms of the Fourier transform of the collision operator will be used to design fast algorithms for computing the Boltzmann collision operator.

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Summary

Broadwell model:

- Derivation of the Broadwell model
- Properties: mass, momentum, and energy conservation; equilibrium; H-theorem

Boltzmann equation:

- Generalization of the Broadwell model
- Properties: mass, momentum, and energy conservation; equilibrium; H-theorem
- Fourier transform of the collision operator