Boltzmann Equation and BGK Model

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Mathematical Aspects of Some Important Equations of Physics
Orange County, Coorg
22-24 February 2018

Density function

- We wish to describe the motion of a rarefied gas, consisting of a very large number of identical particles, moving in a three-dimensional space.
- The statistical description of the dynamics is given in terms of the *one particle distribution function*, denoted by f, which is a function of time t, position x and velocity ξ, i.e.

$$f = f(t, x, \xi), \; t > 0, \; x \in \mathbb{R}^3, \; \xi \in \mathbb{R}^3.$$

- By definition, $f(t, x, \xi)$ is the probability density to find a particle at time t, in the position x, with velocity ξ. Thus, the integral

$$\int_V \int_\Omega f(t, x, \xi) d\xi dx$$

is the probability of finding a particle in the region $V \subset \mathbb{R}^3$ at time t with velocities $\xi \in \Omega \subset \mathbb{R}^3$.

Density function

- When the particles do not collide with each other, the speed ξ of each particle will remain constant in time.
- A particle with speed ξ and located at the point x at the initial time $t = 0$ will move to $x + \tau\xi$ at a later time τ.
- Therefore, $f(\tau, x, \xi) = f(0, x - \tau\xi, \xi)$. In this case, f provides a solution to the linear transport equation:

$$\partial_t f + \xi \cdot \nabla_x f = 0.$$

- When there are collisions between the particles, f satisfies the Boltzmann equation:

$$\partial_t f + \xi \cdot \nabla_x f = Q(f, f),$$

where $Q(f, f)$ is called the collision operator.

Collision operator

- We will assume binary elastic collisions, i.e. only collisions between pair of particles (binary).
- Moreover the collisions are assumed to be elastic, i.e. total momentum and, also the total kinetic energy is conserved during the collision.
- Let ξ, ξ_* denote the velocities of two particles before collision and let ξ', ξ'_*, their velocities after the collision. Conservation requires

$$\xi + \xi_* = \xi' + \xi'_*,$$
$$||\xi||^2 + ||\xi_*||^2 = ||\xi'||^2 + ||\xi'_*||^2.$$

Lemma

A quadruple $(\xi, \xi_*, \xi', \xi'_*)$ solves the above equations if, and only if,

$$\xi' = \xi - \{(\xi - \xi_*) \cdot \nu\}\nu$$
$$\xi'_* = \xi_* + \{(\xi - \xi_*) \cdot \nu\}\nu, \text{ for some } \nu \in \mathbb{S}^2.$$

Collision operator

- The collision operator $Q(f,f)$ is defined by the relation:

$$Q(f,f) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} B(\nu,\xi,\xi_*) \left\{ f(t,x,\xi')f(t,x,\xi_*') - f(t,x,\xi)f(t,x,\xi_*) \right\} d\nu d\xi_*.$$

- Here, $B = B(\nu,\xi,\xi_*)$ is called the collision kernel which tells us how strong is the collision of two particles with velocities ξ, ξ_* and scattering angle ν.
- Under the hard sphere assumption, B takes the form:

$$B(\nu,\xi,\xi_*) = |(\xi - \xi_*) \cdot \nu|.$$

Collisional invariants

Definition

A function $\phi \colon \mathbb{R}^3 \to \mathbb{R}$ *is called collisional invariant, if*

$$\int_{\mathbb{R}^3} \phi(\xi) Q(f,f) d\xi = 0$$

for all solutions f *of the Boltzmann equation.*

Proposition

If ϕ *is a collisional invariant, the the functional* Φ *defined by*

$$\Phi(f) := \int_{\mathbb{R}^3} \phi(\xi) f(\xi) d\xi$$

is a quantity conserved by all solutions of the Boltzmann equation.

Collisional invariants

Proposition

A function $\phi = \phi(\xi)$ is a collisional invariant if, and only if,

$$\phi(\xi) + \phi(\xi_*) = \phi(\xi') + \phi(\xi'_*)$$

and the functions satisfying this condition are characterised by

$$\phi(\xi) = a\xi + b \cdot \xi + c||\xi||^2,$$

where $a, c \in \mathbb{R}$ and $b \in \mathbb{R}^3$.

Conserved quantities

1. Taking $\phi(\xi) = 1$, we obtain the conserved quantity mass

$$\rho(t,x) := \int_{\mathbb{R}^3} f(t,x,\xi)d\xi.$$

2. Taking $\phi(\xi) = e_k \cdot \xi$, we obtain the conserved quantity momentum

$$\rho u(t,x) := \int_{\mathbb{R}^3} \xi f(t,x,\xi)d\xi.$$

3. Taking $\phi(\xi) = ||\xi||^2/2$, we obtain the conserved quantity energy

$$\rho e(t,x) := \int_{\mathbb{R}^3} \frac{||\xi||^2}{2} f(t,x,\xi)d\xi.$$

Boltzmann inequality

Proposition

For every solution $f \geq 0$ of the Boltzmann equation, the following inequality

$$\int_{\mathbb{R}^3} \log f \; Q(f,f) d\xi \leq 0$$

holds and equality happens if, and only if, $\log f$ is an invariant.

As a consequence of the Boltzmann inequality, we can prove

Theorem

The thermodynamic equilibrium states characterised by $Q(f,f) = 0$ are obtained by the Maxwellian distribution:

$$f(\xi) = Ae^{-\beta||(\xi - v)||^2},$$

where $A, \beta > 0$ and $v \in \mathbb{R}^3$ are arbitrary.

Boltzmann H-theorem

Define the entropy and entropy flux pair

$$H(f) := \int_{\mathbb{R}^3} f \log f d\xi, \ \ \Psi(f) := \int_{\mathbb{R}^3} \xi f \log f d\xi.$$

Then, we get the kinetic entropy inequality

$$\partial_t H(f) + \nabla_x \cdot \Psi(f) \leq 0.$$

Integrating with respect to x and assuming suitable decay as $||x|| \to \infty$, we get

Theorem (H-theorem)

The quantity $\mathcal{H}(t)$, where

$$\mathcal{H}(t) = \int_{\mathbb{R}^3} H(t,x) dx$$

decreases in time, i.e. $d\mathcal{H}/dt \leq 0$.

Conservation laws

Define the macroscopic conserved variables

$$\begin{pmatrix} \rho \\ \rho u \\ \rho e \end{pmatrix} (t, x) := \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \xi \\ \frac{||\xi||^2}{2} \end{pmatrix} f(t, x, \xi) d\xi,$$

where ρ is the mass, u is the velocity and e is the specific energy.

The specific energy can be decomposed as

$$\rho e = \int_{\mathbb{R}^3} \frac{||\xi||^2}{2} f(t, x, \xi) d\xi = \int_{\mathbb{R}^3} \frac{||\xi - u||^2}{2} f(t, x, \xi) d\xi + \frac{1}{2} \rho u^2.$$

Let $C = \xi - u$, the peculiar velocity, the term

$$\rho \varepsilon := \int_{\mathbb{R}^3} \frac{||C||^2}{2} f(t, x, \xi) d\xi$$

is called the internal energy.

Conservation laws

- The stress tensor is defined as

$$\pi = \int_{\mathbb{R}^3} C \otimes C \;\, f d\xi.$$

- The internal energy is then $2\rho\varepsilon = \mathrm{tr}(\pi)$.
- The thermodynamic pressure p is defined by

$$p := \frac{2\rho\varepsilon}{3}.$$

- The heat flux vector Q is defined by

$$Q = \int_{\mathbb{R}^3} ||C||^2 C \;\, f d\xi.$$

Conservation laws

Theorem (Conservation laws)

Let $f \geq 0$ be a solution of the Boltzmann equation. Then, the macroscopic conserved variables, defined as before, satisfies the system of conservation laws

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho u) &= 0, \\ \partial_t (\rho u) + \nabla \cdot (\rho u \otimes u + \pi) &= 0, \\ \partial_t (\rho e) + \nabla \cdot (\rho e u + \pi u + Q) &= 0. \end{aligned}$$

- This is the most general form of conservation laws of mass, momentum and energy.
- The form of the stress tensor π and heat flux vector Q are unknown.
- A highly underdetermined system of 5 conservation laws in 14 unknown quantities.

Euler equations

- Suppose $f(\xi) = Ae^{-\beta||(\xi - v)||^2}$, the Maxwellian distribution.
- The unknowns A, β and v can be obtained using the conserved quantities.
- This yields the form:

$$M(t,x,\xi) = \frac{\rho}{(2\pi RT)^{3/2}} e^{-\frac{||\xi - u||^2}{2RT}},$$

where $T = 2\varepsilon/3R$ is the temperature and R is a constant.

- Moreover, $\pi = p\mathrm{Id}$ and $Q = 0$.

Corollary (Euler equations)

Assume f is the Maxwellian. The conserved variables satisfy the Euler equations

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho u) &= 0, \\ \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla p &= 0, \\ \partial_t(\rho e) + \nabla \cdot ((\rho e + p)u) &= 0, \end{aligned}$$

where $p = 2\rho\varepsilon/3$ is the equation of state.

Entropy inequality

- Defining the functional $H(f) = \int_{\mathbb{R}^3} f \log f d\xi$ for the Maxwellian $f = M$ gives the macroscopic entropy
$$H = \int_{\mathbb{R}^3} M(t,x,\xi) \log M(t,x,\xi) d\xi = C_v \log \left(\frac{\varepsilon}{\rho^{\gamma-1}} \right).$$
- The function H is strictly convex function of the conserved variables $U = (\rho, \rho u, \rho\varepsilon)$.

A characterisation of H is given by

Proposition (Brenier, 1992)

H satisfies
$$H = \min \int_{\mathbb{R}^3} H(f) d\xi,$$
where the minimum is taken over all $f \geq 0$ satisfying
$$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \xi \\ \frac{||\xi||^2}{2} \end{pmatrix} f(t, x\xi) d\xi = \begin{pmatrix} \rho \\ \rho u \\ \rho\varepsilon \end{pmatrix} (t,x).$$

BGK Model

- The BGK (Bhatnagar, Gross and Crook) model is given by

$$\partial_t f + \xi \cdot \nabla_x f = \frac{M(\xi) - f}{\tau},$$

where $M(\xi)$ is the Maxwellian distribution and $0 < \tau \ll 1$ is usually known as a relaxation parameter.

- The BGK collision operator $J(f) = (M - f)/\tau$ satisfies

1. $$\int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \xi \\ \frac{||\xi||^2}{2} \end{pmatrix} J(f) d\xi = 0$$

2. $$\int_{\mathbb{R}^3} \log f \; J(f) d\xi \leq 0.$$

BGK model

- The Maxwellian M is a solution of the minimisation problem

$$\min \left\{ H(f) \colon \text{All solutions } f \geq 0 \text{ and } \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \xi \\ \frac{||\xi||^2}{2} \end{pmatrix} f d\xi = \begin{pmatrix} \rho \\ \rho u \\ \rho e \end{pmatrix} \right\}$$

- From numerical applications, it is interesting to consider other equilibra than the Maxwellian.
- Given a convex functional h, satisfying some reasonable assumptions, we consider the minimisation problem $\min h(f)$ where the minimum is taken over

Theorem

The minimisation problem admits a unique solution N and using N we can construct a BGK model with

$$J_N(f) = \frac{N - f}{\tau}.$$

As $\tau \to 0$, the corresponding moments of N satisfy the Euler equations.

Thank You for Your Kind Attention!

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