Summer Course at PKU (July 2020)
Introduction to Kinetic Theory – Lecture Notes*

Jingwei Hu

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Contents

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1 Introduction

These lecture notes are a collection of materials related to various aspects of modern kinetic theory, including physical derivation, mathematical theory, and numerical methods. The main focus is on the Boltzmann-like collisional kinetic equations and their numerical approximations. To begin with, let us take a look at Figure 1 to understand the role of kinetic theory in multiscale modeling hierarchy.

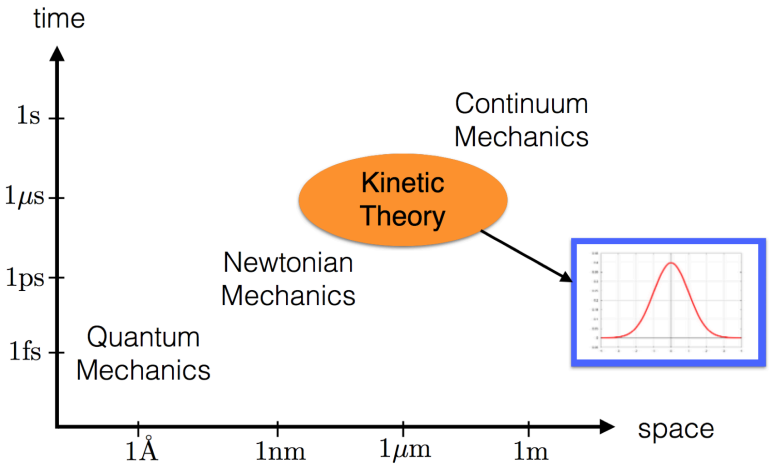

Figure 1: Role of kinetic theory in multiscale modeling hierarchy.

2 The Boltzmann equation for hard spheres

Proposed by Ludwig Boltzmann in 1872, the Boltzmann equation is one of the fundamental equations in kinetic theory. It describes the non-equilibrium dynamics of a gas or system comprised of a large number of particles. In this very first part of the course, we derive the Boltzmann equation for hard sphere molecules. For better understanding, we start with a heuristic derivation and then discuss a more formal derivation from the Liouville equation.

2.1 Heuristic derivation

This part of the presentation mainly follows [8, Chapter 1.2].

Let us start with the function $P^{(1)}(t, x_1, v_1)$, which is the one-particle *probability density function* (PDF). $P^{(1)}\,\mathrm{d}x_1\,\mathrm{d}v_1$ gives the probability of finding one fixed particle (say, the one labeled by 1) in an infinitesimal volume $\mathrm{d}x_1\,\mathrm{d}v_1$ centered at the point (x_1, v_1) of the phase space, where $x_1 \in \mathbb{R}^3$ is the position and $v_1 \in \mathbb{R}^3$ is the particle velocity.

When two particles (say, particles 1 and 2) collide, momentum and energy must be conserved (mass is always conserved). Let v_1, v_2 be the velocities before a collision and (v_1', v_2') the velocities after a collision. From

$$v_1 + v_2 = v_1' + v_2', \quad |v_1|^2 + |v_2|^2 = |v_1'|^2 + |v_2'|^2, \tag{2.1}$$

one can derive that

$$v_1' = v_1 - [(v_1 - v_2) \cdot \omega]\omega, \quad v_2' = v_2 + [(v_1 - v_2) \cdot \omega]\omega, \tag{2.2}$$

where ω is the impact direction (the unit vector connecting the centers of particles 1 and 2). Note from (2.2) that

$$v_2' - v_1' = (v_2 - v_1) - 2[(v_2 - v_1) \cdot \omega]\omega, \tag{2.3}$$

i.e., the relative velocity undergoes a specular reflection at the impact (see Figure 2).

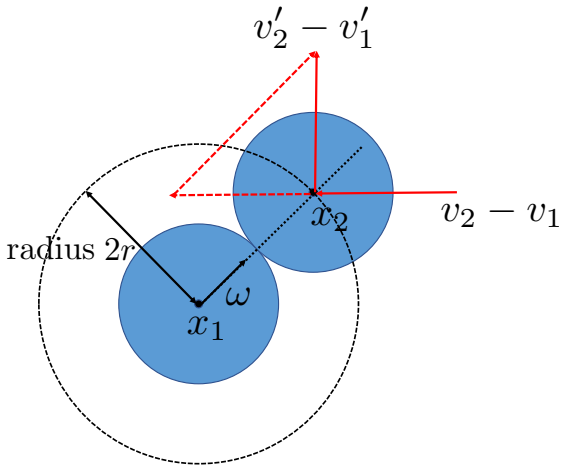

Figure 2: Illustration of particle collisions.

In the absence of collisions and external forces, $P^{(1)}$ would remain unchanged along the trajectory of particle 1. That is, $P^{(1)}$ satisfies

$$\partial_t P^{(1)} + v_1 \cdot \nabla_{x_1} P^{(1)} = 0. \tag{2.4}$$

Now with collisions, one would expect

$$\partial_t P^{(1)} + v_1 \cdot \nabla_{x_1} P^{(1)} = G - L, \tag{2.5}$$

where $L\,\mathrm{d}x_1\,\mathrm{d}v_1\,\mathrm{d}t$ gives the probability of finding particles with position between x_1 and $x_1 + \mathrm{d}x_1$ and velocity between v_1 and $v_1 + \mathrm{d}v_1$ that disappear from these ranges of values because of a collision in the time interval between t and $t + \mathrm{d}t$ (L is often called

the *loss* term of the collision operator), and $G\,\mathrm{d}x_1\,\mathrm{d}v_1\,\mathrm{d}t$ gives the analogous probability of finding particles entering the same range in the same time interval (G is often called the *gain* term of the collision operator). To count these probabilities, imaging particle 1 as a sphere at rest and endowed with twice the actual radius r and the other particles being the point masses with velocity $v_2 - v_1$ (see Figure 2). Fixing particle 1, there are $N-1$ particles (assume there are a total of N particles) that will collide with it, and they are to be found in the cylinder of height $|(v_2 - v_1)\cdot\omega|\,\mathrm{d}t$ and base area $(2r)^2\,\mathrm{d}\omega$. Then

$$\begin{aligned} L\,\mathrm{d}x_1\,\mathrm{d}v_1\,\mathrm{d}t = (N-1)\int_{\mathbb{R}^3}\int_{S^2_-} P^{(2)}(t,x_1,v_1,x_1+2r\omega,&v_2)|(v_2-v_1)\cdot\omega|\,\mathrm{d}t \\ &\times (2r)^2\,\mathrm{d}\omega\,\mathrm{d}v_2\,\mathrm{d}x_1\,\mathrm{d}v_1, \end{aligned} \tag{2.6}$$

where $P^{(2)}$ is the two-particle PDF, and S^2_- is the hemisphere corresponding to $(v_2 - v_1)\cdot\omega < 0$. Therefore,

$$L = (N-1)(2r)^2\int_{\mathbb{R}^3}\int_{S^2_-} P^{(2)}(t,x_1,v_1,x_1+2r\omega,v_2)|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2. \tag{2.7}$$

Similarly,

$$G = (N-1)(2r)^2\int_{\mathbb{R}^3}\int_{S^2_+} P^{(2)}(t,x_1,v_1,x_1+2r\omega,v_2)|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2, \tag{2.8}$$

where S^2_+ is the hemisphere corresponding to $(v_2 - v_1)\cdot\omega > 0$.

Now we make two crucial assumptions:

- Assume $N\to\infty$, $r\to 0$, but Nr^2 is finite. This is the so-called *Boltzmann-Grad limit.*
- Assume $P^{(2)}(t,x_1,v_1,x_2,v_2) = P^{(1)}(t,x_1,v_1)P^{(1)}(t,x_2,v_2)$ for two particles that are about to collide. This is the *molecular chaos assumption.*

Then L becomes

$$\begin{aligned} L &= N(2r)^2\int_{\mathbb{R}^3}\int_{S^2_-} P^{(2)}(t,x_1,v_1,x_1,v_2)|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2 \\ &= N(2r)^2\int_{\mathbb{R}^3}\int_{S^2_-} P^{(1)}(t,x_1,v_1)P^{(1)}(t,x_1,v_2)|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2, \end{aligned} \tag{2.9}$$

where we used the assumption 1 in the first equality and assumption 2 in the second equality. For G, we have

$$\begin{aligned} G &= (N-1)(2r)^2\int_{\mathbb{R}^3}\int_{S^2_+} P^{(2)}(t,x_1,v_1',x_1+2r\omega,v_2')|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2 \\ &= N(2r)^2\int_{\mathbb{R}^3}\int_{S^2_+} P^{(1)}(t,x_1,v_1')P^{(1)}(t,x_1,v_2')|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2 \\ &= N(2r)^2\int_{\mathbb{R}^3}\int_{S^2_-} P^{(1)}(t,x_1,v_1')P^{(1)}(t,x_1,v_2')|(v_2-v_1)\cdot\omega|\,\mathrm{d}\omega\,\mathrm{d}v_2, \end{aligned} \tag{2.10}$$

where the first equality is because $P^{(2)}$ is continuous at a collision, the second equality is obtained for the same reason as above for L (since $(v_2-v_1)\cdot\omega > 0$ implies $(v_2'-v_1')\cdot\omega < 0$), and the third one is a simple change of variable $\omega \to -\omega$.

Putting together G and L, we have

$$\begin{aligned}\partial_t P^{(1)}+v_1\cdot\nabla_{x_1}P^{(1)} = N(2r)^2\int_{\mathbb{R}^3}\int_{S^2_-}|(v_2-v_1)\cdot\omega| \\ \times[P^{(1)}(t,x_1,v_1')P^{(1)}(t,x_1,v_2') - P^{(1)}(t,x_1,v_1)P^{(1)}(t,x_1,v_2)]\,\mathrm{d}\omega\,\mathrm{d}v_2.\end{aligned} \tag{2.11}$$

In this course we will often consider the one-particle *number distribution function* f (i.e., $f = NP^{(1)}$), then f satisfies (changing $x_1 \to x$, $v_1 \to v$, $v_2 \to v_*$, $\omega \to -\omega$)

$$\partial_t f + v\cdot\nabla_x f = (2r)^2\int_{\mathbb{R}^3}\int_{(v-v_*)\cdot\omega<0}|(v-v_*)\cdot\omega|[f'f_*' - ff_*]\,\mathrm{d}\omega\,\mathrm{d}v_*, \tag{2.12}$$

where f, f_*, f', f_*' are short hand notations for $f(t,x,v)$, $f(t,x,v_*)$, $f(t,x,v')$, $f(t,x,v_*')$, and

$$v' = v - [(v-v_*)\cdot\omega]\omega, \quad v_*' = v_* + [(v-v_*)\cdot\omega]\omega. \tag{2.13}$$

Equation (2.12) is the Boltzmann equation for hard spheres.

It is often convenient to integrate ω over the whole sphere S^2 rather than hemisphere, which yields

$$\partial_t f + v\cdot\nabla_x f = 2r^2\int_{\mathbb{R}^3}\int_{S^2}|(v-v_*)\cdot\omega|[f'f_*' - ff_*]\,\mathrm{d}\omega\,\mathrm{d}v_*. \tag{2.14}$$

2.2 Formal derivation from the Liouville equation (BBGKY hierarchy)

In this section, we give a formal derivation of the Boltzmann equation starting from the Liouville equation. The rigorous derivation was an open and challenging problem for a long time. In 1973, Lanford showed that, although for a very short time, the Boltzmann equation can be derived from the mechanical systems.

This part of the presentation mainly follows [6, Chapter 3.2], where one can also find the rigorous treatise.

Consider N hard spheres of radius r. Let x_i, v_i denote the position and velocity of particle i, then the state of the system is given by

$$(x_1, v_1, \ldots, x_N, v_N) \in \Omega^N \times \mathbb{R}^{3N} = \Lambda,$$

where

$$\Omega^N = \{(x_1,\ldots,x_N)\,|\,|x_i - x_j| > 2r, i \neq j\},$$

$$\partial\Lambda = \{(x_1, v_1, \ldots, x_N, v_N)\,|\,|x_i - x_j| = 2r, i \neq j\},$$

since the particles cannot overlap.

Let $P^{(N)}(t, x_1, v_1, \ldots, x_N, v_N)$ be the N-particle PDF, then $P^{(N)}$ satisfies the Liouville equation

$$\partial_t P^{(N)} + \sum_{i=1}^{N} v_i \cdot \nabla_{x_i} P^{(N)} = 0. \tag{2.15}$$

Define the s-particle PDF as

$$P^{(s)}(t, x_1, v_1, \ldots, x_s, v_s) = \int P^{(N)} \, \mathrm{d}x_{s+1} \, \mathrm{d}v_{s+1} \ldots \, \mathrm{d}x_N \, \mathrm{d}v_N, \tag{2.16}$$

then integrating (2.15) one obtains

$$\partial_t P^{(s)} + I_1 + I_2 = 0, \tag{2.17}$$

with

$$\begin{aligned} I_1 &= \sum_{i=1}^{s} \int v_i \cdot \nabla_{x_i} P^{(N)} \, \mathrm{d}x_{s+1} \, \mathrm{d}v_{s+1} \ldots \, \mathrm{d}x_N \, \mathrm{d}v_N, \\ I_2 &= \sum_{i=s+1}^{N} \int v_i \cdot \nabla_{x_i} P^{(N)} \, \mathrm{d}x_{s+1} \, \mathrm{d}v_{s+1} \ldots \, \mathrm{d}x_N \, \mathrm{d}v_N. \end{aligned} \tag{2.18}$$

For I_2, applying the divergence theorem (one can refer to Figure 2 again but with (x_1, v_1) replaced by (x_i, v_i), (x_2, v_2) by (x_j, v_j), and ω by ω_{ij}), one has

$$\begin{aligned} I_2 = \sum_{j=1}^{s} \sum_{i=s+1}^{N} (2r)^2 \int & v_i \cdot \omega_{ij} P^{(N)}(t, x_1, v_1, \ldots, x_{i-1}, v_{i-1}, x_j - 2r\omega_{ij}, v_i, \ldots, x_N, v_N) \\ & \times \mathrm{d}\omega_{ij} \, \mathrm{d}x_{s+1} \ldots \, \mathrm{d}x_{i-1} \, \mathrm{d}x_{i+1} \ldots \, \mathrm{d}x_N \, \mathrm{d}v_{s+1} \ldots \, \mathrm{d}v_N \\ + \sum_{\substack{j=s+1, \\ j \neq i}}^{N} \sum_{i=s+1}^{N} (2r)^2 \int & v_i \cdot \omega_{ij} P^{(N)}(t, x_1, v_1, \ldots, x_{i-1}, v_{i-1}, x_j - 2r\omega_{ij}, v_i, \ldots, x_N, v_N) \\ & \times \mathrm{d}\omega_{ij} \, \mathrm{d}x_{s+1} \ldots \, \mathrm{d}x_{i-1} \, \mathrm{d}x_{i+1} \ldots \, \mathrm{d}x_N \, \mathrm{d}v_{s+1} \ldots \, \mathrm{d}v_N. \end{aligned} \tag{2.19}$$

The second sum in the above equation is completely zero by the Liouville theorem (it is the integral of $\sum_{i=s+1}^{N} v_i \cdot \nabla_{x_i} P^{(N)}$ relative to the dynamics of the last $N - s$ particles). Using the symmetry of $P^{(N)}$, the first term can be further reduced to

$$\begin{aligned} I_2 &= (N-s)(2r)^2 \sum_{j=1}^{s} \int v_{s+1} \cdot \omega_{s+1,j} P^{(N)}(t, x_1, v_1, \ldots, x_s, v_s, x_j - 2r\omega_{s+1,j}, v_{s+1}, \ldots, x_N, v_N) \\ &\qquad \times \mathrm{d}\omega_{s+1,j} \, \mathrm{d}x_{s+2} \ldots \, \mathrm{d}x_N \, \mathrm{d}v_{s+1} \ldots \, \mathrm{d}v_N \\ &= (N-s)(2r)^2 \sum_{j=1}^{s} \int v_{s+1} \cdot \omega_{s+1,j} P^{(s+1)}(t, x_1, v_1, \ldots, x_s, v_s, x_j - 2r\omega_{s+1,j}, v_{s+1}) \, \mathrm{d}\omega_{s+1,j} \, \mathrm{d}v_{s+1}. \end{aligned} \tag{2.20}$$

For I_1, it can be shown that (see below)

$$I_1 = \sum_{i=1}^{s} v_i \cdot \nabla_{x_i} P^{(s)} - (N-s)(2r)^2 \sum_{j=1}^{s} \int v_j \cdot \omega_{s+1,j} \times P^{(s+1)}(t, x_1, v_1, \ldots, x_s, v_s, x_j - 2r\omega_{s+1,j}, v_{s+1}) \, \mathrm{d}\omega_{s+1,j} \, \mathrm{d}v_{s+1}, \tag{2.21}$$

where the second term is due to the integration domain depends on x_i.

Putting together I_1 and I_2, (2.17) becomes

$$\partial_t P^{(s)} + \sum_{i=1}^{s} v_i \cdot \nabla_{x_i} P^{(s)} = (N-s)(2r)^2 \sum_{j=1}^{s} \int (v_j - v_{s+1}) \cdot \omega_{s+1,j} \times P^{(s+1)}(t, x_1, v_1, \ldots, x_s, v_s, x_j - 2r\omega_{s+1,j}, v_{s+1}) \, \mathrm{d}\omega_{s+1,j} \, \mathrm{d}v_{s+1}. \tag{2.22}$$

This is the so-called *BBGKY hierarchy for hard spheres* (the equation of P^s depends on P^{s+1}), named after Bogoliubov, Born, Green, Kirkwood, and Yvon. In particular, taking $s = 1$ in (2.22) gives

$$\begin{aligned}
&\partial_t P^{(1)} + v_1 \cdot \nabla_{x_1} P^{(1)} = (N-1)(2r)^2 \int (v_1 - v_2) \cdot \omega_{21} P^{(2)}(t, x_1, v_1, x_1 - 2r\omega_{21}, v_2) \, \mathrm{d}\omega_{21} \, \mathrm{d}v_2 \\
&= (N-1)(2r)^2 \int (v_2 - v_1) \cdot \omega_{12} P^{(2)}(t, x_1, v_1, x_1 + 2r\omega_{12}, v_2) \, \mathrm{d}\omega_{12} \, \mathrm{d}v_2 \\
&= (N-1)(2r)^2 \int_{(v_2 - v_1)\cdot\omega_{12} > 0} |(v_2 - v_1) \cdot \omega_{12}| P^{(2)}(t, x_1, v_1, x_1 + 2r\omega_{12}, v_2) \, \mathrm{d}\omega_{12} \, \mathrm{d}v_2 \\
&\quad - (N-1)(2r)^2 \int_{(v_2 - v_1)\cdot\omega_{12} < 0} |(v_2 - v_1) \cdot \omega_{12}| P^{(2)}(t, x_1, v_1, x_1 + 2r\omega_{12}, v_2) \, \mathrm{d}\omega_{12} \, \mathrm{d}v_2.
\end{aligned} \tag{2.23}$$

This is the same as equation (2.5) with (2.8) and (2.7) derived in the previous section. The rest of the derivation is the same. That is, the first BBGKY hierarchy yields the Boltzmann equation.

It remains to prove (2.21). Note that in the two-particle case,

$$
\begin{aligned}
&v_1 \cdot \nabla_{x_1} \int_{|x_1-x_2|>2r} P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2 \\
=&\lim_{t\to 0}\frac{1}{t}\left[\int_{|x_1+tv_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2 - \int_{|x_1-x_2|>2r} P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\right] \\
=&\lim_{t\to 0}\frac{1}{t}\left[\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2+tv_1,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2 - \int_{|x_1-x_2|>2r} P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\right] \\
=&\lim_{t\to 0}\frac{1}{t}\left[\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2+tv_1,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2 - \int_{|x_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\right] \\
&+\frac{1}{t}\left[\int_{|x_1-x_2|>2r} P^{(2)}(t,x_1+tv_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2 - \int_{|x_1-x_2|>2r} P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2\right] \\
=&\int_{|x_1-x_2|>2r} (v_1\cdot\nabla_{x_2}+v_1\cdot\nabla_{x_1})P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2 \\
=&(2r)^2\int v_1\cdot\omega_{21}P^{(2)}(t,x_1,v_1,x_1-2r\omega_{21},v_2)\,\mathrm{d}\omega_{21}\,\mathrm{d}v_2 + \int v_1\cdot\nabla_{x_1}P^{(2)}(t,x_1,v_1,x_2,v_2)\,\mathrm{d}x_2\,\mathrm{d}v_2.
\end{aligned}
\tag{2.24}
$$

Analogously,

$$
\begin{aligned}
&\sum_{i=1}^{s} v_i\cdot\nabla_{x_i}\int P^{(N)}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}\ldots\,\mathrm{d}x_N\,\mathrm{d}v_N \\
=&\sum_{i=1}^{s}\int\left(\sum_{k=s+1}^{N} v_i\cdot\nabla_{x_k}+v_i\cdot\nabla_{x_i}\right)P^{(N)}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}\ldots\,\mathrm{d}x_N\,\mathrm{d}v_N \\
=&\sum_{i=1}^{s}\Bigg[(N-s)(2r)^2\int v_i\cdot\omega_{s+1,i}P^{(N)}(t,x_1,v_1,\ldots,x_s,v_s,x_i-2r\omega_{s+1,i},v_{s+1},\ldots,x_N,v_N) \\
&\times\mathrm{d}\omega_{s+1,i}\,\mathrm{d}v_{s+1}\,\mathrm{d}x_{s+2}\ldots\,\mathrm{d}x_N\,\mathrm{d}v_N+\int v_i\cdot\nabla_{x_i}P^{(N)}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}\ldots\,\mathrm{d}x_N\,\mathrm{d}v_N\Bigg].
\end{aligned}
\tag{2.25}
$$

This implies

$$
\begin{aligned}
&\sum_{i=1}^{s} v_i\cdot\nabla_{x_i}P^{(s)}-\sum_{i=1}^{s}(N-s)(2r)^2\int v_i\cdot\omega_{s+1,i}P^{(s+1)}(t,x_1,v_1,\ldots,x_s,v_s,x_i-2r\omega_{s+1,i},v_{s+1})\,\mathrm{d}\omega_{s+1,i}\,\mathrm{d}v_{s+1} \\
&=\sum_{i=1}^{s}\int v_i\cdot\nabla_{x_i}P^{(N)}\,\mathrm{d}x_{s+1}\,\mathrm{d}v_{s+1}\ldots\,\mathrm{d}x_N\,\mathrm{d}v_N,
\end{aligned}
\tag{2.26}
$$

which is (2.21).

3 The Boltzmann equation for general (repulsive) intermolecular potentials

We have seen that the Boltzmann equation for hard spheres is given by (2.12) (2.13). Another way of viewing (2.13) is to note that (v', v_*') must lie on the same sphere determined by (v, v_*) (see Figure 3).

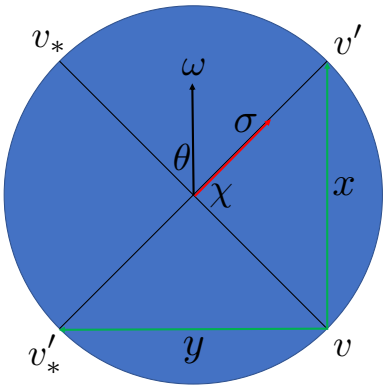

Figure 3: Velocities during a classical elastic collision. ω is the unit vector along the direction of $v' - v$.

To include general interactions other than hard spheres, one can generalize the Boltzmann equation (2.12) as

$$\partial_t f + v \cdot \nabla_x f = \int_{\mathbb{R}^3} \int_{(v-v_*)\cdot\omega<0} B(v - v_*, \omega)[f' f_*' - f f_*] \, \mathrm{d}\omega \, \mathrm{d}v_*. \tag{3.1}$$

Here the function B is called the *collision kernel* and is defined as

$$B(v - v_*, \omega) = |V| \frac{b}{\sin\theta} \left| \frac{\mathrm{d}b}{\mathrm{d}\theta} \right|, \tag{3.2}$$

where $V = v - v_*$ is the relative velocity, $0 < \theta < \pi/2$ is the angle between $-V$ and ω, $b = b(|V|, \theta)$ is the impact parameter (see Figure 4). From the classical scattering theory, we know for hard spheres with radius r,

$$b = 2r \sin\theta. \tag{3.3}$$

Therefore,

$$B = 4r^2 \cos\theta |V| = 4r^2 |V \cdot \omega|, \tag{3.4}$$

i.e., it reduces to the hard sphere case derived before.

Corresponding to the integration over the whole sphere (2.14), we define

$$\partial_t f + v \cdot \nabla_x f = \int_{\mathbb{R}^3} \int_{S^2} B_\omega(|V|, |\cos\theta|)[f' f_*' - f f_*] \, \mathrm{d}\omega \, \mathrm{d}v_*, \tag{3.5}$$

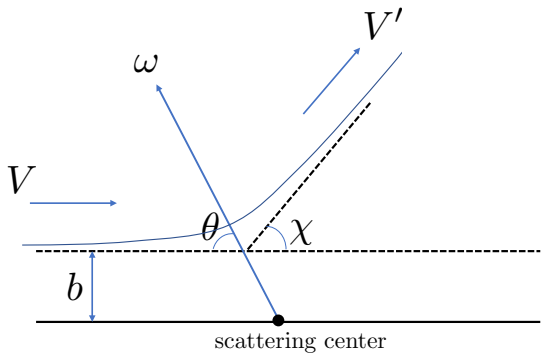

Figure 4: Illustration of particle scattering in a repulsive potential field (notation consistent with Figure 3). b is the impact parameter, χ is the scattering angle, $V = v - v_*$ and $V' = v' - v'_*$.

where

$$B_\omega(|V|, |\cos\theta|) = \frac{1}{2}|V|\frac{b}{\sin\theta}\left|\frac{\mathrm{d}b}{\mathrm{d}\theta}\right|, \tag{3.6}$$

and

$$v' = v - [(v - v_*)\cdot\omega]\omega, \quad v'_* = v_* + [(v - v_*)\cdot\omega]\omega. \tag{3.7}$$

This is what we are going to refer to as the ω-representation.

Another parametrization of the Boltzmann equation that uses the unit vector σ along V' reads

$$\partial_t f + v\cdot\nabla_x f = \int_{\mathbb{R}^3}\int_{S^2} B_\sigma(|V|, \cos\chi)[f'f'_* - ff_*]\,\mathrm{d}\sigma\,\mathrm{d}v_*, \tag{3.8}$$

where

$$B_\sigma(|V|, \cos\chi) = |V|\Sigma(|V|, \chi), \quad \Sigma(|V|, \chi) = \frac{b}{\sin\chi}\left|\frac{\mathrm{d}b}{\mathrm{d}\chi}\right|, \tag{3.9}$$

$\Sigma(|V|, \cos\chi)$ is the *differential cross section* with $0 < \chi < \pi$, and

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2}\sigma, \quad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|}{2}\sigma. \tag{3.10}$$

This is what we are going to refer to as the σ-representation. In particular, the hard sphere collision kernel under this representation reads $B_\sigma(|V|, \cos\chi) = r^2|V|$.

Now for a general (repulsive) intermolecular potential $\phi(r)$ (r is the distance between two particles), b is related to χ implicitly as follows

$$\chi = \pi - 2\int_0^{r_0} \frac{\mathrm{d}r}{\left[1 - r^2 - \frac{4\phi(br^{-1})}{m|V|^2}\right]^{1/2}}, \tag{3.11}$$

where m is the single particle mass, and r_0 is the positive root to the equation

$$1 - r^2 - \frac{4\phi(br^{-1})}{m|V|^2} = 0. \tag{3.12}$$

Let us take a close look of the inverse power law potential

$$\phi(r) = \frac{K}{r^{s-1}}, \quad 2 < s \leq \infty, \quad K \text{ is some positive constant.} \tag{3.13}$$

Then (3.11) becomes

$$\chi = \pi - 2\int_0^{r_0} \frac{\mathrm{d}r}{\left[1 - r^2 - \frac{4Kr^{s-1}}{m|V|^2 b^{s-1}}\right]^{1/2}} = \pi - 2\int_0^{r_0} \frac{\mathrm{d}r}{\left[1 - r^2 - \left(\frac{r}{\beta}\right)^{s-1}\right]^{1/2}}, \tag{3.14}$$

with $\beta := \left(\frac{m|V|^2}{4K}\right)^{\frac{1}{s-1}} b$. Thus the collision kernel B_σ is

$$B_\sigma = |V|\frac{b}{\sin\chi}\left|\frac{\mathrm{d}b}{\mathrm{d}\chi}\right| = |V|\left(\frac{4K}{m|V|^2}\right)^{\frac{2}{s-1}} \frac{\beta}{\sin\chi}\left|\frac{\mathrm{d}\beta}{\mathrm{d}\chi}\right| = \left(\frac{4K}{m}\right)^{\frac{2}{s-1}} |V|^{\frac{s-5}{s-1}} \frac{\beta}{\sin\chi}\left|\frac{\mathrm{d}\beta}{\mathrm{d}\chi}\right|. \tag{3.15}$$

Since β can be solved implicitly from (3.14) to yield $\beta = \beta(\chi)$, (3.15) implies that

$$B_\sigma = b_s(\cos\chi)|V|^{\frac{s-5}{s-1}}, \quad b_s(\cos\chi) = \left(\frac{4K}{m}\right)^{\frac{2}{s-1}} \frac{\beta}{\sin\chi}\left|\frac{\mathrm{d}\beta}{\mathrm{d}\chi}\right|. \tag{3.16}$$

When $s = 5$, B_σ is a function of χ only which will lead to many simplifications (usually referred to as Maxwell molecules). The hard sphere kernel can be considered as a special case of (3.16) when $s = \infty$. Furthermore, (3.16) shows that the velocity dependence in the collision kernel behaves like $|V|^{\frac{s-5}{s-1}+2}$. When $|V|$ is small, this is integrable if $\frac{s-5}{s-1} + 2 > -1$, i.e. $s > 2$. Note that $s = 2$ corresponds to the Coulomb potential. Therefore, the Boltzmann equation should not be used to describe the Coulomb interaction[1].

Based on (3.16), it is common in the kinetic literature to distinguish the kernel by its velocity dependence:

$$B_\sigma = b_\lambda(\cos\chi)|V|^\lambda, \quad -3 < \lambda \leq 1, \tag{3.17}$$

where $\lambda > 0$ is called the *hard potential*, $\lambda < 0$ is the *soft potential*, and $\lambda = 0$ is the *Maxwell kernel*.

Let us analyze a bit the asymptotic behavior of χ w.r.t. β. When $\beta \ll 1$, (3.14) can be approximated as

$$\chi \approx \pi - 2\int_0^{\beta} \frac{\mathrm{d}r}{\left[1 - \left(\frac{r}{\beta}\right)^{s-1}\right]^{1/2}} = \pi - 2\beta\int_0^1 \frac{\mathrm{d}u}{(1-u^{s-1})^{1/2}} = \pi - 2\beta A(s), \tag{3.18}$$

[1]In this limit, one should consider the so-called Landau operator which is a diffusive type operator. We will come back to this later in the course.

so when $\beta \to 0$, $\chi \to \pi$, and $\beta \left| \frac{\mathrm{d}\beta}{\mathrm{d}\chi} \right|$ is well behaved. When $\beta \gg 1$, (3.14) can be approximated as

$$\chi \approx \pi - 2 \int_0^1 \frac{1 + \frac{1}{2}(1-r^2)^{-1} \left(\frac{r}{\beta}\right)^{s-1}}{(1-r^2)^{1/2}} \, \mathrm{d}r = \frac{A(s)}{\beta^{s-1}}, \tag{3.19}$$

so when $\beta \to \infty$, $\chi \to 0$, and

$$\beta \left| \frac{\mathrm{d}\beta}{\mathrm{d}\chi} \right| \sim \chi^{-\frac{2}{s-1}-1}, \tag{3.20}$$

i.e., the collision kernel contains a nonintegrable singularity at $\chi = 0$ for all $s > 2$ (except $s = \infty$). This can be avoided either by cutting off β, so that the potential ϕ is zero for large β, or by the less physical, but mathematically more tractable, method of directly cutting off χ near 0, that is, eliminating grazing collisions from the collision term. This is the so-called *Grad's angular cut-off* assumption.

4 Basic properties of the Boltzmann equation

In this section, we derive some basic properties of the Boltzmann equation, which we rewrite here for clarity[2]:

$$\partial_t f + v \cdot \nabla_x f = Q(f,f), \quad x \in \Omega \subset \mathbb{R}^d, \quad v \in \mathbb{R}^d, \quad d \geq 2, \tag{4.1}$$

where f is the number distribution function, $Q(f,f)$ is the so-called *collision operator*, which is a quadratic integral operator acting only in the velocity space. In fact, it is convenient to introduce a bilinear form of Q as (in both σ- and ω- representations):

$$\begin{aligned} Q(g,f)(v) &= \int_{\mathbb{R}^d} \int_{S^{d-1}} B_\sigma(|v-v_*|, \cos\chi)[g'_* f' - g_* f] \, \mathrm{d}\sigma \, \mathrm{d}v_* \\ &= \int_{\mathbb{R}^d} \int_{S^{d-1}} B_\omega(|v-v_*|, |\cos\theta|)[g'_* f' - g_* f] \, \mathrm{d}\omega \, \mathrm{d}v_*, \end{aligned} \tag{4.2}$$

where

$$v' = \frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma, \quad v'_* = \frac{v+v_*}{2} - \frac{|v-v_*|}{2}\sigma, \quad \cos\chi = \sigma \cdot \widehat{(v-v_*)}, \tag{4.3}$$

$$v' = v - [(v-v_*)\cdot\omega]\omega, \quad v'_* = v_* + [(v-v_*)\cdot\omega]\omega, \quad |\cos\theta| = |\omega \cdot \widehat{(v-v_*)}|. \tag{4.4}$$

Note that the physically relevant case is the dimension $d = 3$ as we considered in previous sections. Here we assume $d \geq 2$ for mathematical generality.

We first derive a very important formula of the collision operator using the ω-representation.

[2]We have deliberately ignored the forcing term like $F(x) \cdot \nabla_v f$ in the discussion so far. With this term, the equation is the so-called Vlasov equation. We will come back to this later in the course.

Proposition 4.1. *(Boltzmann's lemma) For any functions $\varphi(v)$, $f(v)$ such that the integrals make sense, one has*

$$\begin{aligned}\int_{\mathbb{R}^d} Q(f,f)\varphi \,\mathrm{d}v &= \frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - ff_*][\varphi+\varphi_*-\varphi'-\varphi'_*]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\ &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)ff_*[\varphi'-\varphi]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_*.\end{aligned} \tag{4.5}$$

Proof.

$$\begin{aligned}\int_{\mathbb{R}^d} Q(f,f)\varphi \,\mathrm{d}v &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - ff_*]\varphi\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\ &= \int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - ff_*]\varphi_*\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\ &= \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - ff_*][\varphi+\varphi_*]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\ &= \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[ff_* - f'f'_*][\varphi'+\varphi'_*]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \\ &= \frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega(|v-v_*|,|\cos\theta|)[f'f'_* - ff_*][\varphi+\varphi_*-\varphi'-\varphi'_*]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_*,\end{aligned} \tag{4.6}$$

where in the second line we swapped v and v_* (hence v' and v'_*); in the fourth line we changed (v, v_*) to (v', v'_*) (hence (v', v'_*) becomes (v, v_*)) for a fixed ω and used the fact that $\mathrm{d}v\,\mathrm{d}v_* = \mathrm{d}v'\,\mathrm{d}v'_*$ (the transform has the unit Jacobian).

The second equality in (4.5) is obtained by changing (v, v_*) to (v', v'_*) only to the gain term. □

4.1 Collision invariants and local conservation laws

Definition 4.2. *A collision invariant is a continuous function $\varphi = \varphi(v)$ such that for each $v, v_* \in \mathbb{R}^d$ and $\omega \in S^{d-1}$, one has*

$$\varphi + \varphi_* = \varphi' + \varphi'_*. \tag{4.7}$$

Since during collisions, mass, momentum and energy are conserved, it is obvious that functions 1, v, and $|v|^2$, and any linear combination of them are the collision invariants. In fact, it can be shown that these are the *only* collision invariants (this is a non-trivial result, for proof one may refer to [9, p. 36-42]).

Using the Boltzmann's lemma, it is clear that

Corollary 4.3.

$$\int_{\mathbb{R}^d} Q(f,f)\,\mathrm{d}v = \int_{\mathbb{R}^d} Q(f,f)v\,\mathrm{d}v = \int_{\mathbb{R}^d} Q(f,f)|v|^2\,\mathrm{d}v = 0. \tag{4.8}$$

Using the Corollary 4.3, if we multiply the Boltzmann equation (4.1) by m, mv, $m|v|^2/2$, and integrate w.r.t. v, we obtain

$$\begin{cases} \partial_t \displaystyle\int_{\mathbb{R}^d} mf \,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^d} mvf \,\mathrm{d}v = 0, \\ \partial_t \displaystyle\int_{\mathbb{R}^d} mvf \,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^d} mv \otimes vf \,\mathrm{d}v = 0, \\ \partial_t \displaystyle\int_{\mathbb{R}^d} \frac{1}{2} m|v|^2 f \,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^d} \frac{1}{2} mv|v|^2 f \,\mathrm{d}v = 0. \end{cases} \tag{4.9}$$

These are the local *conservation laws* (conservation of mass, momentum, and energy).

To better view the connection of f (number distribution function) and macroscopic quantities such as density, temperature, etc., let us define

$$n = \int_{\mathbb{R}^d} f \,\mathrm{d}v, \quad \rho = mn, \quad u = \frac{1}{n} \int_{\mathbb{R}^d} vf \,\mathrm{d}v, \tag{4.10}$$

where n is the *number density*, ρ is the *mass density*, and u is the *bulk velocity*. Further, with the *peculiar velocity*

$$c = v - u, \tag{4.11}$$

we define

$$T = \frac{1}{dnR} \int_{\mathbb{R}^d} |c|^2 f \,\mathrm{d}v, \quad \mathbb{P} = \int_{\mathbb{R}^d} mc \otimes cf \,\mathrm{d}v, \quad q = \int_{\mathbb{R}^d} \frac{1}{2} mc|c|^2 f \,\mathrm{d}v, \tag{4.12}$$

where T is the *temperature*, $\mathbb{P}$ is the *stress tensor*, and q is the *heat flux vector*. $R = k_B/m$ is the gas constant (k_B is the Boltzmann's constant).

Finally, the *pressure* p is defined as

$$p = \frac{1}{d} \mathrm{tr}(\mathbb{P}) = \rho RT. \tag{4.13}$$

With the above definitions, we can recast the local conservation laws (4.9) using macroscopic quantities:

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho u) = 0, \\ \partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + \mathbb{P}) = 0, \\ \partial_t E + \nabla_x \cdot (Eu + \mathbb{P}u + q) = 0, \end{cases} \tag{4.14}$$

where $E = \frac{d}{2}\rho RT + \frac{1}{2}\rho u^2$ is the total energy. The system (4.14) is completely equivalent to (4.9), hence to the Boltzmann equation. Note that this system is not closed because $\mathbb{P}$ and q, generally speaking, cannot be represented in terms of ρ, u, and T.

4.2 Boltzmann's H-theorem and Maxwellian

Proposition 4.4. *(Boltzmann's H-theorem)*

$$\int_{\mathbb{R}^d} Q(f,f)\ln f \,\mathrm{d}v \le 0, \tag{4.15}$$

and the equality holds if and only if $f = \exp(a + b\cdot v + c|v|^2)$.

Proof. Taking $\varphi = \ln f$ in the Boltzmann's lemma yields

$$\int_{\mathbb{R}^d} Q(f,f)\ln f \,\mathrm{d}v = -\frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega[f'f'_* - ff_*][\ln(f'f'_*) - \ln(ff_*)]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_* \le 0, \tag{4.16}$$

where the inequality is due to $\ln x$ is a monotonically increasing function, so $(x-y)(\ln x - \ln y) \ge 0$ for any $x, y > 0$. The equality holds iff $\ln f$ is a collision invariant, i.e., $f = \exp(a + b\cdot v + c|v|^2)$, with a, b, c being some constants. □

If a function f is of the form $\exp(a + b\cdot v + c|v|^2)$, it can be rewritten as

$$f = \exp\left(c\left|v + \frac{b}{2c}\right|^2 - \frac{|b|^2}{4c} + a\right). \tag{4.17}$$

For f to be integrable, c must be negative. Choosing $c' = -c$, $b' = -\frac{b}{2c}$, $a' = \exp(-\frac{|b|^2}{4c} + a)$ gives

$$f = a'\exp(-c'|v - b'|^2). \tag{4.18}$$

Using the definition of n, u and T given in the previous section, we can see that[3]

$$f = \frac{n}{(2\pi RT)^{d/2}}\exp\left(-\frac{|v-u|^2}{2RT}\right) := \mathcal{M}. \tag{4.19}$$

(4.19) is called the *Maxwellian*.

Corollary 4.5. *The following statements are equivalent.*

$$\int_{\mathbb{R}^d} Q(f,f)\ln f \,\mathrm{d}v = 0 \iff f = \mathcal{M} \iff Q(f,f) = 0. \tag{4.20}$$

Corollary 4.6.

$$\partial_t \int_{\mathbb{R}^d} f\ln f \,\mathrm{d}v + \nabla_x \cdot \int_{\mathbb{R}^d} vf\ln f \,\mathrm{d}v = -D(f) \le 0, \tag{4.21}$$

where

$$D(f) = \frac{1}{4}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\int_{S^{d-1}} B_\omega[f'f'_* - ff_*][\ln(f'f'_*) - \ln(ff_*)]\,\mathrm{d}\omega\,\mathrm{d}v\,\mathrm{d}v_*. \tag{4.22}$$

[3]Note the Gaussian integrals $\int_{-\infty}^{\infty} e^{-\alpha v^2}\,\mathrm{d}v = \left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}}$, $\int_{-\infty}^{\infty} v^2 e^{-\alpha v^2}\,\mathrm{d}v = \frac{1}{2\alpha}\left(\frac{\pi}{\alpha}\right)^{\frac{1}{2}}$.

If we assume f decays fast enough as $x \to \infty$, or is periodic in x, then (4.21) upon further integration in x yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(t) \leq 0, \tag{4.23}$$

where $\mathcal{H}(t) := \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} f \ln f \,\mathrm{d}v\,\mathrm{d}x$ is the *H function*. (4.23) shows that $\mathcal{H}$ is always non-increasing and reaches its minimum value iff f reaches the Maxwellian (local equilibrium). This is consistent to the second law of thermodynamics.

4.3 Boundary condition

The commonly used boundary condition for the Boltzmann equation consists of the following: for a boundary point $x \in \partial\Omega$ and outward pointing normal $n(x)$,

- Maxwell diffusive boundary:

$$f(t,x,v) = \rho_w(t,x) f_w(t,x,v), \quad (v-u_w)\cdot n < 0, \tag{4.24}$$

  with

$$f_w(t,x,v) = \exp\left(-\frac{|v-u_w|^2}{2RT_w}\right), \tag{4.25}$$

  where $u_w(t,x)$ and $T_w(t,x)$ are the wall velocity and temperature. $\rho_w(t,x)$ is determined by

$$\rho_w(t,x) = -\frac{\int_{(v-u_w)\cdot n\geq 0}(v-u_w)\cdot n f \,\mathrm{d}v}{\int_{(v-u_w)\cdot n<0}(v-u_w)\cdot n f_w \,\mathrm{d}v}. \tag{4.26}$$

- Reflective boundary:

$$f(t,x,v) = f(t,x,v-2[(v-u_w)\cdot n]n), \quad (v-u_w)\cdot n < 0. \tag{4.27}$$

- Inflow boundary:

$$f(t,x,v) = g(t,x,v), \quad (v-u_w)\cdot n < 0, \tag{4.28}$$

  where $g(t,x,v)$ is the prescribed function.

5 Fluid limits of the Boltzmann equation

We have seen how the Boltzmann equation can be derived from the N-body particle system under the Boltzmann-Grad limit. Let us now see how the Boltzmann equation can be connected to macroscopic fluid equations. To this end, we need to introduce a proper scaling, hence nondimensionalization of the equation (4.1) is needed. For more discussion of the topics in this section, the readers are referred to [3] or [6, Chapter 2.2].

5.1 Nondimensionalization of the Boltzmann equation

Let us choose first macroscopic scales of length x_0 and time t_0, and a reference temperature T_0. This defines two distinct velocity scales: x_0/t_0 is the macroscopic velocity, $v_0 = \sqrt{RT_0}$ is the thermal speed. In addition, we define the reference number density $n_0 = N/x_0^d$. We then rescale t, x, v and f as follows:

$$\hat{t} = \frac{t}{t_0}, \quad \hat{x} = \frac{x}{x_0}, \quad \hat{v} = \frac{v}{v_0}, \quad \hat{f} = \frac{f}{n_0/v_0^d}. \tag{5.1}$$

The collision kernel, according to the hard sphere case, can be rescaled as

$$\hat{B} = \frac{B}{\sqrt{2}\pi v_0 d_0^{d-1}}, \tag{5.2}$$

where d_0 is the reference diameter of the particle. Then the equation (4.1) becomes

$$\frac{1}{t_0}\partial_{\hat{t}}\hat{f} + \frac{v_0}{x_0}\hat{v}\cdot\nabla_{\hat{x}}\hat{f} = \left(\frac{n_0}{v_0^d}\right)(\sqrt{2}\pi v_0 d_0^{d-1})v_0^d\hat{Q}(\hat{f},\hat{f}), \tag{5.3}$$

i.e.,

$$\frac{x_0}{v_0 t_0}\partial_{\hat{t}}\hat{f} + \hat{v}\cdot\nabla_{\hat{x}}\hat{f} = \sqrt{2}\pi n_0 x_0 d_0^{d-1}\hat{Q}(\hat{f},\hat{f}). \tag{5.4}$$

The factor

$$\frac{x_0}{v_0 t_0} = \frac{\frac{x_0}{t_0}}{v_0} := \mathrm{St} \tag{5.5}$$

is the ratio of the macroscopic velocity and thermal speed, which is called the *kinetic Strouhal number*. The factor

$$\frac{1}{\sqrt{2}\pi n_0 x_0 d_0^{d-1}} = \frac{\frac{x_0^d}{\sqrt{2}\pi N d_0^{d-1}}}{x_0} := \mathrm{Kn} \tag{5.6}$$

is the ratio of the mean free path and macroscopic length scale, which is called the *Knudsen number*. Kn characterizes the degree of rarefaction of the system.

Therefore, the Boltzmann equation in dimensionless form reads as (dropping $\hat{}$ for simplicity)

$$\mathrm{St}\,\partial_t f + v\cdot\nabla_x f = \frac{1}{\mathrm{Kn}}Q(f,f). \tag{5.7}$$

Accordingly, we rescale the macroscopic quantities as

$$\hat{n} = \frac{n}{n_0}, \quad \hat{\rho} = \frac{\rho}{mn_0}, \quad \hat{u} = \frac{u}{v_0}, \quad \hat{T} = \frac{T}{T_0}, \quad \hat{\mathbb{P}} = \frac{\mathbb{P}}{mn_0 v_0^2}, \quad \hat{q} = \frac{q}{mn_0 v_0^3}, \tag{5.8}$$

then in rescaled variables (again dropping $\hat{}$ for simplicity),

$$n = \rho = \int_{\mathbb{R}^d} f\,\mathrm{d}v, \quad u = \frac{1}{\rho}\int_{\mathbb{R}^d} vf\,\mathrm{d}v, \quad c = v - u, \tag{5.9}$$

$$T = \frac{1}{d\rho}\int_{\mathbb{R}^d}|c|^2 f\,\mathrm{d}v, \quad \mathbb{P} = \int_{\mathbb{R}^d} c\otimes cf\,\mathrm{d}v, \quad q = \int_{\mathbb{R}^d}\frac{1}{2}c|c|^2 f\,\mathrm{d}v, \tag{5.10}$$

$$p = \rho T, \quad E = \frac{d}{2}\rho T + \frac{1}{2}\rho u^2, \tag{5.11}$$

and the Maxwellian is

$$\mathcal{M} = \frac{\rho}{(2\pi T)^{d/2}} \exp\left(-\frac{|v-u|^2}{2T}\right). \tag{5.12}$$

We will derive the compressible Euler and Navier-Stokes limits of the Boltzmann equation in the following, for which we assume

$$\mathrm{St} = 1, \quad \mathrm{Kn} = \varepsilon \ll 1. \tag{5.13}$$

Then (5.7) can be written as

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f). \tag{5.14}$$

5.2 Compressible Euler limit

In (5.14), let $\varepsilon \to 0$, formally we have $Q(f, f) \to 0$. By Corollary 4.5, this implies $f \to \mathcal{M}$. If $f = \mathcal{M}$, we have

$$\mathbb{P} = \int_{\mathbb{R}^d} c \otimes c\mathcal{M} \, \mathrm{d}v = \rho T \, \mathrm{Id} = p\mathrm{Id}, \quad q = \int_{\mathbb{R}^d} \frac{1}{2} c|c|^2 \mathcal{M} \, \mathrm{d}v = 0, \tag{5.15}$$

where Id is the identity matrix. Therefore, the local conservation law (4.14) becomes

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho u) = 0, \\ \partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + p \, \mathrm{Id}) = 0, \\ \partial_t E + \nabla_x \cdot ((E + p)u) = 0. \end{cases} \tag{5.16}$$

This is the well-known compressible Euler equation.

5.3 Compressible Navier-Stokes limit

Compared to the Euler limit, derivation of the Navier-Stokes limit of the Boltzmann equation is much more involved and can be done via the so-called *Chapman-Enskog expansion*. We will also need the linearized collision operator which we introduce below.

5.3.1 Linearized Boltzmann collision operator

If we are interested in the behavior of the collision operator around the local Maxwellian (5.12), we can expand it as

$$Q(\mathcal{M}(1+f), \mathcal{M}(1+f)) = Q(\mathcal{M}, \mathcal{M}) + [Q(\mathcal{M}, \mathcal{M}f) + Q(\mathcal{M}f, \mathcal{M})] + Q(\mathcal{M}f, \mathcal{M}f). \tag{5.17}$$

The *linearized Boltzmann collision operator* is defined as

$$L_{\mathcal{M}} f = \frac{1}{\mathcal{M}} [Q(\mathcal{M}, \mathcal{M}f) + Q(\mathcal{M}f, \mathcal{M})], \tag{5.18}$$

which, written out explicitly, reads

$$
\begin{aligned}
L_{\mathcal{M}} f &= \frac{1}{\mathcal{M}} \int_{\mathbb{R}^d} \int_{S^{d-1}} B_\omega(|v-v_*|, |\cos\theta|)[\mathcal{M}'\mathcal{M}'_* f'_* + \mathcal{M}'_*\mathcal{M}' f' - \mathcal{M}\mathcal{M}_* f_* - \mathcal{M}_*\mathcal{M} f] \,\mathrm{d}\omega \,\mathrm{d}v_* \\
&= \int_{\mathbb{R}^d} \int_{S^{d-1}} B_\omega(|v-v_*|, |\cos\theta|)[f' + f'_* - f - f_*]\mathcal{M}_* \,\mathrm{d}\omega \,\mathrm{d}v_* \\
&= \int_{\mathbb{R}^d} \int_{S^{d-1}} B_\omega(|v-v_*|, |\cos\theta|)[f' + f'_* - f_*]\mathcal{M}_* \,\mathrm{d}\omega \,\mathrm{d}v_* \\
&\quad - \int_{\mathbb{R}^d} \int_{S^{d-1}} B_\omega(|v-v_*|, |\cos\theta|)\mathcal{M}_* \,\mathrm{d}\omega \,\mathrm{d}v_* f := K_{\mathcal{M}}(f)(v) - \nu_{\mathcal{M}}(v) f(v),
\end{aligned}
\tag{5.19}
$$

where we used $\mathcal{M}\mathcal{M}_* = \mathcal{M}'\mathcal{M}'_*$.

Proposition 5.1. *Define the weighted inner product $\langle f, g\rangle_{\mathcal{M}} = \int_{\mathbb{R}^d} fg\mathcal{M} \,\mathrm{d}v$. Then the linearized collision operator satisfies*

(a) $\langle L_{\mathcal{M}} f, g\rangle_{\mathcal{M}} = \langle f, L_{\mathcal{M}} g\rangle_{\mathcal{M}}$ *(self-adjoint).*

(b) $\langle L_{\mathcal{M}} f, f\rangle_{\mathcal{M}} \le 0$ *(nonpositive).*

(c) $\langle L_{\mathcal{M}} f, f\rangle_{\mathcal{M}} = 0 \Longleftrightarrow f = a + b\cdot v + c|v|^2 \Longleftrightarrow L_{\mathcal{M}} f = 0.$

Proof. Start with the obvious equality

$$
\begin{aligned}
&\langle L_{\mathcal{M}} f, g\rangle_{\mathcal{M}} = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \int_{S^{d-1}} B_\omega(|v-v_*|, |\cos\theta|)[f' + f'_* - f - f_*] g\mathcal{M}\mathcal{M}_* \,\mathrm{d}\omega \,\mathrm{d}v \,\mathrm{d}v_* \\
&= -\frac{1}{4} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \int_{S^{d-1}} B_\omega(|v-v_*|, |\cos\theta|)[f' + f'_* - f - f_*][g' + g'_* - g - g_*]\mathcal{M}\mathcal{M}_* \,\mathrm{d}\omega \,\mathrm{d}v \,\mathrm{d}v_* \\
&= \langle f, L_{\mathcal{M}} g\rangle_{\mathcal{M}},
\end{aligned}
\tag{5.20}
$$

where the second line is obtained following exactly the same procedure as we proved the Boltzmann's lemma (Proposition 4.1). Taking $g = f$ in the above equation, it is clear

$$
\langle L_{\mathcal{M}} f, f\rangle_{\mathcal{M}} = -\frac{1}{4} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \int_{S^{d-1}} B_\omega(|v-v_*|, |\cos\theta|)[f' + f'_* - f - f_*]^2 \mathcal{M}\mathcal{M}_* \,\mathrm{d}\omega \,\mathrm{d}v \,\mathrm{d}v_* \le 0,
\tag{5.21}
$$

and the equality holds iff $f' + f'_* - f - f_* = 0$, then part (c) is straightforward. □

The above proposition implies that the spectrum of the linear operator $L_{\mathcal{M}}$ is nonpositive, and eigenvalue zero is a common eigenvalue of eigenfunctions 1, v, $|v|^2$. In fact, for Maxwell molecules, the complete eigenvalues/eigenfunctions are known.

If the collision kernel $B_\omega(|v-v_*|, |\cos\theta|)$ is a hard cut-off kernel, one can show that $L_{\mathcal{M}}$ is a Fredholm operator. Then $R(L_{\mathcal{M}}) = \ker(L^*_{\mathcal{M}})^\perp$. By self-adjointness of $L_{\mathcal{M}}$, we have $R(L_{\mathcal{M}}) = \ker(L_{\mathcal{M}})^\perp$ (note that $\ker(L_{\mathcal{M}}) = \mathrm{span}\{1, v, |v|^2\}$, then $f \in$

$\ker(L_{\mathcal{M}})^{\perp} \iff \int_{\mathbb{R}^d} f(1, v, |v|^2)^T \mathcal{M}\,\mathrm{d}v = 0)$. Therefore, $L_{\mathcal{M}}$ admits a pseudoinverse from $\ker(L_{\mathcal{M}})^{\perp}$ to $\ker(L_{\mathcal{M}})^{\perp}$, and is denoted by $L_{\mathcal{M}}^{-1}$. Furthermore, consider

$$A(v) = v \otimes v - \frac{1}{d}|v|^2 \mathrm{Id}, \quad B(v) = \left(\frac{|v|^2}{2} - \frac{d+2}{2}\right) v, \tag{5.22}$$

one has

$$\begin{aligned} L_{\mathcal{M}}^{-1} A\left(\frac{v-u}{\sqrt{T}}\right) &= -\frac{1}{\rho}\alpha\left(T, \frac{v-u}{\sqrt{T}}\right) A\left(\frac{v-u}{\sqrt{T}}\right), \\ L_{\mathcal{M}}^{-1} B\left(\frac{v-u}{\sqrt{T}}\right) &= -\frac{1}{\rho}\beta\left(T, \frac{v-u}{\sqrt{T}}\right) B\left(\frac{v-u}{\sqrt{T}}\right), \end{aligned} \tag{5.23}$$

where α and β are some scalar functions.

5.3.2 Chapman-Enskog expansion

From the Euler limit, it is clear that as $\varepsilon \to 0$, $f \to \mathcal{M}$. Hence we write f as

$$f = \mathcal{M} + \varepsilon g, \tag{5.24}$$

where $g = O(1)$ is the remainder. Furthermore, we know

$$\int_{\mathbb{R}^d} f(1, v, |v|^2/2)^T \,\mathrm{d}v = \int_{\mathbb{R}^d} \mathcal{M}(1, v, |v|^2/2)^T \,\mathrm{d}v = (\rho, \rho u, E)^T, \tag{5.25}$$

which implies $g/\mathcal{M} \in \ker(L_{\mathcal{M}})^{\perp}$.

Substituting (5.24) into (5.14) yields

$$\partial_t f + v \cdot \nabla_x f = \mathcal{M} L_{\mathcal{M}}\left(\frac{g}{\mathcal{M}}\right) + \varepsilon Q(g, g), \tag{5.26}$$

that is,

$$\begin{aligned} g &= \mathcal{M} L_{\mathcal{M}}^{-1}\left(\frac{1}{\mathcal{M}}(\partial_t f + v \cdot \nabla_x f)\right) + O(\varepsilon) \\ &= \mathcal{M} L_{\mathcal{M}}^{-1}\left(\frac{1}{\mathcal{M}}(\partial_t \mathcal{M} + v \cdot \nabla_x \mathcal{M})\right) + O(\varepsilon), \end{aligned} \tag{5.27}$$

where we used (5.24) in the second line.

On the other hand, substituting (5.24) into the local conservation law (4.14) yields

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho u) = 0, \\ \partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + p\,\mathrm{Id}) = \varepsilon \nabla_x \cdot \mathbb{P}^{(1)}, \\ \partial_t E + \nabla_x \cdot ((E+p)u) = \varepsilon \nabla_x \cdot \left(\mathbb{P}^{(1)} u + q^{(1)}\right), \end{cases} \tag{5.28}$$

where

$$\mathbb{P}^{(1)} := -\int_{\mathbb{R}^d} (v-u) \otimes (v-u) g \,\mathrm{d}v, \quad q^{(1)} := -\int_{\mathbb{R}^d} \frac{1}{2}(v-u)|v-u|^2 g \,\mathrm{d}v. \tag{5.29}$$

The remaining task is to evaluate $\mathbb{P}^{(1)}$ and $q^{(1)}$ using (5.27).

First of all, for the Maxwellian function defined in (5.12), it is easy to see

$$\mathrm{d}\mathcal{M} = \mathcal{M}\left[\frac{1}{\rho}\,\mathrm{d}\rho + \frac{(v-u)}{T}\cdot\,\mathrm{d}u + \left(\frac{|v-u|^2}{2T^2} - \frac{d}{2T}\right)\mathrm{d}T\right]. \tag{5.30}$$

Then,

$$\begin{aligned}\frac{1}{\mathcal{M}}(\partial_t\mathcal{M} + v\cdot\nabla_x\mathcal{M}) =& \frac{1}{\rho}(\partial_t\rho + v\cdot\nabla_x\rho) + \frac{(v-u)}{T}\cdot(\partial_t u + v\cdot\nabla_x u)\\ &+ \left(\frac{|v-u|^2}{2T^2} - \frac{d}{2T}\right)(\partial_t T + v\cdot\nabla_x T).\end{aligned} \tag{5.31}$$

Since we already knew that ρ, u, and T satisfy the compressible Euler equations to the leading order, we could use the spatial derivatives of these functions to replace their time derivatives which gives

$$\begin{aligned}\frac{1}{\mathcal{M}}(\partial_t\mathcal{M} + v\cdot\nabla_x\mathcal{M}) =& \left(\frac{|v-u|^2}{2T} - \frac{d+2}{2}\right)\frac{(v-u)\cdot\nabla_x T}{T}\\ &+ \frac{1}{2}\left(\frac{(v-u)\otimes(v-u)}{T} - \frac{|v-u|^2}{dT}\mathrm{Id}\right) : \sigma(u) + O(\varepsilon),\end{aligned} \tag{5.32}$$

with

$$\sigma(u) = \nabla_x u + (\nabla_x u)^T - \frac{2}{d}(\nabla_x\cdot u)\mathrm{Id}, \tag{5.33}$$

where $\nabla_x u$ is a matrix with ij-th component given by $\frac{\partial u_i}{\partial x_j}$ and the operation : between two matrices is defined as $A : B = \sum_{ij} a_{ij}b_{ij}$.

Then

$$\begin{aligned}&L_{\mathcal{M}}^{-1}\left(\frac{1}{\mathcal{M}}(\partial_t\mathcal{M} + v\cdot\nabla_x\mathcal{M})\right)\\ =&\frac{1}{2}L_{\mathcal{M}}^{-1}\left(\frac{(v-u)\otimes(v-u)}{T} - \frac{|v-u|^2}{dT}\mathrm{Id}\right) : \sigma(u) + L_{\mathcal{M}}^{-1}\left(\left(\frac{|v-u|^2}{2T} - \frac{d+2}{2}\right)\frac{(v-u)}{\sqrt{T}}\right)\cdot\frac{\nabla_x T}{\sqrt{T}} + O(\varepsilon)\\ =&-\frac{1}{\rho}\alpha\left(T, \frac{v-u}{\sqrt{T}}\right)\frac{1}{2}A\left(\frac{v-u}{\sqrt{T}}\right) : \sigma(u) - \frac{1}{\rho}\beta\left(T, \frac{v-u}{\sqrt{T}}\right)B\left(\frac{v-u}{\sqrt{T}}\right)\cdot\frac{\nabla_x T}{\sqrt{T}} + O(\varepsilon),\end{aligned} \tag{5.34}$$

where we used the property of the linearized collision operator introduced in the previous section.

To sum up, we have obtained

$$g = -\frac{\mathcal{M}}{\rho}\alpha\left(T, \frac{v-u}{\sqrt{T}}\right)\frac{1}{2}A\left(\frac{v-u}{\sqrt{T}}\right) : \sigma(u) - \frac{\mathcal{M}}{\rho}\beta\left(T, \frac{v-u}{\sqrt{T}}\right)B\left(\frac{v-u}{\sqrt{T}}\right)\cdot\frac{\nabla_x T}{\sqrt{T}} + O(\varepsilon). \tag{5.35}$$

It is interesting to note that g does not depend on ρ.

Finally, substituting (5.35) into (5.29), one can find that

$$\mathbb{P}^{(1)} = \mu(T)\sigma(u) + O(\varepsilon), \quad q^{(1)} = \kappa(T)\nabla_x T + O(\varepsilon), \tag{5.36}$$

with

$$\sigma(u) = \nabla_x u + (\nabla_x u)^T - \frac{2}{d}(\nabla_x \cdot u)\mathrm{Id}, \tag{5.37}$$

where μ and κ are some non-negative functions of T only. Indeed, for Maxwell molecules, $\mu \sim T$; and for hard spheres, $\mu \sim \sqrt{T}$. μ is called the dynamic viscosity and κ is the thermal conductivity.

Plugging (5.36) into (5.28) and dropping $O(\varepsilon^2)$ terms yields

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho u) = 0, \\ \partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + p\,\mathrm{Id}) = \varepsilon \nabla_x \cdot (\mu \sigma(u)), \\ \partial_t E + \nabla_x \cdot ((E+p)u) = \varepsilon \nabla_x \cdot (\mu \sigma(u) u + \kappa \nabla_x T)\,, \end{cases} \tag{5.38}$$

which is the well-known compressible Navier-Stokes equation.

Remark 5.2. *One can also continue the same procedure to go beyond the second-order expansion. This will yield the Burnett and super Burnett equations, which are generally unstable hence less used in practice.*

Remark 5.3. *Incompressible fluid limits of the Boltzmann equation can be derived in a similar fashion by assuming a different scaling: $St = \varepsilon$, $Kn = \varepsilon$.*

6 Other kinetic models/equations and a brief summary of mathematical theory

6.1 The BGK model and its variants

Due to the complicated structure of the Boltzmann collision operator, various simpler kinetic models have been proposed to mimic its properties. One of the most popular models was introduced by Bhatnagar, Gross, and Krook [4]:

$$\partial_t f + v \cdot \nabla_x f = Q^{\mathrm{BGK}}(f), \tag{6.1}$$

with

$$Q^{\mathrm{BGK}}(f) = \nu(\mathcal{M}[f] - f), \tag{6.2}$$

where $\mathcal{M}[f]$ is the Maxwellian (4.19) (with $d = 3$) and ν is the collision frequency given by $\nu = p/\mu$ ($p = \rho RT$ is the pressure, μ is the dynamic viscosity which is a function of T).

It is easy to check that the BGK operator conserves mass, momentum and energy as the Boltzmann operator (Corollary 4.3). It also satisfies the H-theorem (Proposition 4.4). Following the same procedure as in Section 5, one can also derive the compressible Euler and Navier-Stokes equations as its fluid limits. However, the resulting

coefficient κ is not satisfactory: the Prandtl number ($\mathrm{Pr} := c_p\mu/\kappa$, c_p is the specific heat) in the BGK model is $\mathrm{Pr} \equiv 1$, which is inconsistent to the Boltzmann equation or experiments (in many gases $\mathrm{Pr} < 1$).

To correct this defect, the so-called ES-BGK model was introduced by Holway [26], in which the Maxwellian is replaced by a general Gaussian distribution:

$$Q^{\mathrm{ESBGK}}(f) = \mathrm{Pr}\nu(\mathcal{G}[f] - f), \tag{6.3}$$

where

$$\mathcal{G}[f] = \frac{n}{\sqrt{\det(2\pi R\mathbb{T})}} \exp\left(-\frac{1}{2R}(v-u)^T\mathbb{T}^{-1}(v-u)\right), \tag{6.4}$$

with

$$\mathbb{T} = \frac{1}{\mathrm{Pr}} T\mathrm{Id} + \left(1 - \frac{1}{\mathrm{Pr}}\right)\frac{\mathbb{P}}{\rho R}. \tag{6.5}$$

More details and properties of this model can be found in [1], wherein it is shown that the ESBGK operator satisfies the H-theorem as well.

Another model that can produce the correct Prandtl number is the so-called Shakov model [44]:

$$Q^{\mathrm{Shakov}}(f) = \nu(\mathcal{S}[f] - f), \tag{6.6}$$

where

$$\mathcal{S}[f] = \mathcal{M}[f]\left[1 + \frac{1-\mathrm{Pr}}{5}\frac{q\cdot(v-u)}{\rho(RT)^2}\left(\frac{|v-u|^2}{RT} - 5\right)\right]. \tag{6.7}$$

This model does not satisfy the H-theorem since the distribution function f may become negative.

6.2 The Landau operator

We have seen in Section 3 that the Boltzmann collision operator diverges in the case of Coulomb potential, for which the collision kernel (3.16) is given by

$$B_\sigma = C\frac{1}{|V|^3\sin^4\frac{\chi}{2}}. \tag{6.8}$$

One can do a Taylor expansion w.r.t. $|V|\sin\frac{\chi}{2}$ to derive that the leading order of the Boltzmann collision operator behaves as (apart from some dimensional constant):

$$Q^{\mathrm{Landau}}(f,f) = \nabla_v \cdot \int_{\mathbb{R}^3} A(v-v_*)[f(v_*)\nabla_v f(v) - f(v)\nabla_{v_*}f(v_*)]\,\mathrm{d}v_*, \tag{6.9}$$

where A is a matrix given by

$$A(z) = \frac{1}{|z|}\left(\mathrm{Id} - \frac{z\otimes z}{|z|^2}\right). \tag{6.10}$$

Interested readers can refer to [13] for a careful derivation.

6.3 The Fokker-Planck operator

The Landau operator discussed above is a diffusive type operator. A similar operator, which appears in many other fields as well, is the Fokker-Planck operator:

$$Q^{\mathrm{FP}}(f) = \rho \nabla_v \cdot (T \nabla_v f + (v-u) f), \tag{6.11}$$

where ρ, u and T are defined by the moments of f.

6.4 The Vlasov equation

A kinetic model widely used in plasma physics is the Vlasov equation. Compared with the Boltzmann equation, it contains a field term while neglects the collision effects. The equation reads

$$\partial_t f_s + v \cdot \nabla_x f_s + \frac{q_s}{m_s}(E + v \times B) \cdot \nabla_v f_s = 0, \tag{6.12}$$

where f_s is the number distribution function of species s, q_s and m_s are the charge and mass of particles. The electromagnetic field is determined self-consistently via the Maxwell equation

$$\nabla_x \cdot E = \frac{\rho}{\varepsilon_0}, \quad \nabla_x \cdot B = 0, \quad \partial_t B = -\nabla_x \times E, \quad \partial_t E = \frac{1}{\varepsilon_0 \mu_0} \nabla_x \times B - \frac{1}{\varepsilon_0} J, \tag{6.13}$$

where ε_0 and μ_0 are, respectively, permittivity and permeability of space. The charge density ρ and current density J are given by

$$\rho = \sum_s q_s \int_{\mathbb{R}^3} f_s \, \mathrm{d}v, \quad J = \sum_s q_s \int_{\mathbb{R}^3} v f_s \, \mathrm{d}v. \tag{6.14}$$

When the electric field E and magnetic field B are not, or only very little, time dependent, we get the stationary Maxwell equation

$$\nabla_x \cdot E = \frac{\rho}{\varepsilon_0}, \quad \nabla_x \cdot B = 0, \quad \nabla_x \times E = 0, \quad \nabla_x \times B = \mu_0 J. \tag{6.15}$$

In many cases, because B itself is small, or its contribution in the Lorentz force $v \times B$ is small, we shall only need the electric field. The third equation of (6.15) implies that E derives from a scalar potential $E = -\nabla_x \phi$, and then the first equation of (6.15) implies the Poisson equation

$$-\Delta_x \phi = \frac{\rho}{\varepsilon_0}, \tag{6.16}$$

which, together with

$$\partial_t f_s + v \cdot \nabla_x f_s - \frac{q_s}{m_s} \nabla_x \phi \cdot \nabla_v f_s = 0, \tag{6.17}$$

constitute the Vlasov-Poisson equation.

For a mathematical review on the Vlasov type equations, the readers are referred to [23] and [6, Chapter 1].

6.5 Other generalization of the classical Boltzmann equation

The Boltzmann equation we have considered so far is for classical, single species, monoatomic gases. To describe real systems, one usually needs to generalize it to include more effects.

When quantum effects of the particles are non-negligible, for example, only one fermion can occupy one quantum state and infinitely many bosons can occupy the same quantum state, one can consider the so-called quantum Boltzmann equation, or Nordheim-Uehling-Uhlenbeck equation, whose equilibrium is the Bose-Einstein distribution or Fermi-Dirac distribution. See [19] for more details about this equation and its generalization to the relativistic case.

If during particle collisions, only mass and momentum are conserved while the energy is dissipative, this will result in the so-called inelastic Boltzmann equation, which can be used to describe granular materials. For a nice review in this direction, one may refer to [48].

Other generalizations include the Boltzmann equation for mixtures, polyatomic gases, chemical reactions, etc., see [8, Chapter 6] for a brief introduction.

6.6 The linear Boltzmann equation or linear transport equation

In many circumstances, one is interested in the interaction of particles with background environment rather than particle interaction themselves. Then the following linear Boltzmann equation is more appropriate

$$\partial_t f + v \cdot \nabla_x f = \int_{\mathbb{R}^d} [s(v_*, v) f(v_*) - s(v, v_*) f(v)] \, \mathrm{d}v_*, \tag{6.18}$$

where $s(v, v_*)$ describes the transition rate from v to v_* and may take various forms depending on the approximation. In fact, our previous discussion on the linearized Boltzmann collision operator (Section 5.3.1) resembles many properties of such linear operators.

Many transport equations fall into this umbrella, for example, the semiconductor Boltzmann equation, the neutron transport equation, etc. A general mathematical introduction to linear transport equations can be found in [11, Chapter 21].

6.7 Mathematical theory for the Boltzmann-like equations

Finally, let us come back to the Boltzmann-like collisional kinetic equations and summarize (very briefly) some existing mathematical theory. For more details and references, see [9, 47].

- Spatially homogeneous setting:

$$\partial_t f = Q(f, f), \quad f = f(t, v). \tag{6.19}$$

Theory regarding the existence, uniqueness, propagation of smoothness, trend to equilibrium, etc. is rather complete for hard potentials with Grad's angular cut-off assumption. The study of singular kernels (soft potentials or potentials with non-integrable angular singularity) is quite recent.

- Perturbative setting:

$$\partial_t h + v \cdot \nabla_x h = L_M h. \tag{6.20}$$

Consider the Boltzmann equation when it is close to a global Maxwellian M (whose ρ, u, T are constant). L_M is the linearized collision operator.

- Renormalized solutions:

Introduced by DiPerna and Lions at the end of eighties, this theory is at the moment the only framework where existence results (not uniqueness) for the full Boltzmann equation can be proven. It relies on two main ingredients: velocity-averaging lemma and renormalization. Simply speaking, the velocity averaging say that the velocity average $\int g(t,x,v)\varphi(v)\,\mathrm{d}v$ of the solution to the transport equation $\partial_t g + v\cdot\nabla_x g = S$ gains regularity in t and x. The renormalization amounts to multiplying a test function $\beta'(f) \sim 1/(1+f)$ to the Boltzmann equation

$$\partial_t \beta(f) + v \cdot \nabla_x \beta(f) = \beta'(f) Q(f,f), \tag{6.21}$$

so that the right hand side is almost linear.

Along this line, there are many studies on justifying the fluid limit of the Boltzmann equation. The high point is the rigorous limit from the DiPerna-Lions renormalized solutions to Leray's weak solutions of the incompressible Navier-Stokes equation by Golse and Saint-Raymond.

7 Numerical methods for the Boltzmann equation

Despite its long history, numerical approximation of the Boltzmann equation presents a huge computational challenge, even on today's supercomputers. This is mainly due to its high dimensionality and nonlinear, nonlocal structure of the collision integral.

Two approaches have been primarily employed for solving the Boltzmann equation:

- **stochastic**: particle based simulation – direct simulation Monte Carlo (DSMC) methods
- **deterministic**: grid based methods – discrete velocity methods (DVM) and Fourier spectral methods

In this section, we will discuss the above methods in an antichronological order and highlight their pros and cons. First of all, it is common practice to solve the Boltzmann equation in a time-splitting manner[4]:

$$\partial_t f + v \cdot \nabla_x f = 0, \tag{7.1}$$

$$\partial_t f = Q(f, f). \tag{7.2}$$

The convection part (7.1), due to its linearity and hyperbolic structure, can be solved using many well-known methods, finite volume/difference method, semi-Lagrangian method, discontinuous Galerkin method, etc. The collision part (7.2) definitely presents the main difficulty and will be our focus here.

7.1 Fourier spectral methods

In this section, we review the Fourier-Galerkin spectral methods for solving the spatially homogeneous Boltzmann equation. We will start with the original direct version, and then present two fast algorithms. The readers can consult [17, Chapter 5-6] for more details.

7.1.1 Direct Fourier spectral method for the spatially homogeneous Boltzmann equation

This part of the presentation mainly follows [41].

In order to apply the method, we first need to truncate the problem somehow. This leads us to consider the following approximated problem of (7.2) on a torus $\mathcal{D}_L = [-L, L]^d$:

$$\begin{cases} \partial_t f = Q^R(f, f), \quad t > 0,\ v \in \mathcal{D}_L, \\ f(0, v) = f^0(v), \end{cases} \tag{7.3}$$

where the initial condition f^0 is assumed to be a non-negative periodic function, Q^R is the truncated collision operator given by

$$Q^R(g, f)(v) = \int_{\mathcal{B}_R} \int_{S^{d-1}} B_\sigma(|q|, \sigma \cdot \hat{q}) \left[g(v'_*) f(v') - g(v - q) f(v) \right] \mathrm{d}\sigma \, \mathrm{d}q, \tag{7.4}$$

where a change of variable $v_* \to q = v - v_*$ is applied to the σ-representation of the collision operator (c.f. (4.2)), and the new variable q is truncated to a ball $\mathcal{B}_R$ with radius R centered at the origin. We write $q = |q|\hat{q}$ with $|q|$ being the magnitude and $\hat{q}$ being the direction. Accordingly,

$$v' = v - \frac{q - |q|\sigma}{2}, \quad v'_* = v - \frac{q + |q|\sigma}{2}. \tag{7.5}$$

[4]From a parallel computing viewpoint, splitting method has its merit in that: 1) the convection part is naturally parallelizable in v; 2) the collision part is naturally parallelizable in x.

In practice, the values of L and R are often chosen by an anti-aliasing argument: assume that $\mathrm{Supp}(f^0(v)) \subset \mathcal{B}_S$, then one can take

$$R = 2S, \quad L \geq \frac{3+\sqrt{2}}{2} S. \tag{7.6}$$

Given an integer $N \geq 0$, we then seek a truncated Fourier series expansion of f as

$$f(t,v) \approx f_N(t,v) = \sum_{k=-N/2}^{N/2} f_k(t) \mathrm{e}^{\mathrm{i}\frac{\pi}{L}k\cdot v} \in \mathbb{P}_N, \tag{7.7}$$

where

$$\mathbb{P}_N = \mathrm{span}\left\{ \mathrm{e}^{\mathrm{i}\frac{\pi}{L}k\cdot v} \middle| -N/2 \leq k \leq N/2 \right\}^{5}, \tag{7.8}$$

equipped with inner product

$$\langle f, g \rangle = \frac{1}{(2L)^d} \int_{\mathcal{D}_L} f \bar{g} \, \mathrm{d}v. \tag{7.9}$$

Substituting f_N into (7.3) and conducting the Galerkin projection onto the space $\mathbb{P}_N$ yields

$$\begin{cases} \partial_t f_N = \mathcal{P}_N Q^R(f_N, f_N), \quad t > 0, \ v \in \mathcal{D}_L, \\ f_N(0,v) = \mathcal{P}_N f^0(v), \end{cases} \tag{7.10}$$

where $\mathcal{P}_N$ is the projection operator: for any function $g(v)$,

$$\mathcal{P}_N g(v) = \sum_{k=-N/2}^{N/2} \hat{g}_k \mathrm{e}^{\mathrm{i}\frac{\pi}{L}k\cdot v}, \quad \hat{g}_k = \langle g, \mathrm{e}^{\mathrm{i}\frac{\pi}{L}k\cdot v} \rangle. \tag{7.11}$$

Writing out each Fourier mode of (7.10), we obtain

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} f_k = Q_k^R, \quad -N/2 \leq k \leq N/2, \\ f_k(0) = f_k^0, \end{cases} \tag{7.12}$$

with

$$Q_k^R := \langle Q^R(f_N, f_N), \mathrm{e}^{\mathrm{i}\frac{\pi}{L}k\cdot v} \rangle, \quad f_k^0 := \langle f_N^0, \mathrm{e}^{\mathrm{i}\frac{\pi}{L}k\cdot v} \rangle. \tag{7.13}$$

Using the orthogonality of the Fourier basis, we can derive that

$$Q_k^R = \sum_{\substack{l,m=-N/2 \\ l+m=k}}^{N/2} G(l,m) f_l f_m, \tag{7.14}$$

[5] Note here $k = (k_1, \ldots, k_d)$ is a vector, $-N/2 \leq k \leq N/2$ means $-N/2 \leq k_j \leq N/2$, $j = 1, \ldots, d$, and $\sum_{k=-N/2}^{N/2} := \sum_{k_1=-N/2}^{N/2} \cdots \sum_{k_d=-N/2}^{N/2}$.

where G is given by

$$G(l,m)=\int_{\mathcal{B}_R}\int_{S^{d-1}} B_\sigma(|q|,\sigma\cdot\hat{q})\left[\mathrm{e}^{-\mathrm{i}\frac{\pi}{2L}(l+m)\cdot q+\mathrm{i}\frac{\pi}{2L}|q|(l-m)\cdot\sigma}-\mathrm{e}^{-\mathrm{i}\frac{\pi}{L}m\cdot q}\right]\mathrm{d}\sigma\,\mathrm{d}q. \quad (7.15)$$

(7.12) is the final Galerkin system one needs to solve. In practice, the weight $G(l,m)$ can be precomputed to high accuracy and stored for future use (note that the memory requirement is $O(N^{2d})$). In the online computation, the sum (7.14) is evaluated directly, whose numerical complexity is $O(N^{2d})$ per time step.

Although the Fourier spectral method can be expensive for large N in terms of memory and computational complexity, it does offer a superior accuracy compared with other deterministic methods such as the DVM. The stability of the method was proved in [21] using the "spreading" property of the collision operator. A simple proof is given recently in [30], where the key is to utilize the mass conservation property and to control the L^2 norm of the negative part of the solution.

7.1.2 A fast Fourier spectral method based on Carleman representation

As we have just seen, the memory requirement and computational complexity of the direct Fourier spectral method may become a bottleneck when N is large. In [39], a fast Fourier spectral method was introduced, though it only works for certain collision kernels.

The method is based on the same Fourier-Galerkin framework but starts with yet another representation of the collision operator, the so-called Carleman form:

$$Q(g,f)(v)=\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} B_c(x,y)\delta(x\cdot y)[g'_*f'-g_*f]\,\mathrm{d}x\,\mathrm{d}y, \quad (7.16)$$

where

$$v_*=v+x+y,\quad v'=v+x,\quad v'_*=v+y. \quad (7.17)$$

The new variables x and y are given in Figure 3, where their perpendicular relation is obvious. The collision kernel changes accordingly and is a complicated function of x and y. We only mention two special cases where B_c is a constant (in fact, these are the cases the fast algorithm will apply): $B_\sigma=C$ in 2D and $B_\sigma=C|v-v_*|$ in 3D.

For simplicity, we shall assume $B_c\equiv 1$ in the following. The procedure presented in the previous section will lead us to the same Galerkin system (7.12) except that the weight $G(l,m)$ is given by

$$G(l,m)=\int_{\mathcal{B}_R}\int_{\mathcal{B}_R}\delta(x\cdot y)\left[\mathrm{e}^{\mathrm{i}\frac{\pi}{L}l\cdot x}\mathrm{e}^{\mathrm{i}\frac{\pi}{L}m\cdot y}-\mathrm{e}^{\mathrm{i}\frac{\pi}{L}m\cdot x}\mathrm{e}^{\mathrm{i}\frac{\pi}{L}m\cdot y}\right]\mathrm{d}x\,\mathrm{d}y. \quad (7.18)$$

Note that the truncation now is performed in the variables x and y instead of q.

The idea of the fast algorithm is to find a separated expansion of the weight $G(l,m)$ (in fact, we only need to do this for the gain term because the loss term is readily a convolution) as

$$G^+(l,m) \approx \sum_{t=1}^{T} \alpha_t(l)\beta_t(m), \tag{7.19}$$

where T is small, so that the weighted convolution (7.14) can be rendered into a few pure convolutions

$$Q_k^{R,+} \approx \sum_{t=1}^{T} \sum_{\substack{l,m=-N/2 \\ l+m=k}}^{N/2} (\alpha_t(l) f_l)(\beta_t(m) f_m), \tag{7.20}$$

hence can be speed up by the fast Fourier transform (FFT).

To achieve this goal, we simplify the gain term of (7.18) as

$$\begin{aligned} G^+(l,m) &= \int_{S^{d-1}} \int_{S^{d-1}} \int_0^R \int_0^R \delta(\hat{x}\cdot\hat{y})\, \mathrm{e}^{\mathrm{i}\frac{\pi}{L}|x|l\cdot\hat{x}} \mathrm{e}^{\mathrm{i}\frac{\pi}{L}|y|m\cdot\hat{y}} |x|^{d-2}|y|^{d-2}\, \mathrm{d}|x|\, \mathrm{d}|y|\, \mathrm{d}\hat{x}\, \mathrm{d}\hat{y} \\ &= \int_{S^{d-1}} \int_{S^{d-1}} \delta(\hat{x}\cdot\hat{y}) \left(\int_0^R \mathrm{e}^{\mathrm{i}\frac{\pi}{L}|x|l\cdot\hat{x}} |x|^{d-2}\, \mathrm{d}|x| \right) \left(\int_0^R \mathrm{e}^{\mathrm{i}\frac{\pi}{L}|y|m\cdot\hat{y}} |y|^{d-2}\, \mathrm{d}|y| \right) \mathrm{d}\hat{x}\, \mathrm{d}\hat{y} \\ &= \int_{S^{d-1}} \int_{S^{d-1}} \delta(\hat{x}\cdot\hat{y}) \alpha(l\cdot\hat{x}) \alpha(m\cdot\hat{y})\, \mathrm{d}\hat{x}\, \mathrm{d}\hat{y}, \end{aligned} \tag{7.21}$$

where

$$\alpha(s) := \int_0^R \mathrm{e}^{\mathrm{i}\frac{\pi}{L}\rho s} \rho^{d-2}\, \mathrm{d}\rho. \tag{7.22}$$

In particular, in 2D, we can write (3D can be done similarly):

$$G^+(l,m) = 2\int_{S^1} \alpha(l\cdot\sigma)\alpha(\sqrt{|m|^2-(m\cdot\sigma)^2})\, \mathrm{d}\sigma, \tag{7.23}$$

that is, the final integration is reduced to a circle (sphere) only. Now if we approximate the final integral by a quadrature rather than precompute it, $G^+(l,m)$ would be a separated expansion of l and m:

$$G^+(l,m) \approx 2\sum_{\sigma\in S^1} w_\sigma\, \alpha(l\cdot\sigma)\alpha(\sqrt{|m|^2-(m\cdot\sigma)^2}), \tag{7.24}$$

where w_σ is the weight of the quadrature.

To summarize, with this trick, the total cost to evaluate Q_k^R is reduced to $O(MN^d \log N)$, with M being the total number of points on the sphere S^{d-1}. In practice, M can usually be chosen much smaller than N^d, hence offers a significant speedup compared to $O(N^{2d})$ complexity of the direct Fourier spectral method.

7.1.3 A fast Fourier spectral method based on σ-representation

The previously introduced fast algorithm leverages on a perpendicular structure of the collision operator. However, it only applies to special kernels. In [22], a different fast algorithm was proposed based on the σ-representation. Indeed, the framework is quite generic and can be applied to a large class of collision operators [28, 35, 29].

The idea is very simple. We go back to the original formulation (7.15) and look for a separated expansion of the weight $G^+(l,m)$ as

$$G^+(l,m) \approx \sum_{t=1}^{T} \alpha_t(l+m)\beta_t(l)\gamma(m). \tag{7.25}$$

If this is possible, then the weighted convolution (7.14) can be written as

$$Q_k^{R,+} \approx \sum_{t=1}^{T} \alpha_t(k) \sum_{\substack{l,m=-N/2 \\ l+m=k}}^{N/2} (\beta_t(l)f_l)(\gamma_t(m)f_m), \tag{7.26}$$

hence can be speed up by FFT.

To realize this, it is sufficient to write the gain term of (7.15) as

$$G^+(l,m) = \int_0^R \int_{S^{d-1}} F(l+m,|q|,\sigma)\mathrm{e}^{\mathrm{i}\frac{\pi}{2L}|q|(l-m)\cdot\sigma}|q|^{d-1}\,\mathrm{d}\sigma\,\mathrm{d}|q|, \tag{7.27}$$

where

$$F(l+m,|q|,\sigma) := \int_{S^{d-1}} B_\sigma(|q|,\sigma\cdot\hat{q})\mathrm{e}^{-\mathrm{i}\frac{\pi}{2L}|q|(l+m)\cdot\hat{q}}\,\mathrm{d}\hat{q}. \tag{7.28}$$

We then precompute F but use a quadrature to approximate the integrals in (7.27) which results in

$$G^+(l,m) \approx \sum_{|q|,\sigma} w_{|q|}w_\sigma F(l+m,|q|,\sigma)|q|^{d-1}\mathrm{e}^{\mathrm{i}\frac{\pi}{2L}|q|l\cdot\sigma}\mathrm{e}^{-\mathrm{i}\frac{\pi}{2L}|q|m\cdot\sigma}. \tag{7.29}$$

Therefore, the total cost to evaluate Q_k^R is reduced to $O(MN_{|q|}N^d\log N)$, with M being the total number of points on the sphere S^{d-1} and $N_{|q|}$ being the number of points in the radial direction $[0,R]$. In practice, we found $N_{|q|}\sim O(N)$ due to the oscillation in $|q|$, and M can usually be chosen smaller than N^{d-1}.

7.2 Discrete velocity methods (DVM)

The discrete velocity methods (DVM) represent early attempts of solving the Boltzmann equation deterministically. Compared with Fourier spectral methods, they are able to preserve the main physical properties of the equation like positivity, conservation, and entropy decay. However, they often converge very slowly and the computational cost is quite high due to the lack of fast algorithms (there are some fast variants of the DVM

proposed recently [40, 7]). Here we give a minimum description of the basic principle of the methods. For more details, the readers can refer to [17].

The DVM starts from a finite computational domain $\mathcal{D}_L = [-L, L]^d$ and assumes uniform discrete velocity points in $\mathcal{D}_L$ with the index set:

$$K = \{k = (k_1, \cdots, k_d) \in \mathbb{Z}^d \mid v_k = k\Delta v \in \mathcal{D}_L\}.$$

Then the distribution function $f_i(t)$ at velocity point v_i is evolved as

$$\frac{\mathrm{d}}{\mathrm{d}t} f_i = Q_i := \sum_{j,k,l \in K} A_{ij}^{kl}(f_k f_l - f_i f_j), \quad i \in K, \tag{7.30}$$

where the kernel $A_{ij}^{kl} \geq 0$ is given by

$$A_{ij}^{kl} = \mathbf{1}(i + j - k - l)\mathbf{1}(|i|^2 + |j|^2 - |k|^2 - |l|^2)W_{ij}^{kl}, \tag{7.31}$$

and the choice of the weight W_{ij}^{kl} distinguishes different DVM. The common requirement is that A_{ij}^{kl} should satisfy the symmetry property:

$$A_{ij}^{kl} = A_{ji}^{kl} = A_{kl}^{ij}. \tag{7.32}$$

Using this property, one can easily derive that

$$\sum_{i \in K} Q_i \phi_i = \frac{1}{4} \sum_{i,j,k,l \in K} A_{ij}^{kl}(f_k f_l - f_i f_j)(\phi_i + \phi_j - \phi_k - \phi_l), \tag{7.33}$$

where ϕ_i is a test function at velocity point v_i. Choosing $\phi_i = 1, v_i, |v_i|^2$, we obtain conservation of mass, momentum and energy:

$$\sum_{i \in K} Q_i = \sum_{i \in K} Q_i v_i = \sum_{i \in K} Q_i |v_i|^2 = 0. \tag{7.34}$$

Choosing $\phi_i = \ln f_i$, we obtain

$$\sum_{i \in K} Q_i \ln f_i = -\frac{1}{4} \sum_{i,j,k,l \in K} A_{ij}^{kl}(f_k f_l - f_i f_j)(\ln(f_k f_l) - \ln(f_i f_l)) \leq 0, \tag{7.35}$$

which implies entropy decay

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{i \in K} f_i \ln f_i = \sum_{i \in K} Q_i(\ln f_i + 1) \leq 0. \tag{7.36}$$

7.3 Direct simulation Monte Carlo methods (DSMC)

8 Structure-preserving numerical methods for stiff kinetic equations

Our focus so far has been on the approximation of the Boltzmann collision operator (i.e., the discretization in the velocity space). To have a robust solver for the full kinetic

equation, we need to consider time and spatial discretization as well. In this section, we will consider the following prototype kinetic equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f), \tag{8.1}$$

where $Q(f)$ can be the Boltzmann collision operator or other operators that share a similar structure, for example, the ones we mentioned in Section 6. Furthermore, we will put emphasis in the regime that is close to the fluid limit, i.e., the Knudsen number ε could be small. The reasons are two-fold: 1) applicationwise, kinetic equations serve as more accurate models compared to fluid equations, hence are often used in the near fluid regime; 2) computationwise, small Knudsen number results in a stiff equation whose numerical approximation is more challenging.

8.1 Asymptotic-preserving (AP) schemes for the BGK equation

Let us take a closer look of the structure of equation (8.1). As we mentioned earlier, the convection part is linear and non-stiff, hence many generic explicit spatial discretization methods (e.g., the finite difference/volume/element methods [38, 45]) can be used. On the other hand, the collision part presents strong stiffness when $\varepsilon \ll 1$, hence it is better to use implicit scheme (explicit scheme would require $\Delta t \sim O(\varepsilon)$). This, as a result, brings several concerns: 1) The collision operator is often nonlinear for which implicit discretization would require iteration. Can we avoid this? 2) We know that as $\varepsilon \to 0$, the continuous equation (formally) converges to the compressible Euler equations. Can we preserve this limit at the discrete level?

The so-called *asymptotic-preserving (AP) schemes* [36] exactly answer the above two questions, whose main idea can be illustrated by Figure 5. For a comprehensive review about AP schemes, the readers can refer to [37, 27, 12].

As a starting example, let us consider the following BGK equation:

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} (\mathcal{M}[f] - f). \tag{8.2}$$

Recall that the Maxwellian $\mathcal{M}$ is defined via the moments of f:

$$\mathcal{M} = \frac{\rho}{(2\pi T)^{d/2}} \exp\left(-\frac{|v-u|^2}{2T}\right), \tag{8.3}$$

with

$$\rho = \int_{\mathbb{R}^d} f \, \mathrm{d}v, \quad u = \frac{1}{\rho} \int_{\mathbb{R}^d} v f \, \mathrm{d}v, \quad T = \frac{1}{d\rho} \int_{\mathbb{R}^d} |v-u|^2 f \, \mathrm{d}v. \tag{8.4}$$

Leaving aside discretization in velocity and physical space, perhaps the simplest way to solve (8.2) is to use the Lie splitting (assume f^n is the numerical solution at time

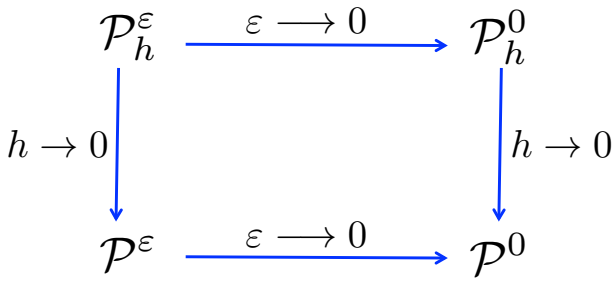

Figure 5: Illustration of AP schemes. $\mathcal{P}^\varepsilon$ is a microscopic equation that depends on the small scale ε (e.g., the equation (8.1)), and $\mathcal{P}^0$ is its macroscopic limit as $\varepsilon \to 0$ (e.g., the Euler equations). Denote the numerical approximation of $\mathcal{P}^\varepsilon$ by $\mathcal{P}_h^\varepsilon$, where h is the discretization parameter such as the time step or mesh size. The asymptotic limit of $\mathcal{P}_h^\varepsilon$ as $\varepsilon \to 0$ (with h fixed), if exists, is denoted by $\mathcal{P}_h^0$. If $\mathcal{P}_h^0$ is a good (consistent and stable) approximation of $\mathcal{P}^0$, then the scheme $\mathcal{P}_h^\varepsilon$ is called AP.

$t_n = n\Delta t$, $n \geq 0$):

$$\begin{cases} \dfrac{f^* - f^n}{\Delta t} + v \cdot \nabla_x f^n = 0, \\ \dfrac{f^{n+1} - f^*}{\Delta t} = \dfrac{1}{\varepsilon}(\mathcal{M}^{n+1} - f^{n+1}), \end{cases} \tag{8.5}$$

where the forward Euler is applied to the non-stiff convection step and backward Euler to the stiff collision step. At first sight, the collision step seems implicit since $\mathcal{M}^{n+1}$ depends on f^{n+1}. However, recall that the BGK operator is conservative, i.e.,

$$\langle \phi f \rangle = \langle \phi \mathcal{M} \rangle := U = (\rho, \rho u, E)^T, \quad \phi = (1, v, |v|^2/2)^T, \quad \langle \cdot \rangle := \int_{\mathbb{R}^d} \cdot \, \mathrm{d}v. \tag{8.6}$$

Then if we take the moments $\langle \phi \, \cdot \rangle$ in the second step of (8.5), we obtain

$$\langle \phi f^{n+1} \rangle = \langle \phi f^* \rangle \implies U^{n+1} = U^*, \tag{8.7}$$

i.e., the macroscopic quantity U remains unchanged in the second step. Therefore, we can use f^* found in the first step to define U^* or U^{n+1} (hence $\mathcal{M}^{n+1}$), then the second step is explicitly solvable (no iteration is needed).

Let us now add the spatial discretization (assume $d = 1$ for simplicity)[6]:

$$\begin{cases} \dfrac{f_i^* - f_i^n}{\Delta t} + \dfrac{\hat{f}_{i+1/2}^n - \hat{f}_{i-1/2}^n}{\Delta x} = 0, \\ \dfrac{f_i^{n+1} - f_i^*}{\Delta t} = \dfrac{1}{\varepsilon}(\mathcal{M}_i^{n+1} - f_i^{n+1}), \end{cases} \tag{8.8}$$

[6]The velocity variable is treated as continuous, or discrete by assuming that the domain is chosen large enough so that the quadrature error in v can be ignored.

where i is the spatial index and the numerical flux $\hat{f}_{i+1/2}$ is defined by the upwind flux splitting:

$$\hat{f}_{i+1/2} = \hat{f}^+_{i+1/2} + \hat{f}^-_{i+1/2}, \tag{8.9}$$

with

$$\hat{f}^+_{i+1/2} = \frac{v+|v|}{2} f^-_{i+1/2}, \quad \hat{f}^-_{i+1/2} = \frac{v-|v|}{2} f^+_{i+1/2}. \tag{8.10}$$

$f^\pm_{i+1/2}$ are the reconstructed values of f at cell interface $x_{i+1/2}$ using neighboring f_i's. The simplest first order choice is $f^-_{i+1/2} = f_i$ and $f^+_{i+1/2} = f_{i+1}$.

Now if we send $\varepsilon \to 0$, the second step of (8.8) implies

$$f_i^n \to \mathcal{M}_i^n, \quad n \geq 1. \tag{8.11}$$

On the other hand, taking the moments $\langle \phi \, \cdot \rangle$ in the first step yields

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \frac{\langle \phi \hat{f}^n_{i+1/2} \rangle - \langle \phi \hat{f}^n_{i-1/2} \rangle}{\Delta x} = 0, \tag{8.12}$$

where we used $U_i^{n+1} = U_i^*$ explained earlier. Finally replacing f_i^n by $\mathcal{M}_i^n$ in the flux definition we obtain

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \frac{F^n_{i+1/2} - F^n_{i-1/2}}{\Delta x} = 0, \quad n \geq 1, \tag{8.13}$$

where

$$F^n_{i+1/2} = \left\langle \phi \frac{v+|v|}{2} \mathcal{M}^{n,-}_{i+1/2} \right\rangle + \left\langle \phi \frac{v-|v|}{2} \mathcal{M}^{n,+}_{i+1/2} \right\rangle. \tag{8.14}$$

(8.13) is a consistent (first order in time) scheme for the limiting compressible Euler equations (5.16). In fact, the flux function can be expressed in terms of ρ, u and T, resulting in the so-called *kinetic flux vector spliting (KFVS) scheme* [14, 43]. Therefore, we have verified that the scheme (8.8) is AP.

If we take a second look at (8.8), we notice that there is an alternative way to solve the collision step: since $\mathcal{M}$ remains unchanged during this step, this is essentially an ODE which can be solved exactly:

$$f_i^{n+1} = \mathrm{e}^{-\frac{\Delta t}{\varepsilon}} f_i^* + \left(1 - \mathrm{e}^{-\frac{\Delta t}{\varepsilon}}\right) \mathcal{M}_i^*. \tag{8.15}$$

This scheme is also AP because as $\varepsilon \to 0$, we still have (8.11).

Furthermore, if we add the two steps in (8.8) together, we obtain

$$\frac{f_i^{n+1} - f_i^n}{\Delta t} + \frac{\hat{f}^n_{i+1/2} - \hat{f}^n_{i-1/2}}{\Delta x} = \frac{1}{\varepsilon}(\mathcal{M}_i^{n+1} - f_i^{n+1}). \tag{8.16}$$

Taking the moments $\langle \phi \, \cdot \rangle$ on both sides of this scheme yields

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} + \frac{\langle \phi \hat{f}^n_{i+1/2} \rangle - \langle \phi \hat{f}^n_{i-1/2} \rangle}{\Delta x} = 0. \tag{8.17}$$

At every time step, we solve (8.17) first to obtain U_i^{n+1}, which consequently defines $\mathcal{M}_i^{n+1}$. Then we solve (8.16) to obtain f_i^{n+1}. This way of viewing the scheme as an unsplit version will play an essential role in construction of high order (in time) schemes as we shall see next.

8.2 High-order AP schemes for the BGK equation

The above discussed schemes are all first order in time which is a bit crude. A natural question is: can we construct a high order scheme? It seems that a simple solution is to apply a high order operator splitting (say, Strang splitting) and then use a high order scheme for each substep. For example, we could do half-step collision, one-step convection, and half-step collision. Over each substep, we use a second order Runge-Kutta (RK) scheme.

Now for the convection step, we apply, say, the second order Heun's method:

$$f^{(1)} = f^n - \Delta t v \cdot \nabla_x f^n, \quad f^{n+1} = f^n - \frac{\Delta t}{2} v \cdot \nabla_x f^n - \frac{\Delta t}{2} v \cdot \nabla_x f^{(1)}, \tag{8.18}$$

which, upon taking the moments $\langle \phi \cdot \rangle$, yields

$$U^{(1)} = U^n - \Delta t \nabla_x \cdot \langle v\phi f^n \rangle, \quad U^{n+1} = U^n - \frac{\Delta t}{2} \nabla_x \cdot \langle v\phi f^n \rangle - \frac{\Delta t}{2} \nabla_x \cdot \langle v\phi f^{(1)} \rangle. \tag{8.19}$$

Let us examine what happens when $\varepsilon \to 0$. Assume that the collision step is solved accurately, then it will project f^n to the corresponding Maxwellian $\mathcal{M}^n$. However, nothing guarantees $f^{(1)} \to \mathcal{M}^{(1)}$. Generally, we will have

$$U^{(1)} = U^n - \Delta t \nabla_x \cdot \langle v\phi \mathcal{M}^n \rangle, \quad U^{n+1} = U^n - \frac{\Delta t}{2} \nabla_x \cdot \langle v\phi \mathcal{M}^n \rangle - \frac{\Delta t}{2} \langle v\phi \mathcal{M}^{(1)} \rangle + O(\Delta t^2), \tag{8.20}$$

i.e., the scheme reduces to first order in the limit.

To get around the order reduction and achieve a high order AP scheme in both kinetic ($\varepsilon \sim O(1)$) and fluid regimes ($\varepsilon \to 0$), a nice framework is the so-called *IMEX (implicit-explicit) schemes*, which can be viewed as high order extension of the first order scheme (8.16)-(8.17). There are both multi-stage and multi-step versions.

8.2.1 IMEX-RK schemes

A s-stage IMEX-RK scheme reads:

$$f^{(i)} = f^n - \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} v \cdot \nabla_x f^{(j)} + \frac{\Delta t}{\varepsilon} \sum_{j=1}^{i} a_{ij} (\mathcal{M}^{(j)} - f^{(j)}), \quad i = 1, \dots, s, \tag{8.21}$$

$$f^{n+1} = f^n - \Delta t \sum_{i=1}^{s} \tilde{w}_i v \cdot \nabla_x f^{(i)} + \frac{\Delta t}{\varepsilon} \sum_{i=1}^{s} w_i (\mathcal{M}^{(i)} - f^{(i)}), \tag{8.22}$$

where the matrices $\tilde{A} = (\tilde{a}_{ij})$, $\tilde{a}_{ij} = 0$ for $j \geq i$ and $A = (a_{ij})$, $a_{ij} = 0$ for $j > i$ are $s \times s$ matrices such that the scheme is explicit for the convection part and implicit for the collision part. Along with the vectors $\tilde{\mathbf{w}} = (\tilde{w}_1, \ldots, \tilde{w}_s)^T$, $\mathbf{w} = (w_1, \ldots, w_s)^T$, they can be represented by a double Butcher tableau:

$$\begin{array}{c|c} \tilde{\mathbf{c}} & \tilde{A} \\ \hline & \tilde{\mathbf{w}}^T \end{array} \qquad \begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{w}^T \end{array}$$

where the vectors $\tilde{\mathbf{c}} = (\tilde{c}_1, \ldots, \tilde{c}_s)^T$, $\mathbf{c} = (c_1, \ldots, c_s)^T$ are defined as

$$\tilde{c}_i = \sum_{j=1}^{i-1} \tilde{a}_{ij}, \quad c_i = \sum_{j=1}^{i} a_{ij}. \tag{8.23}$$

At every stage of (8.21), since the collision part is implicit, one has to obtain $\mathcal{M}^{(i)}$ first in order to evaluate $f^{(i)}$. This can be achieved similarly as the first order scheme (8.16)-(8.17): taking the moments $\langle \phi \cdot \rangle$ on both sides of (8.21) yields

$$U^{(i)} = U^n - \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} \nabla_x \cdot \langle v \phi f^{(j)} \rangle, \tag{8.24}$$

which consequently defines $\mathcal{M}^{(i)}$.

Some preliminary notions about the IMEX-RK schemes are necessary before we discuss their asymptotic properties. First of all, the double Butcher tableau must satisfy the order conditions (standard order conditions for each tableau and coupling conditions) [25, 42]. Then according to the structure of matrix A in the implicit tableau, one can further classify the schemes into the following categories [5, 16]:

- **Type A**: if the matrix A is invertible.
- **Type CK**: if the matrix A can be written as

$$\begin{pmatrix} 0 & 0 \\ \mathbf{a} & \hat{A} \end{pmatrix}, \tag{8.25}$$

  and the submatrix $\hat{A} \in \mathbb{R}^{(s-1)\times(s-1)}$ is invertible; in particular, if the vector $\mathbf{a} = 0$, $w_1 = 0$, the scheme is of type ARS.
- If $a_{si} = w_i$, $\tilde{a}_{si} = \tilde{w}_i$, $i = 1, \ldots, s$, i.e., $f^{n+1} = f^{(s)}$, the scheme is said to be **globally stiffly accurate (GSA)**.

To save the space, we list only two examples of IMEX-RK schemes: ARS type schemes of first and second order [2]. More tables can be found in the aforementioned references. Note that the first order ARS scheme is nothing but the forward-backward Euler scheme (8.16).

We have the following straightforward result.

0	0	0
1	1	0
	1	0

0	0	0
1	0	1
	0	1

Table 1: ARS(1,1,1) scheme.

0	0	0	0
γ	γ	0	0
1	δ	$1-\delta$	0
	δ	$1-\delta$	0

0	0	0	0
γ	0	γ	0
1	0	$1-\gamma$	γ
	0	$1-\gamma$	γ

$\gamma = 1 - \frac{\sqrt{2}}{2},\ \delta = 1 - \frac{1}{2\gamma}.$

Table 2: ARS(2,2,2) scheme.

Proposition 8.1. *If the IMEX-RK scheme (8.21)-(8.22) is of type A, then for fixed Δt, in the limit $\varepsilon \to 0$, the scheme becomes the explicit RK scheme characterized by $(\tilde{A}, \tilde{\mathbf{w}})$ applied to the limiting compressible Euler equations (5.16).*

Proof. For ease of presentation, we first rewrite (8.21)-(8.22) using vector notations:

$$\mathbf{F} = f^n \mathbf{e} - \Delta t \tilde{A} v \cdot \nabla_x \mathbf{F} + \frac{\Delta t}{\varepsilon} A(\mathcal{M}[\mathbf{F}] - \mathbf{F}), \tag{8.26}$$

$$f^{n+1} = f^n - \Delta t \tilde{\mathbf{w}}^T v \cdot \nabla_x \mathbf{F} + \frac{\Delta t}{\varepsilon} \mathbf{w}^T (\mathcal{M}[\mathbf{F}] - \mathbf{F}), \tag{8.27}$$

where $\mathbf{F} := (f^{(1)}, \dots, f^{(s)})^T$, $\mathbf{e} := (1, \dots, 1)^T$, and $\mathcal{M}[\mathbf{F}] := (\mathcal{M}^{(1)}, \dots, \mathcal{M}^{(s)})^T$. Taking the moments $\langle \phi \cdot \rangle$ on both sides of (8.26)-(8.27) yields

$$\langle \phi \mathbf{F} \rangle = \langle \phi f^n \rangle \mathbf{e} - \Delta t \tilde{A} \nabla_x \cdot \langle v \phi \mathbf{F} \rangle, \tag{8.28}$$

$$\langle \phi f^{n+1} \rangle = \langle \phi f^n \rangle - \Delta t \tilde{\mathbf{w}}^T \nabla_x \cdot \langle v \phi \mathbf{F} \rangle. \tag{8.29}$$

If $\varepsilon \to 0$ in (8.26), one has $A(\mathcal{M}[\mathbf{F}] - \mathbf{F}) = 0$, which implies $\mathbf{F} = \mathcal{M}[\mathbf{F}]$ since A is invertible. Therefore, as $\varepsilon \to 0$, the moment equations (8.28)-(8.29) become

$$\langle \phi \mathbf{F} \rangle = \langle \phi f^n \rangle \mathbf{e} - \Delta t \tilde{A} \nabla_x \cdot \langle v \phi \mathcal{M}[\mathbf{F}] \rangle, \tag{8.30}$$

$$\langle \phi f^{n+1} \rangle = \langle \phi f^n \rangle - \Delta t \tilde{\mathbf{w}}^T \nabla_x \cdot \langle v \phi \mathcal{M}[\mathbf{F}] \rangle, \tag{8.31}$$

which is the explicit RK scheme characterized by $(\tilde{A}, \tilde{\mathbf{w}})$ applied to the compressible Euler equations. □

Proposition 8.2. *If the IMEX-RK scheme (8.21)-(8.22) is of type CK and GSA, and the initial data is consistent:*

$$f^0 = \mathcal{M}[f^0] + O(\varepsilon), \tag{8.32}$$

then for fixed Δt, in the limit $\varepsilon \to 0$, the scheme becomes the explicit RK scheme characterized by $(\tilde{A}, \tilde{\mathbf{w}})$ applied to the limiting compressible Euler equations (5.16), and

$$f^n \to \mathcal{M}[f^n], \quad n \geq 1. \tag{8.33}$$

Proof. If a scheme is of type CK and GSA, then $f^{(1)} = f^n$, $f^{n+1} = f^{(s)}$. Rewriting $\mathbf{F} = (f^{(1)}, \hat{\mathbf{F}})$, $\mathbf{e} = (1, \hat{\mathbf{e}})$, $\mathcal{M}[\mathbf{F}] = (\mathcal{M}[f^{(1)}], \mathcal{M}[\hat{\mathbf{F}}])$, then (8.26) becomes

$$\hat{\mathbf{F}} = f^n \hat{\mathbf{e}} - \Delta t \tilde{\mathbf{a}} v \cdot \nabla_x f^n - \Delta t \hat{\tilde{A}} v \cdot \nabla_x \hat{\mathbf{F}} + \frac{\Delta t}{\varepsilon} \mathbf{a}(\mathcal{M}[f^n] - f^n) + \frac{\Delta t}{\varepsilon} \hat{A}(\mathcal{M}[\hat{\mathbf{F}}] - \hat{\mathbf{F}}), \quad (8.34)$$

where we have used a similar notation for matrix $\tilde{A}$ as that in (8.25):

$$\begin{pmatrix} 0 & 0 \\ \tilde{\mathbf{a}} & \hat{\tilde{A}} \end{pmatrix}. \quad (8.35)$$

Taking the moments $\langle \phi \cdot \rangle$ on both sides of (8.34) yields

$$\langle \phi \hat{\mathbf{F}} \rangle = \langle \phi f^n \rangle \hat{\mathbf{e}} - \Delta t \tilde{\mathbf{a}} \nabla_x \cdot \langle v \phi f^n \rangle - \Delta t \hat{\tilde{A}} \nabla_x \cdot \langle v \phi \hat{\mathbf{F}} \rangle. \quad (8.36)$$

Now sending $\varepsilon \to 0$ in (8.34), one has $\mathbf{a}(\mathcal{M}[f^n] - f^n) + \hat{A}(\mathcal{M}[\hat{\mathbf{F}}] - \hat{\mathbf{F}}) = 0$, which reduces to $\hat{A}(\mathcal{M}[\hat{\mathbf{F}}] - \hat{\mathbf{F}}) = 0$ for consistent initial data. This further implies $\hat{\mathbf{F}} = \mathcal{M}[\hat{\mathbf{F}}]$ since $\hat{A}$ is invertible. Therefore, as $\varepsilon \to 0$, the moment equation (8.36) becomes

$$\langle \phi \hat{\mathbf{F}} \rangle = \langle \phi f^n \rangle \hat{\mathbf{e}} - \Delta t \tilde{\mathbf{a}} \nabla_x \cdot \langle v \phi \mathcal{M}[f^n] \rangle - \Delta t \hat{\tilde{A}} \nabla_x \cdot \langle v \phi \mathcal{M}[\hat{\mathbf{F}}] \rangle, \quad (8.37)$$

i.e., the explicit RK scheme characterized by $(\tilde{A}, \tilde{\mathbf{w}})$ applied to the compressible Euler equations. Since the scheme is GSA, we have $f^{n+1} = \mathcal{M}[f^{n+1}]$, thus the initial data remains consistent at the next time step. □

8.2.2 IMEX-BDF schemes

There is also a multi-step version of the IMEX schemes, see [18] for more details. Here we will only mention a subclass – IMEX backward differentiation formulas (BDF) due to their particular nice properties.

A s-step IMEX-BDF scheme reads:

$$f^{n+1} = -\sum_{j=1}^{s} \alpha_j f^{n+1-j} - \Delta t \sum_{j=1}^{s} \gamma_j v \cdot \nabla_x f^{n+1-j} + \frac{\Delta t}{\varepsilon} \beta(\mathcal{M}^{n+1} - f^{n+1}), \quad (8.38)$$

where $\alpha = (\alpha_1, \ldots, \alpha_s)^T$, $\gamma = (\gamma_1, \ldots, \gamma_s)^T$, and β are given in Table 3. Unlike IMEX-RK schemes which are self-starting, multi-step schemes need s starting values $f^0, f^1, \ldots, f^{s-1}$, which can often be prepared using IMEX-RK schemes. (8.38) can be solved explicitly using the same trick as before: taking the moments $\langle \phi \cdot \rangle$ on both sides of the scheme yields

$$U^{n+1} = -\sum_{j=1}^{s} \alpha_j U^{n+1-j} - \Delta t \sum_{j=1}^{s} \gamma_j \nabla_x \cdot \langle v \phi f^{n+1-j} \rangle, \quad (8.39)$$

hence U^{n+1} can be found first to define $\mathcal{M}^{n+1}$.

Regarding the AP property, we have the following straightforward result.

s	α^T	γ^T	β
1	-1	1	1
2	$(-\frac{4}{3}, \frac{1}{3})$	$\left(\frac{4}{3}, -\frac{2}{3}\right)$	$\frac{2}{3}$
3	$\left(-\frac{18}{11}, \frac{9}{11}, -\frac{2}{11}\right)$	$\left(\frac{18}{11}, -\frac{18}{11}, \frac{6}{11}\right)$	$\frac{6}{11}$
4	$\left(-\frac{48}{25}, \frac{36}{25}, -\frac{16}{25}, \frac{3}{25}\right)$	$\left(\frac{48}{25}, -\frac{72}{25}, \frac{48}{25}, -\frac{12}{25}\right)$	$\frac{12}{25}$

Table 3: Coefficients of IMEX-BDF schemes up to fourth order [34].

Proposition 8.3. *If the initial data are consistent:*

$$f^n = \mathcal{M}[f^n] + O(\varepsilon), \quad n = 0, \dots, s-1, \tag{8.40}$$

then for fixed Δt, in the limit $\varepsilon \to 0$, the IMEX-BDF scheme (8.38) becomes the explicit multi-step scheme characterized by (α, γ) applied to the limiting compressible Euler equations (5.16), and

$$f^n \to \mathcal{M}[f^n], \quad n \geq s. \tag{8.41}$$

Proof. When $\varepsilon \to 0$, (8.38) implies

$$f^n \to \mathcal{M}^n, \quad n \geq s, \tag{8.42}$$

which, together with the consistent initial data, gives

$$f^n \to \mathcal{M}^n, \quad n \geq 0. \tag{8.43}$$

Therefore, as $\varepsilon \to 0$, the moment equation (8.39) becomes

$$U^{n+1} = -\sum_{j=1}^{s} \alpha_j U^{n+1-j} - \Delta t \sum_{j=1}^{s} \gamma_j \nabla_x \cdot \langle v\phi \mathcal{M}^{n+1-j} \rangle, \tag{8.44}$$

which is the explicit multi-step scheme characterized by (α, γ) applied to the compressible Euler equations. □

Let's also take a look at the Navier-Stokes asymptotics of the IMEX-BDF scheme. To this aim, we again use the vector representation: define $\mathbf{F} = (f^n, f^{n-1}, \dots, f^{n+1-s})^T$, then (8.38) can be written as

$$f^{n+1} = -\alpha^T \mathbf{F} - \Delta t \gamma^T \mathcal{T}_{\Delta x}(\mathbf{F}) + \frac{\Delta t}{\varepsilon} \beta (\mathcal{M}^{n+1} - f^{n+1}), \tag{8.45}$$

where we assume a p-th order spatial discretization $\mathcal{T}_{\Delta x}$ is applied to the convection term $v \cdot \nabla_x$. From (8.45), we obtain

$$\begin{aligned} f^{n+1} &= \mathcal{M}^{n+1} - \frac{\varepsilon}{\beta} \left(\frac{f^{n+1} + \alpha^T \mathbf{F}}{\Delta t} + \gamma^T \mathcal{T}_{\Delta x}(\mathbf{F}) \right) \\ &= \mathcal{M}^{n+1} - \frac{\varepsilon}{\beta} \left(\frac{f^{n+1} + \alpha^T \mathbf{F}}{\Delta t} + \gamma^T v \cdot \nabla_x \mathbf{F} \right) + O(\varepsilon \Delta x^p) \\ &= \mathcal{M}^{n+1} - \varepsilon \left(\partial_t f^{n+1} + v \cdot \nabla_x f^{n+1} \right) + O(\varepsilon \Delta t^s + \varepsilon \Delta x^p) \\ &= \mathcal{M}^{n+1} - \varepsilon \left(\partial_t \mathcal{M}^{n+1} + v \cdot \nabla_x \mathcal{M}^{n+1} \right) + O(\varepsilon^2 + \varepsilon \Delta t^s + \varepsilon \Delta x^p). \end{aligned} \tag{8.46}$$

On the other hand, taking the moments $\langle \phi \cdot \rangle$ on both sides of (8.45) yields

$$U^{n+1} = -\alpha^T \mathbf{U} - \Delta t \gamma^T \langle \mathcal{T}_{\Delta x}(\mathbf{F}) \phi \rangle, \tag{8.47}$$

which implies

$$\partial_t U^{n+1} + \nabla_x \cdot \langle v f^{n+1} \phi \rangle = O(\Delta t^s + \Delta x^p). \tag{8.48}$$

Finally substituting (8.46) into the above equation yields

$$\partial_t U^{n+1} + \nabla_x \cdot \langle v \left(\mathcal{M}^{n+1} - \varepsilon \left(\partial_t \mathcal{M}^{n+1} + v \cdot \nabla_x \mathcal{M}^{n+1} \right) \right) \phi \rangle = O(\Delta t^s + \Delta x^p + \varepsilon(\Delta t^s + \Delta x^p) + \varepsilon^2). \tag{8.49}$$

This means the scheme (8.45) is a consistent discretization to the Navier-Stokes equation when ε is small (provided the initial data are consistent up to order $O(\varepsilon)$). Since the viscosity term is of order $O(\varepsilon)$, one needs Δt^s and Δx^p to resolve $O(\varepsilon)$.

The IMEX-RK and IMEX-BDF schemes are high order in the kinetic regime $\varepsilon \sim O(1)$ (guaranteed by the order condition). Under certain assumptions, they can maintain the same order of accuracy in the fluid regime when $\varepsilon \to 0$ (guaranteed by the AP property). What about the intermediate regime (when ε is neither too big nor too small)? Generally speaking, there would be order reductions, especially for IMEX-RK schemes [34]. On the other hand, the IMEX-BDF schemes can exhibit uniform accuracy for a wide range of ε, which makes them particularly attractive for handling multiscale problems. This fact has recently been proved rigorously for the linear hyperbolic system with stiff relaxation [31].

8.3 Penalty based IMEX and exponential AP schemes for the homogeneous Boltzmann equation

We have focused exclusively on the stiff BGK equation (8.2). How about the stiff Boltzmann equation? Due to the complexity of the Boltzmann collision operator, the previous trick (obtaining $\mathcal{M}^{n+1}$ first and then solving for f^{n+1} would not work). Here we introduce two methods for the spatially homogeneous Boltzmann equation

$$\partial_t f = \frac{1}{\varepsilon} Q(f, f). \tag{8.50}$$

One is of IMEX flavor and one is of exponential flavor. The starting point of both methods is to rewrite (8.50) as

$$\partial_t f = \frac{1}{\varepsilon} P(f) - \frac{1}{\varepsilon} \mu f, \quad P(f) := Q(f, f) + \mu f, \tag{8.51}$$

where μ is a constant chosen large enough such that $P(f) \geq 0$. We know that the Boltzmann collision operator can be written as

$$Q(f, f) = Q^+(f, f) - L(f) f, \quad L(f) = A * f, \quad A(v) = \int_{S^{d-1}} B_\sigma(|v|, \sigma \cdot \hat{v}) \, \mathrm{d}\sigma, \tag{8.52}$$

hence μ can be chosen as $\|L(f)\|_{L^\infty}$ or $\rho\|A\|_{L^\infty}$.

In the IMEX method, one discretizes (8.51) as

$$\frac{f^{n+1}-f^n}{\Delta t}=\frac{1}{\varepsilon}P(f^n)-\frac{1}{\varepsilon}\mu f^{n+1}. \tag{8.53}$$

The rationale is that after penalization the stiff collision term $P(f)$ becomes less stiff, hence can be treated explicitly. The linear term μf is stiff but can be easily treated implicitly. (8.53) can be written as a convex combination

$$f^{n+1}=\frac{\varepsilon}{\varepsilon+\mu\Delta t}f^n+\frac{\mu\Delta t}{\varepsilon+\mu\Delta t}\frac{P(f^n)}{\mu}. \tag{8.54}$$

When $\varepsilon\to 0$, it implies $f^{n+1}\to P(f^n)/\mu$. Now if we start with consistent initial data $f^n=\mathcal{M}+O(\varepsilon)$. As $\varepsilon\to 0$, we would have $f^{n+1}\to\mathcal{M}$, i.e., the scheme is AP. Furthermore, if we start with $f^n\geq 0$, we still have $f^{n+1}\geq 0$. The similar idea can be applied to the spatially inhomogeneous Boltzmann equation, see [20] for more details.

In the exponential method [15], one further writes (8.51) as

$$\partial_t\left[(f-\mathcal{M})\mathrm{e}^{\frac{\mu}{\varepsilon}t}\right]=\frac{1}{\varepsilon}(P(f)-\mu\mathcal{M})\mathrm{e}^{\frac{\mu}{\varepsilon}t}, \tag{8.55}$$

since $\mathcal{M}$ remains unchanged during the collision step. This reformulation removes the stiffness and one can apply the standard explicit RK scheme to (8.55). Here we only mention two special cases. One is the forward Euler method:

$$f^{n+1}=f^n\mathrm{e}^{-\frac{\mu}{\varepsilon}\Delta t}+\mathcal{M}\left(1-\mathrm{e}^{-\frac{\mu}{\varepsilon}\Delta t}-\frac{\mu\Delta t}{\varepsilon}\mathrm{e}^{-\frac{\mu}{\varepsilon}\Delta t}\right)+\frac{P(f^n)}{\mu}\frac{\mu\Delta t}{\varepsilon}\mathrm{e}^{-\frac{\mu}{\varepsilon}\Delta t}. \tag{8.56}$$

The other is the explicit midpoint method:

$$\begin{cases} f^{(1)}=f^n\mathrm{e}^{-\frac{\mu}{2\varepsilon}\Delta t}+\mathcal{M}\left(1-\mathrm{e}^{-\frac{\mu}{2\varepsilon}\Delta t}-\frac{\mu\Delta t}{2\varepsilon}\mathrm{e}^{-\frac{\mu}{2\varepsilon}\Delta t}\right)+\frac{P(f^n)}{\mu}\frac{\mu\Delta t}{2\varepsilon}\mathrm{e}^{-\frac{\mu}{2\varepsilon}\Delta t},\\ f^{n+1}=f^n\mathrm{e}^{-\frac{\mu}{\varepsilon}\Delta t}+\mathcal{M}\left(1-\mathrm{e}^{-\frac{\mu}{\varepsilon}\Delta t}-\frac{\mu\Delta t}{\varepsilon}\mathrm{e}^{-\frac{\mu}{2\varepsilon}\Delta t}\right)+\frac{P(f^{(1)})}{\mu}\frac{\mu\Delta t}{\varepsilon}\mathrm{e}^{-\frac{\mu}{2\varepsilon}\Delta t}. \end{cases} \tag{8.57}$$

First of all, for both schemes, if we send $\varepsilon\to 0$, we have $f^{n+1}\to\mathcal{M}$. Secondly, it is easy to see that each step is a convex combination of positive functions. Therefore, if we start with $f^n\geq 0$, we still have $f^{n+1}\geq 0$.

8.4 A second-order positivity-preserving and AP scheme for stiff kinetic equations

We have discussed many AP schemes for the stiff kinetic equation (8.1). Now if we ask ourself the following question: in addition to just preserving the asymptotic limit, can we make the scheme positivity-preserving? For kinetic simulations, positivity is an important property as the basic unknown is the PDF. If f becomes negative, many

things can go wrong, say, the temperature is not well-defined, not even to mention the entropy.

By now it should be fairly clear that we can certainly do so if we are content with the first order (in time) scheme. For instance, one can do the splitting as in (8.5). The convection step can be easily made positive if we use, say, the first-order upwind scheme under certain CFL condition[7]. The collision step can also be made positive easily, not just for the BGK operator, even for the Boltzmann operator (see the previous section[8]). How about the second order (in time) scheme? A second thought will convince you that it is not so obvious: 1) the Strang splitting would not work (suffer from the order reduction when $\varepsilon \to 0$); 2) the IMEX schemes would not work because they generally do not preserve the positivity[9].

Therefore, we have to jump out of the conventional toolbox and think about something unconventional. In [33], second-order positivity-preserving and AP schemes are constructed for the BGK equation, which rely on a key correction step utilizing the Frechet derivative of the BGK operator. In [32], a more general framework is introduced which allows one to treat a large class of stiff kinetic equations of the form (8.1). We briefly describe the method here.

Suppose that the solution at time $t = t_0 + s$ to the homogeneous equation $\partial_t f = Q(f)$ with initial data $f|_{t_0} = g$ is denoted by $\varphi^s g$. Then the scheme for (8.1) reads:

$$\begin{aligned} f^{(0)} &= \varphi^{a\Delta t/\varepsilon} f^n, \\ f^{(1)} &= \varphi^{(1-2a)\Delta t/\varepsilon} \left[f^{(0)} - \Delta t v \cdot \nabla_x f^{(0)} \right], \\ f^{(2)} &= f^{(1)} - \Delta t v \cdot \nabla_x f^{(1)}, \\ f^{n+1} &= \varphi^{a\Delta t/\varepsilon} \left[\frac{1}{2} f^{(2)} + \frac{1}{2} \varphi^{(1-a)\Delta t/\varepsilon} f^n \right], \end{aligned} \tag{8.58}$$

where a is a constant satisfying $0 < a < 1/2$.

One can verify that (8.58) is second order when $\varepsilon = O(1)$. The positivity-preserving property is clear, provided the transport step is positivity-preserving. To check the AP property, we take the moments $\langle \phi \cdot \rangle$ on (8.58) to obtain

$$\begin{aligned} U^{(0)} &= U^n, \\ U^{(1)} &= U^{(0)} - \Delta t \nabla_x \cdot \langle v \phi f^{(0)} \rangle, \\ U^{(2)} &= U^{(1)} - \Delta t \nabla_x \cdot \langle v \phi f^{(1)} \rangle, \\ U^{n+1} &= \frac{1}{2}(U^{(2)} + U^n). \end{aligned} \tag{8.59}$$

[7]Higher order positivity-preserving spatial discretization is also possible, see for instance [49].

[8]Of course to solve the Boltzmann equation, one also needs a positivity-preserving scheme for the collision operator.

[9]In fact, there is an order barrier: there does not exist unconditionally strong stability preserving (SSP) implicit RK or multi-step schemes of order higher than one [24].

On the other hand, as $\varepsilon \to 0$, from (8.58) we know $f^{(0)} \to \mathcal{M}^{(0)}$, $f^{(1)} \to \mathcal{M}^{(1)}$, $f^{n+1} \to \mathcal{M}^{n+1}$. Therefore, (8.59) becomes

$$\begin{aligned} U^{(1)} &= U^n - \Delta t \nabla_x \cdot \langle v\phi \mathcal{M}^n \rangle, \\ U^{(2)} &= U^{(1)} - \Delta t \nabla_x \cdot \langle v\phi \mathcal{M}^{(1)} \rangle, \\ U^{n+1} &= \frac{1}{2}(U^{(2)} + U^n), \end{aligned} \tag{8.60}$$

which is the second order Heun's method applied to the limiting Euler equations, i.e., the scheme is AP.

To implement the scheme (8.58), we need to provide the solution map φ^s for the equation $\partial_t f = Q(f)$. This can be relaxed to an approximate solver as long as it is second order accurate, positivity-preserving, and AP. For example, the exponential method introduced in the previous section can be used when $Q(f)$ is the Boltzmann operator.

8.5 An entropic finite difference scheme for the Fokker-Planck equation

Let us consider the following spatially homogeneous Fokker-Planck equation:

$$\partial_t f = \frac{1}{\varepsilon} Q^{\mathrm{FP}}(f), \tag{8.61}$$

where Q^{FP} is given in (6.11). Here for simplicity, we ignore the factor ρT and consider

$$Q^{\mathrm{FP}}(f) = \nabla_v \cdot \left(\nabla_v f + \frac{(v-u)}{T} f \right) = \nabla_v \cdot \left(\mathcal{M} \nabla_v \left(\frac{f}{\mathcal{M}} \right) \right). \tag{8.62}$$

It can be checked that this operator conserves mass, momentum and energy, and satisfies the H-theorem (like the BGK operator).

Note that (8.61) is a diffusive type equation, if we use the explicit scheme, the time step needs to be $\Delta t \sim O(\varepsilon \Delta v^2)$, which can be quite restrictive if ε is small. Here we introduce a simple implicit finite difference scheme which possesses many nice features. For simplicity, we consider $d = 1$ and no-flux boundary condition. As before, we assume that the domain is large enough so that the quadrature error in v can be ignored.

The key is to discretize the second representation in (8.62):

$$Q_j^{\mathrm{FP},\Delta v} := \frac{1}{\Delta v^2} \left[\hat{\mathcal{M}}_{j+1/2} \left(\frac{f_{j+1}^{n+1}}{\mathcal{M}_{j+1}} - \frac{f_j^{n+1}}{\mathcal{M}_j} \right) - \hat{\mathcal{M}}_{j-1/2} \left(\frac{f_j^{n+1}}{\mathcal{M}_j} - \frac{f_{j-1}^{n+1}}{\mathcal{M}_{j-1}} \right) \right], \tag{8.63}$$

where $\mathcal{M}_j$ is defined as

$$\mathcal{M}_j = \frac{\rho}{\sqrt{2\pi T}} \mathrm{e}^{-\frac{|v_j - u|^2}{2T}}, \tag{8.64}$$

with ρ, u, T determined by the moments of the initial condition f^0. $\hat{\mathcal{M}}_{j+1/2}$ is a second-order positive approximation of $\mathcal{M}$ at grid point $v_{j+1/2}$, for example, one could choose $\hat{\mathcal{M}}_{j+1/2} = (\mathcal{M}_j + \mathcal{M}_{j+1})/2$. Then the scheme reads:

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} = \frac{1}{\varepsilon} Q_j^{\mathrm{FP},\Delta v}. \tag{8.65}$$

First of all, the scheme conserves mass by no-flux boundary condition:

$$\sum_j f_j^{n+1} = \sum_j f_j^n. \tag{8.66}$$

Secondly, the scheme is positivity-preserving: if $f_j^n \geq 0$, then $f_j^{n+1} \geq 0$. To see this, we assume that $f_j^{n+1}/\mathcal{M}_j$ attains its minimum at v_i, then we must have $f_i^{n+1} = f_i^n + \frac{\Delta t}{\varepsilon} Q_i^{\mathrm{FP},\Delta v} \geq 0$, hence all j, $f_j^{n+1}/\mathcal{M}_j \geq f_i^{n+1}/\mathcal{M}_i \geq 0$.

Furthermore, we have (by discrete integration by parts)

$$\begin{aligned}
&\sum_j Q_j^{\mathrm{FP},\Delta v} \ln\left(\frac{f_j^{n+1}}{\mathcal{M}_j}\right) \Delta v \\
=&\sum_j \frac{1}{\Delta v}\left[\hat{\mathcal{M}}_{j+1/2}\left(\frac{f_{j+1}^{n+1}}{\mathcal{M}_{j+1}} - \frac{f_j^{n+1}}{\mathcal{M}_j}\right) - \hat{\mathcal{M}}_{j-1/2}\left(\frac{f_j^{n+1}}{\mathcal{M}_j} - \frac{f_{j-1}^{n+1}}{\mathcal{M}_{j-1}}\right)\right] \ln\left(\frac{f_j^{n+1}}{\mathcal{M}_j}\right) \\
=&-\sum_j \frac{1}{\Delta v}\hat{\mathcal{M}}_{j+1/2}\left(\frac{f_{j+1}^{n+1}}{\mathcal{M}_{j+1}} - \frac{f_j^{n+1}}{\mathcal{M}_j}\right)\left[\ln\left(\frac{f_{j+1}^{n+1}}{\mathcal{M}_{j+1}}\right) - \ln\left(\frac{f_j^{n+1}}{\mathcal{M}_j}\right)\right] \\
\leq& 0,
\end{aligned} \tag{8.67}$$

and the equality holds iff $f_j^{n+1} = c\mathcal{M}_j$ for all j, and the constant $c = 1$ by mass conservation. Therefore, we have proved

$$\sum_j Q_j^{\mathrm{FP},\Delta v} \ln\left(\frac{f_j^{n+1}}{\mathcal{M}_j}\right) \Delta v = 0 \iff f_j^{n+1} = \mathcal{M}_j,\ \forall j \iff Q_j^{\mathrm{FP},\Delta v} = 0,\ \forall j. \tag{8.68}$$

This means the scheme (8.65) is AP: as $\varepsilon \to 0$, $f_j^{n+1} \to \mathcal{M}_j$ for all j.

Finally, the scheme decays the relative entropy: define

$$H^n = \sum_j f_j^n \ln\left(\frac{f_j^n}{\mathcal{M}_j}\right) \Delta v, \tag{8.69}$$

then

$$H^{n+1} \leq H^n. \tag{8.70}$$

Indeed,

$$\begin{aligned} H^{n+1} - H^n &= \sum_j \left(f_j^{n+1} \ln\left(\frac{f_j^{n+1}}{\mathcal{M}_j}\right) - f_j^n \ln\left(\frac{f_j^n}{\mathcal{M}_j}\right)\right) \Delta v \\ &= \sum_j \left((f_j^{n+1} - f_j^n) \ln\left(\frac{f_j^{n+1}}{\mathcal{M}_j}\right) + f_j^n \ln\left(\frac{f_j^{n+1}}{f_j^n}\right)\right) \Delta v \\ &:= I_1 + I_2, \end{aligned} \tag{8.71}$$

where

$$\begin{aligned} I_1 &= \sum_j (f_j^{n+1} - f_j^n) \ln\left(\frac{f_j^{n+1}}{\mathcal{M}_j}\right) \Delta v = \frac{\Delta t}{\varepsilon} \sum_j Q_j^{\mathrm{FP},\Delta v} \ln\left(\frac{f_j^{n+1}}{\mathcal{M}_j}\right) \Delta v \le 0, \\ I_2 &= \sum_j f_j^n \ln\left(\frac{f_j^{n+1}}{f_j^n}\right) \Delta v \le \sum_j f_j^n \left(\frac{f_j^{n+1}}{f_j^n} - 1\right) \Delta v = 0, \end{aligned} \tag{8.72}$$

by inequality $\ln x \le x - 1$ and mass conservation.

9 Numerical methods for the Vlasov equation

In this section, we review some numerical methods for solving the Vlasov equation (see Section 6.4). For simplicity, we will consider the following (dimensionless) Vlasov-Poisson equation describing the electron distribution:

$$\partial_t f + v \cdot \nabla_x f + E \cdot \nabla_v f = 0, \tag{9.1}$$

$$E = -\nabla_x \phi, \quad -\Delta_x \phi = \rho - 1, \quad \rho = \int_{\mathbb{R}^d} f \,\mathrm{d}v. \tag{9.2}$$

Note that (9.1) can be written in a conservative form:

$$\partial_t f + \nabla_x \cdot (vf) + \nabla_v \cdot (Ef) = 0. \tag{9.3}$$

This system possesses a number of conservation properties. Define

$$J = \int_{\mathbb{R}^d} vf \,\mathrm{d}v, \quad I = \int_{\mathbb{R}^d} \frac{1}{2}|v|^2 f \,\mathrm{d}v, \tag{9.4}$$

and assume periodic boundary condition, we have conservation of mass, momentum and energy:

$$\int_\Omega \rho \,\mathrm{d}x = \int_\Omega 1 \,\mathrm{d}x, \quad \int_\Omega J \,\mathrm{d}x = \mathrm{Const}, \quad \int_\Omega \left(I + \frac{1}{2}|E|^2\right) \mathrm{d}x = \mathrm{Const}. \tag{9.5}$$

To see this, multiply (9.1) by 1, v, $|v|^2/2$, and integrate in v and x, we obtain

$$\partial_t \int_\Omega \rho \,\mathrm{d}x = 0, \quad \partial_t \int_\Omega J \,\mathrm{d}x = \int_\Omega \rho E \,\mathrm{d}x, \quad \partial_t \int_\Omega I \,\mathrm{d}x = \int_\Omega J \cdot E \,\mathrm{d}x. \tag{9.6}$$

On the other hand, using the identity

$$0 = \int_\Omega E \times (\nabla_x \times E)\,\mathrm{d}x = \frac{1}{2}\int_\Omega \nabla_x |E|^2\,\mathrm{d}x - \int_\Omega (E\cdot\nabla_x)E\,\mathrm{d}x = \int_\Omega (\nabla_x\cdot E)E\,\mathrm{d}x, \quad (9.7)$$

we have

$$\int_\Omega \rho E\,\mathrm{d}x = \int_\Omega (\nabla_x\cdot E + 1)E\,\mathrm{d}x = 0. \quad (9.8)$$

Using the mass conservation, we have

$$\begin{aligned} &\int_\Omega J\cdot E\,\mathrm{d}x = -\int_\Omega J\cdot\nabla_x\phi\,\mathrm{d}x = \int_\Omega \phi\nabla_x\cdot J\,\mathrm{d}x = -\int_\Omega \phi\partial_t\rho\,\mathrm{d}x \\ =& -\int_\Omega \phi\nabla_x\cdot(\partial_t E)\,\mathrm{d}x = \int_\Omega \nabla_x\phi\cdot\partial_t E\,\mathrm{d}x = -\int_\Omega E\cdot\partial_t E\,\mathrm{d}x \\ =& -\int_\Omega \frac{1}{2}\partial_t|E|^2\,\mathrm{d}x. \end{aligned} \quad (9.9)$$

9.1 Semi-Lagrangian methods

To numerically solve the Vlasov equation (9.1), the simplest way is to use the operator splitting:

$$\partial_t f + v\cdot\nabla_x f = 0, \quad (9.10)$$

$$\partial_t f + E(t,x)\cdot\nabla_v f = 0. \quad (9.11)$$

Then over each substep, we get a "constant" coefficient advection equation[10]. Indeed, (9.10) can be viewed as an advection equation in the physical space with constant velocity v. For (9.11), if we integrate over v, we get $\partial_t\rho = 0$, hence ρ remains unchanged over this step, consequently ϕ or E remains unchanged. Therefore, (9.11) can be viewed as an advection equation in the velocity space with constant velocity E. After splitting, each substep can be solved exactly by tracing back the characteristics. However, the characteristics may not pass through the grid points, hence some interpolation is needed. This is the basic idea of the classical semi-Lagrangian method [10].

In this section, we give a brief description of the above method for the 1D Vlasov-Poisson equation. For more details, the readers can consult the lecture notes [46]. In 1D, the equation reads:

$$\partial_t f + v\partial_x f + E\partial_v f = 0, \quad x\in[x_L, x_R], \quad (9.12)$$

$$E = -\partial_x\phi, \quad -\partial_{xx}\phi = \rho - 1, \quad \rho = \int_{-L}^{L} f\,\mathrm{d}v, \quad (9.13)$$

where we assume the periodic boundary condition in x. For v, we assume L is chosen large enough so that the domain truncation error is negligible.

[10] From a parallel computing viewpoint, splitting method has its merit in that: 1) the convection part is naturally parallelizable in v; 2) the field part is naturally parallelizable in x.

The first ingredient we need is the interpolation. A commonly used one is the B-splines, which are constructed recursively as follows: the degree 0 B-spline is defined by

$$S^0(x) = \begin{cases} 1, & |x| \le \frac{1}{2}, \\ 0, & \text{elsewhere.} \end{cases} \tag{9.14}$$

High-order B-splines of degree $m \ge 1$ are defined by

$$S^m(x) = S^0 * S^{m-1}(x) = \int_{-\frac{1}{2}}^{\frac{1}{2}} S^{m-1}(x-u)\,\mathrm{d}u = \int_{x-\frac{1}{2}}^{x+\frac{1}{2}} S^{m-1}(u)\,\mathrm{d}u. \tag{9.15}$$

In particular, the degree 1 B-spline is

$$S^1(x) = \begin{cases} 1 - |x|, & |x| \le 1, \\ 0, & \text{elsewhere;} \end{cases} \tag{9.16}$$

the degree 2 B-spline is

$$S^2(x) = \begin{cases} \frac{1}{2}\left(\frac{3}{2} - |x|\right)^2, & \frac{1}{2} \le |x| \le \frac{3}{2}, \\ \frac{3}{4} - |x|^2, & |x| \le \frac{1}{2}, \\ 0, & \text{elsewhere;} \end{cases} \tag{9.17}$$

and the degree 3 B-spline is

$$S^3(x) = \begin{cases} \frac{1}{6}\left(2 - |x|\right)^3, & 1 \le |x| \le 2, \\ \frac{2}{3} - |x|^2 + \frac{1}{2}|x|^3, & |x| \le 1, \\ 0, & \text{elsewhere.} \end{cases} \tag{9.18}$$

Now consider the interval $[a, b]$ with uniform grid points: $x_i = a + i\Delta x$, $i = 0, \ldots, N$, $\Delta x = (b-a)/N$. Suppose we are given the function values $f(x_i)$ at all grid points, then a cubic spline interpolant $f_{\Delta x}(x)$ of $f(x)$ is given by

$$f_{\Delta x}(x) = \sum_{j=0}^{N-1} a_j S^m\left(\frac{x - x_j}{\Delta x}\right). \tag{9.19}$$

with the coefficients a_j determined by the interpolation condition: $f_{\Delta x}(x_i) = f(x_i)$, $i = 1, \ldots, N$, $f_{\Delta x}(x)$ is a cubic polynomial over each subinterval, and $f_{\Delta x}(x) \in C^2[a, b]$ (note that we still need two additional conditions which could be the periodic boundary conditions $f_{\Delta x}(a) = f_{\Delta x}(b)$, $f'_{\Delta x}(a) = f'_{\Delta x}(b)$). In particular, if $f(x_i) \equiv C$, we have $a_i \equiv C$.

The B-splines verify the following important properties: $S^m(x) \ge 0$, symmetric, and has compact support. Furthermore,

- Unit mean:
$$\int_{-\infty}^{\infty} S^m(x)\,\mathrm{d}x = 1.$$
- Partition of unity:
$$\sum_{j=0}^{N-1} S^m\left(\frac{x - x_j}{\Delta x}\right) = 1.$$

The full algorithm proceeds as follows:

- Initialization: Given $f^0(x_i, v_j)$, deduce $\rho^0(x_i) = \sum_j f^0(x_i, v_j)\Delta v$, and solve the Poisson equation to obtain $\phi^0(x_i)$, hence $E^0(x_i)$.
- At time step t^n, given $f^n(x_i, v_j)$ and $E^n(x_i)$,
  - Solve $\partial_t f + E^n \partial_v f = 0$ for a half time step $\Delta t/2$ using the semi-Lagrangian method to obtain $f^*(x_i, v_j) = f^n(x_i, v_j - E^n(x_i)\Delta t/2)$.
  - Solve $\partial_t f + v\partial_x f = 0$ for a full time step Δt using the semi-Lagrangian method to obtain $f^{**}(x_i, v_j) = f^*(x_i - v_j\Delta t, v_j)$.
  - Compute $\rho^{n+1}(x_i) = \sum_j f^{**}(x_i, v_j)\Delta v$, and solve the Poisson equation to obtain $\phi^{n+1}(x_i)$, hence $E^{n+1}(x_i)$.
  - Solve $\partial_t f + E^{n+1}\partial_v f = 0$ for a half time step $\Delta t/2$ using the semi-Lagrangian method to obtain $f^{n+1}(x_i, v_j) = f^{**}(x_i, v_j - E^{n+1}(x_i)\Delta t/2)$.

  Note that the spline interpolation is needed to get value $f^n(x_i, v_j - E^n(x_i)\Delta t/2)$ using $f^n(x_i, v_j)$, and similarly for other semi-Lagrangian steps.

9.2 Particle in cell (PIC) methods

We seek a particle solution as

$$f_N(t, x, v) = \sum_{p=1}^{N} w_p \delta(x - x_p(t))\delta(v - v_p(t)), \tag{9.20}$$

then the particle position and velocity $x_p(t)$ and $v_p(t)$ solve

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} x_p = v_p, \\ \dfrac{\mathrm{d}}{\mathrm{d}t} v_p = E_p(t) + v_p \times B_p(t). \end{cases} \tag{9.21}$$

Correspondingly,

$$\begin{aligned} \rho_N(t, x) &= \int f_N(t, x, v)\,\mathrm{d}v = \sum_{p=1}^{N} w_p \delta(x - x_p(t)), \\ J_N(t, x) &= \int v f_N(t, x, v)\,\mathrm{d}v = \sum_{p=1}^{N} w_p \delta(x - x_p(t)) v_p(t). \end{aligned} \tag{9.22}$$

To define them on the grid x_i, we convolve with a spline function $S_\varepsilon(x) = \frac{1}{\varepsilon^3} S^m\left(\frac{x}{\varepsilon}\right)$:

$$\begin{aligned} \rho_i(t) &= \rho_N * S_\varepsilon = \sum_{p=1}^N w_p S_\varepsilon(x_i - x_p(t)), \\ J_i(t) &= J_N * S_\varepsilon = \sum_{p=1}^N w_p S_\varepsilon(x_i - x_p(t)) v_p(t). \end{aligned} \tag{9.23}$$

Then using these values to solve the Maxwell equation to obtain $E_i(t)$ and $B_i(t)$. Finally to get them back to the particle position x_p, we take

$$E_p(t) = \sum_i E_i(t) S_\varepsilon(x_p - x_i), \quad B_p(t) = \sum_i B_i(t) S_\varepsilon(x_p - x_i). \tag{9.24}$$

Let's check the conservation properties. Conservation of mass is obvious:

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{p=1}^N w_p = 0. \tag{9.25}$$

Conservation of momentum:

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t} \left(\sum_{p=1}^N w_p v_p + \sum_i E_i \times B_i \right) \\ =& \sum_{p=1}^N w_p (E_p + v_p \times B_p) + \sum_i \partial_t (E_i \times B_i) \\ =& \sum_i (\rho_i E_i + J_i \times B_i) + \sum_i (\partial_t E_i \times B_i + E_i \times \partial_t B_i) = ...0. \end{aligned} \tag{9.26}$$

Conservation of energy:

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}t} \left(\sum_{p=1}^N w_p \frac{1}{2} |v_p|^2 + \sum_i \frac{1}{2} (|E_i|^2 + |B_i|^2) \right) \\ =& \sum_{p=1}^N w_p v_p \cdot (E_p + v_p \times B_p) + \sum_i (E_i \cdot \partial_t E_i + B_i \cdot \partial_t B_i) \\ =& \sum_i J_i \cdot E_i + \sum_i (E_i \cdot \partial_t E_i + B_i \cdot \partial_t B_i) = ...0. \end{aligned} \tag{9.27}$$

For entropy, define

$$H(t) = \int \int \left(\sum_{p=1}^N w_p S_\varepsilon(x - x_p) S_\varepsilon(v - v_p) \right) \ln \left(\sum_{p=1}^N w_p S_\varepsilon(x - x_p) S_\varepsilon(v - v_p) \right) \mathrm{d}v \, \mathrm{d}x \tag{9.28}$$

Then

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}H(t) &= \sum_{p=1}^{N} w_p \int\int \left(S_\varepsilon(v-v_p)\nabla_{x_p} S_\varepsilon(x-x_p)\cdot\frac{\mathrm{d}x_p}{\mathrm{d}t} + S_\varepsilon(x-x_p)\nabla_{v_p} S_\varepsilon(v-v_p)\cdot\frac{\mathrm{d}v_p}{\mathrm{d}t}\right) \\ &\quad \times \ln\left(\sum_{p=1}^{N} w_p S_\varepsilon(x-x_p)S_\varepsilon(v-v_p)\right)\,\mathrm{d}v\,\mathrm{d}x \\ &= \sum_{p=1}^{N} w_p \int\int \left(S_\varepsilon(v-v_p)\nabla_{x_p} S_\varepsilon(x-x_p)\cdot v_p + S_\varepsilon(x-x_p)\nabla_{v_p} S_\varepsilon(v-v_p)\cdot(E_p(t)+v_p\times B_p(t))\right) \\ &\quad \times \ln\left(\sum_{p=1}^{N} w_p S_\varepsilon(x-x_p)S_\varepsilon(v-v_p)\right)\,\mathrm{d}v\,\mathrm{d}x = 0.\end{aligned} \tag{9.29}$$

For time discretization, one could do the Stormer-Verlet algorithm:

$$\begin{cases} v_p^{n+1/2} = v_p^n + \dfrac{\Delta t}{2}E_p^n, \\ x_p^{n+1} = x_p^n + \Delta t v_p^{n+1/2}, \\ v_p^{n+1} = v_p^{n+1/2} + \dfrac{\Delta t}{2}E_p^{n+1}, \end{cases} \tag{9.30}$$

where to compute E_p^{n+1}, we use x_p^{n+1} to define ρ_i^{n+1} on the grid, then solve the Poisson equation to obtain E_i^{n+1}, and finally get back to E_p^{n+1} at the particle position.

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