Accurate Deterministic Solutions for the Classic Boltzmann Shock Profile

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ACCURATE DETERMINISTIC SOLUTIONS FOR THE CLASSIC BOLTZMANN SHOCK PROFILE

by

YUBEI YUE

A dissertation submitted to the Graduate Faculty in Physics in partial fulfillment of
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Abstract

ACCUARATE DETERMINISTIC SOLUTIONS FOR THE CLASSIC BOLTZMANN SHOCK PROFILE

by

YUBEI YUE

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The Boltzmann equation or Boltzmann transport equation is a classical kinetic equation devised by Ludwig Boltzmann in 1872. It is regarded as a fundamental law in rarefied gas dynamics. Rather than using macroscopic quantities such as density, temperature, and pressure to describe the underlying physics, the Boltzmann equation uses a distribution function in phase space to describe the physical system, and all the macroscopic quantities are weighted averages of the distribution function. The information contained in the Boltzmann equation is surprisingly rich, and the Euler and Navier-Stokes equations of fluid dynamics can be derived from it using series expansions. Moreover, the Boltzmann equation can reach regimes far from the capabilities of fluid dynamical equations, such as the realm of rarefied gases – the topic of this thesis. Although the Boltzmann equation is very powerful, it is extremely difficult to solve in most situations. Thus the only hope is to solve it numerically. But soon one finds that even a numerical simulation of the equation is extremely difficult, due to both the complex and high-dimensional integral in the collision operator, and the hyperbolic phase-space advection terms. For
this reason, until few years ago most numerical simulations had to rely on Monte Carlo techniques. In this thesis I will present a new and robust numerical scheme to compute direct deterministic solutions of the Boltzmann equation, and I will use it to explore some classical gas-dynamical problems. In particular, I will study in detail one of the most famous and intrinsically nonlinear problems in rarefied gas dynamics, namely the accurate determination of the Boltzmann shock profile for a gas of hard spheres.
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# Contents

Contents vii

List of Figures ix

List of Tables xi

1 Introduction to Boltzmann equation 1
   1.1 History and concepts . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 1
   1.2 Basic equation . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 2
   1.3 Molecule model . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 9
   1.4 Collision invariants . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 10
   1.5 The Maxwell distribution . . . . . . . . . . . . . . . . . . . . . . . . . . 13
   1.6 The H-Theorem . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 15
   1.7 The macroscopic equations . . . . . . . . . . . . . . . . . . . . . . . . . . 17
   1.8 Model equations . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 22
   1.9 Knudsen number and dimensionless Boltzmann equation . . . . . . . . . 24
   1.10 The linearized collision operator . . . . . . . . . . . . . . . . . . . . . . 25
   1.11 Linearized Boltzmann equation . . . . . . . . . . . . . . . . . . . . . . . 28

2 Calculating the Collision Operator 30
   2.1 Background . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 30
   2.2 Transforming from velocity space to the spectral space . . . . . . . . . . 32
   2.3 Evaluating the collision operator . . . . . . . . . . . . . . . . . . . . . . 33
   2.4 Time relaxation process in the spatially homogeneous case . . . . . . . . 37
   2.5 GPU acceleration . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 46

3 Solving the transport equation 48
   3.1 Background . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 48
   3.2 The splitting method . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 49
   3.3 Solving the 1-d transport equation . . . . . . . . . . . . . . . . . . . . . . 51
   3.4 WENO method . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 53
3.4.1 Time Advance ....................................................... 53
3.4.2 WENO Reconstruction ........................................... 53
3.4.3 Flux Calculation ................................................... 56
3.4.4 Maximum-principle-satisfying flux limiter ...................... 58
3.5 PFC ................................................................. 59

4 Shock waves in the Boltzmann equation .............................. 63
  4.1 Shock waves ....................................................... 63
  4.2 Analytical study ................................................... 64
  4.3 Numerical study ................................................... 75

5 Shock curvature correction ............................................. 82
  5.1 Background ....................................................... 82
  5.2 Introduction ....................................................... 83
  5.3 Jump conditions .................................................. 84
    5.3.1 Zero-order conditions ...................................... 86
    5.3.2 First-order conditions ..................................... 87
  5.4 1-1 momentum flow discontinuity ................................ 89
  5.5 Concluding remarks ............................................. 93

Bibliography ............................................................ 94
# List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Collision between a pair of molecules</td>
<td>4</td>
</tr>
<tr>
<td>1.2</td>
<td>Possible collision pair</td>
<td>5</td>
</tr>
<tr>
<td>2.1</td>
<td>Periodic distribution in the phase space</td>
<td>33</td>
</tr>
<tr>
<td>2.2</td>
<td>Collision algorithm flow chart</td>
<td>39</td>
</tr>
<tr>
<td>2.3</td>
<td>n=64 time step=0</td>
<td>40</td>
</tr>
<tr>
<td>2.4</td>
<td>n=64 time step=50</td>
<td>40</td>
</tr>
<tr>
<td>2.5</td>
<td>n=64 time step=200</td>
<td>41</td>
</tr>
<tr>
<td>2.6</td>
<td>n=81 time step=0</td>
<td>41</td>
</tr>
<tr>
<td>2.7</td>
<td>n=81 time step=50</td>
<td>42</td>
</tr>
<tr>
<td>2.8</td>
<td>n=81 time step=200</td>
<td>42</td>
</tr>
<tr>
<td>2.9</td>
<td>n=100 time step=0</td>
<td>43</td>
</tr>
<tr>
<td>2.10</td>
<td>n=100 time step=50</td>
<td>43</td>
</tr>
<tr>
<td>2.11</td>
<td>n=100 time step=200</td>
<td>44</td>
</tr>
<tr>
<td>2.12</td>
<td>n=100 time step=250, X-Y intersection at Z=50</td>
<td>44</td>
</tr>
<tr>
<td>2.13</td>
<td>n=250 time step=250, intersection at the center</td>
<td>45</td>
</tr>
<tr>
<td>2.14</td>
<td>Compare CPU and GPU time (in seconds)</td>
<td>46</td>
</tr>
<tr>
<td>3.1</td>
<td>Splitting algorithm</td>
<td>51</td>
</tr>
<tr>
<td>3.2</td>
<td>Finite volume grid</td>
<td>52</td>
</tr>
<tr>
<td>3.3</td>
<td>WENO computational cells</td>
<td>54</td>
</tr>
<tr>
<td>3.4</td>
<td>PFC: Integral at the right boundary for a positive velocity</td>
<td>61</td>
</tr>
<tr>
<td>3.5</td>
<td>PFC: Integral at the left boundary for a negative velocity</td>
<td>62</td>
</tr>
<tr>
<td>4.1</td>
<td>Mach 1.2 density profile</td>
<td>70</td>
</tr>
<tr>
<td>4.2</td>
<td>Mach 1.59 density profile</td>
<td>71</td>
</tr>
<tr>
<td>4.3</td>
<td>Mach 2.0 density profile</td>
<td>72</td>
</tr>
<tr>
<td>4.4</td>
<td>Mach 2.5 density profile</td>
<td>73</td>
</tr>
<tr>
<td>4.5</td>
<td>Mach 3.0 density profile</td>
<td>74</td>
</tr>
<tr>
<td>4.6</td>
<td>Density</td>
<td>77</td>
</tr>
<tr>
<td>4.7</td>
<td>Temperature</td>
<td>77</td>
</tr>
<tr>
<td>4.8</td>
<td>DSMC</td>
<td>80</td>
</tr>
<tr>
<td>4.9</td>
<td>WENO-LF</td>
<td>80</td>
</tr>
<tr>
<td>Figure</td>
<td>Description</td>
<td>Page</td>
</tr>
<tr>
<td>--------</td>
<td>-----------------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>4.10</td>
<td>WENO-LF with fix</td>
<td>80</td>
</tr>
<tr>
<td>4.11</td>
<td>WENO-Rusanov</td>
<td>80</td>
</tr>
<tr>
<td>4.12</td>
<td>PFC</td>
<td>80</td>
</tr>
<tr>
<td>4.13</td>
<td>WENO-Godunov</td>
<td>80</td>
</tr>
<tr>
<td>4.14</td>
<td>WENO-Godunov vs. DSMC comparison</td>
<td>81</td>
</tr>
<tr>
<td>4.15</td>
<td>DSMC</td>
<td>81</td>
</tr>
<tr>
<td>4.16</td>
<td>WENO-Godunov</td>
<td>81</td>
</tr>
<tr>
<td>5.1</td>
<td>Local coordinate system at a point on the shock</td>
<td>85</td>
</tr>
<tr>
<td>5.2</td>
<td>$M = 2$ shock profiles</td>
<td>90</td>
</tr>
<tr>
<td>5.3</td>
<td>$v_2^2$ moment for $M = 2$</td>
<td>91</td>
</tr>
<tr>
<td>5.4</td>
<td>Odd and Even part of the $v_2^2$ moment</td>
<td>92</td>
</tr>
<tr>
<td>5.5</td>
<td>Odd and even parts of the $v_2^2$ moment for $M = 2$</td>
<td>92</td>
</tr>
<tr>
<td>5.6</td>
<td>$\int_{-\infty}^{+\infty} dX \int v_2^2 (\tilde{f}_0^* - \hat{f}) , dv$ as a function of the Mach number</td>
<td>92</td>
</tr>
</tbody>
</table>
List of Tables

2.1 Compare CPU and GPU time (in seconds) ........................................ 47
4.1 MFP for the hot side ................................................................. 68
4.2 comparing 1-norm and 2-norm .................................................. 69
4.3 Best $\beta$ .............................................................................. 69
4.4 Mach 1.2 density: estimated best $\beta = 0.35$ ............................. 70
4.5 Mach 1.59 density: estimated best $\beta = 1.28$ ............................ 71
4.6 Mach 2.0 density: estimated best $\beta = 2.30$ ............................ 72
4.7 Mach 2.5 density: estimated best $\beta = 3.39$ ............................ 73
4.8 Mach 3.0 density: estimated best $\beta = 4.18$ ............................ 74
Dedicated to my parents and sister for their constant support and unconditional love.
Chapter 1

Introduction to Boltzmann equation

1.1 History and concepts

The Boltzmann transport equation is a member of a wide family of kinetics equation used in describing non-equilibrium phenomena. In the kinetic theory of gases, one studies microscopic collisions and translations at the molecular level. Due to the vast number of molecules in the system, it is not possible to follow the dynamics of each molecule, and a continuous description is the only choice. The (normalized) distribution function takes scalar values between 0 and 1, and represents the probability of molecules at a specific space position and with a specific velocity. The macroscopic quantities are obtained by integrating out the velocity variables. In this way, macroscopic quantities such as temperature, density and pressure can be obtained from the microscopic information. A key component in any kinetic equation is the so-called collision operator, and it is the collision operator that distinguishes various kinetic models.

The Boltzmann equation is widely used in gas dynamics, and there are many molecular collision models used in the equation, such as Maxwellian molecules, hard sphere molecules and others that we will discuss in the subsequent section. The Boltzmann equation is a non-linear equation and contains very rich information. Indeed if one defines a scalar called Knudsen number to be the ratio of the average spatial separation between two subsequent collisions of a molecule to the typical length in the macroscopic
flow under consideration, then for very small Knudsen number the classical Euler equation and Navier-Stokes equations of fluid mechanics can be derived from the Boltzmann using series expansion, as we will also see later. In the other limiting case of a very large Knudsen number, one recovers a much simpler situation, the collision-free transport flow.

The main focus of this thesis is on the middle ground between these two limiting cases, the so-called the transition regime. There are many interesting problems in this regime that we will explore later on. In order to describe a rarefied gas flow, one also needs appropriate boundary conditions. The boundary conditions describe the gas-surfaces interactions, and connect the theory to solid state physics, forming a research field of their own. In this thesis, we will encounter only two simple boundary conditions, reverse and specular reflection with an ideal wall.

1.2 Basic equation

Let us start by deriving the Boltzmann equation from the collision dynamics between a pair of hard sphere molecules (see details in [5]). Let \( P^{(1)}(x_1, \xi_1, t) \) denotes the probability density of finding particle 1 at position \( x_1 \) and with velocity \( \xi_1 \). The 3-d coordinate space and 3-d velocity space span a six-dimension phase space. The probability density is associated with each point in this phase space. Assuming an elastic collision takes place between two molecules, using classical energy and momentum conservation laws we have,

\[
\begin{align*}
\xi'_1 &= \xi_1 - n \cdot (\xi_1 - \xi_2) \\
\xi'_2 &= \xi_2 + n \cdot (\xi_1 - \xi_2).
\end{align*}
\]

(1.1)

In the above equations, \( \xi_1 \) and \( \xi_2 \) are the velocities of molecule 1 and 2 before the collision, and \( \xi'_1 \) and \( \xi'_2 \) are the velocities after the collision. The vector \( n \) is a unit vector, defined as

\[
n = \frac{\xi_1 - \xi'_1}{|\xi_1 - \xi'_1|}.
\]

(1.2)

One can verify that the above relations between pre- and post-collisional velocities conserve energy and momentum. To get a better understanding of this, we subtract the two
equations in 1.1, and get
\[ V' = V - 2n(n \cdot V), \] (1.3)
where \( V \) and \( V' \) are the relative velocities defined as
\[ V = \xi_1 - \xi_2, \]
\[ V' = \xi_1' - \xi_2'. \] (1.4)

Eqn.1.3 states that the post collision relative velocity \( V' \) is actually a specular reflection of the pre-collision relative velocity \( V \) at the collision point. To see this, taking the dot product with \( n \) on both sides we get
\[ n \cdot V' = -n \cdot V. \] (1.5)

That is to say, \( V' \) and \( V \) have the same amplitude but "reverse" angles relative to \( n \).

We can split \( V \) into a normal component \( V_n \) parallel to \( n \) and a transversal component \( V_t \) orthogonal to \( n \). Then Eqn.1.5 becomes
\[ V'_n = -V_n. \] (1.6)

Projecting Eqn.1.3 (orthogonally to \( n \)) we get
\[ V'_t = V_t. \] (1.7)

The relative velocity changes sign in the normal direction after a collision, but remains unchanged in the transversal direction. The relation is also illustrated in the figure below.

In the absence of collisions, we have the continuity equation
\[ \frac{\partial P^{(1)}(x_1, \xi_1, t)}{\partial t} + \xi_1 \cdot \frac{\partial P^{(1)}(x_1, \xi_1, t)}{\partial x_1} = 0. \] (1.8)

Now we need take the collisional effects into account. We denote by \( G \) the gain term, such that \( Gdx_1d\xi_1dt \) is the expected number of molecules entering into the region between \( x_1 \) and \( x_1 + dx_1 \) with velocity between \( \xi_1 \) and \( \xi_1 + d\xi_1 \) within time interval \( dt \) coming from other 6-d phase space points. We denote by \( L \) the loss term, such that \( Ldx_1d\xi_1dt \) is the
expected number of molecules leaving the region between \( \mathbf{x}_1 \) and \( \mathbf{x}_1 + d\mathbf{x}_1 \) with velocity between \( \mathbf{\xi}_1 \) and \( \mathbf{\xi}_1 + d\mathbf{\xi}_1 \) within time interval \( dt \) and flowing into other 6-d phase space points. Then the full equation reads

\[
\frac{\partial P^{(1)}(\mathbf{x}_1, \mathbf{\xi}_1, t)}{\partial t} + \mathbf{\xi}_1 \cdot \frac{\partial P^{(1)}(\mathbf{x}_1, \mathbf{\xi}_1, t)}{\partial \mathbf{x}_1} = G - L. \tag{1.9}
\]

The gain term \( G \) and loss term \( L \) are non-local terms, because in order to evaluate their effect at one phase space point \( (\mathbf{x}_1, \mathbf{\xi}_1) \), one always need another phase space point \( (\mathbf{x}_2, \mathbf{\xi}_2) \) and a new probability \( P^{(2)}(\mathbf{x}_1, \mathbf{\xi}_1, \mathbf{x}_2, \mathbf{\xi}_2, t) \), the probability of having the first molecule at phase space point \( (\mathbf{x}_1, \mathbf{\xi}_1) \) and the second molecule at phase space point \( (\mathbf{x}_2, \mathbf{\xi}_2) \) at time \( t \), which is the prerequisite for an occurrence of a collision. Integrating out all possible phase space points \( (\mathbf{x}_2, \mathbf{\xi}_2) \), will give the final expression for the gain and loss terms.

Let us consider a \( N \)-particle system, and randomly pick one particle at the phase space
Chapter 1. Introduction to Boltzmann equation

Figure 1.2: Possible collision pair

point \((x_1, \xi_1)\). We can choose the reference frame so that the molecule is static and with an effective diameter of \(2\sigma\), where \(\sigma\) is the physical diameter, and assume all other particles are ideal point masses with velocity \(\xi_i - \xi_1\), where the index \(i\) refers to all the particles from 2 to \(N\). Because all particles are identical and indistinguishable, we must have

\[
G = (N-1)g \\
L = (N-1)l,
\]

(1.10)

where lower-case \(g\) and \(l\) are the gain term and loss term associated with only one molecule which collides with \((x_1, \xi_1)\), for example, the particle at \((x_2, \xi_2)\). Let \(x_1\) be the center of the first molecule, then the position of the second molecule with respect to it is \(x_2 = x_1 + \sigma n\), where \(n\) is a unit vector joining the center of molecule 1 and point mass molecule 2. We need to count all the molecules with velocity \(\xi_2\) that could have a collision with
molecule 1 during time \( t \) to \( t + dt \). To do so we need integrate over a cylinder volume with height \( |(\xi_2 - \xi_1) \cdot n| dt \), and with a base area \( dS = \sigma^2 d\mathbf{n} \). This cylinder with volume \( \sigma^2 d\mathbf{n}|(\xi_2 - \xi_1) \cdot n| dt \) contains all the particles with velocity \( \xi_2 \) that will collide with particle 1 within the time interval \( dt \). Thus the total collision probability between particle 1 and 2 is \( P^{(2)}(x_1, \xi_1, x_2, \xi_2, t) dx_1 d\xi_1 d\xi_2 \sigma^2 d\mathbf{n}|(\xi_2 - \xi_1) \cdot n| dt \). We also have to integrate with \( d\xi_2 \) and \( dx_2 \) (which is equivalent to integrating over \( d\mathbf{n} \)).

We obtain

\[
\begin{aligned}
ldx_1 d\xi_1 dt &= dx_1 d\xi_1 dt \int_{R^3} \int_{B^-} P^{(2)}(x_1, \xi_1, x_1 + \sigma n, \xi_2, t) \sigma^2 |(\xi_2 - \xi_1) \cdot n| d\mathbf{n} d\xi_2, \\
gdx_1 d\xi_1 dt &= d\mathbf{x}_1 d\xi_1 dt \int_{R^3} \int_{B^+} P^{(2)}(x_1, \xi_1, x_1 + \sigma n, \xi_2, t) \sigma^2 |(\xi_2 - \xi_1) \cdot n| d\mathbf{n} d\xi_2,
\end{aligned}
\]

where \( B^- \) is the hemisphere \( \mathbf{V} \cdot \mathbf{n} < 0 \) such that the particles are moving toward each other and about to have a collision, and the collision will send particle 1 away. So this term indeed has a “loss” effect on the probability density at phase point \((x_1, \xi_1)\). The corresponding gain term is obtained analogously,

\[
\begin{aligned}
l dx_1 d\xi_1 dt &= d\mathbf{x}_1 d\xi_1 dt \int_{R^3} \int_{B^-} P^{(2)}(x_1, \xi_1, x_1 + \sigma n, \xi_2, t) \sigma^2 |(\xi_2 - \xi_1) \cdot n| d\mathbf{n} d\xi_2, \\
g d\xi_1 d\xi_1 dt &= dx_1 d\xi_1 dt \int_{R^3} \int_{B^+} P^{(2)}(x_1, \xi_1, x_1 + \sigma n, \xi_2, t) \sigma^2 |(\xi_2 - \xi_1) \cdot n| d\mathbf{n} d\xi_2,
\end{aligned}
\]

where \( B^+ \) is the hemisphere with \( \mathbf{V} \cdot \mathbf{n} > 0 \), such that the particles are moving away from each other after undergoing a collision. Thus, the collision brought particle 1 into its current position, producing a gain effect.

Then, we can immediately write out the \( N \) particle gain and loss terms,

\[
L = (N - 1) \sigma^2 \int_{R^3} \int_{B^-} P^{(2)}(x_1, \xi_1, x_1 + \sigma n, \xi_2, t) |(\xi_2 - \xi_1) \cdot n| d\mathbf{n} d\xi_2, \\G = (N - 1) \sigma^2 \int_{R^3} \int_{B^+} P^{(2)}(x_1, \xi_1, x_1 + \sigma n, \xi_2, t) |(\xi_2 - \xi_1) \cdot n| d\mathbf{n} d\xi_2.
\]

In the above equations, the probability \( P^{(2)}(x_1, \xi_1, x_1 + \sigma n, \xi_2, t) \) is the pre-collision probability. We would like a post-collision probability \( P^{(2)}(x_1, \xi_1', x_1 + \sigma n, \xi_2', t) \), where the \( \xi_1 \) and \( \xi_2 \) are defined in Eqn.1.1. We will shortly see why we need relate the post-collision probability and the pre-collision probabilities. It turns out that the following
equation holds,

\[ P^{(2)}(x_1, \xi_1, x_1 + \sigma n, \xi_2, t) = P^{(2)}(x_1, \xi'_1, x_1 + \sigma n, \xi'_2, t). \]  \hspace{1cm} (1.15)

It means that although the velocities of particle 1 and particle 2 undergo a discontinuous change during a collision, the probability of finding the pair of particles at \((x_1, \xi_1)\) and \((x_2, \xi_2)\) is as the same as finding the pair at \((x_1, \xi'_1)\) and \((x_2, \xi'_2)\). Equivalently, the probability during a collision is continuous. The reason is that for each collision, before and after collision, the velocity pair is related by a one to one map. They cannot go to any other value. So now we apply the probability continuity property to the gain term in Eqn.1.14 and get

\[ G = (N - 1)\sigma^2 \int_{R^3} \int_{B^+} P^{(2)}(x_1, \xi'_1, x_1 + \sigma n, \xi'_2, t)(\xi'_2 - \xi_1) \cdot n |dn| d\xi'_2. \]  \hspace{1cm} (1.16)

but leave the loss term be unchanged.

To proceed further, one needs the so-called molecule chaos assumption (see [5] for further explanation),

\[ P^{(2)}(x_1, \xi_1, x_2, \xi_2, t) = P^{(1)}(x_1, \xi_1, t)P^{(1)}(x_2, \xi_2, t), \]  \hspace{1cm} (1.17)

for

\[ n \cdot (\xi_1 - \xi_2) < 0. \]  \hspace{1cm} (1.18)

This assumption means that the collision pair is randomly chosen, and that the probability of finding a collision pair with first particle at \((x_1, \xi_1)\) and second at \((x_1, \xi_1)\) is just the probability of finding a particle at \((x_1, \xi_1)\) times the probability of finding a particle at \((x_2, \xi_2)\). Using the above assumption, the Boltzmann-Grad limit for the loss term expressed in Eqn.1.13 is

\[ L = N\sigma^2 \int_{R^3} \int_{B^-} P^{(1)}(x_1, \xi_1, t)P^{(1)}(x_1 + \sigma n, \xi_2, t)(\xi_2 - \xi_1) \cdot n |dn| d\xi_2. \]  \hspace{1cm} (1.19)

However, we cannot apply directly the chaos assumption to Eqn.1.14; rather we apply it to Eqn.1.16 because a pre-collision \((\xi_1, \xi_2)\) is related to a post-collision \((\xi'_1, \xi'_2)\) by a one to one map. Then, we get the analogous expression for the gain term, with \(B^+\) changing
to $B^-$ because of the map.

$$G = N\sigma^2 \int_{R^3} \int_{B^-} P^{(1)}(x_1, \xi_1, t) P^{(1)}(x_1 + \sigma n, \xi_2, t) |(\xi_2 - \xi_1) \cdot n| d\xi_2. \quad (1.20)$$

Because we are taking the limit of $\sigma \to 0$, we can neglect the difference between $x_1$ and $x_1 + \sigma n$, and write

$$L = N\sigma^2 \int_{R^3} \int_{B^-} P^{(1)}(x_1, \xi_1, t) P^{(1)}(x_1, \xi_2, t) |(\xi_2 - \xi_1) \cdot n| d\xi_2, \quad (1.21)$$

and

$$G = N\sigma^2 \int_{R^3} \int_{B^-} P^{(1)}(x_1, \xi_1', t) P^{(1)}(x_1, \xi_2, t) |(\xi_2 - \xi_1) \cdot n| d\xi_2. \quad (1.22)$$

By substituting the above gain and loss term into Eqn.1.9, we finally get the full Boltzmann equation,

$$\frac{\partial P^{(1)}(x_1, \xi_1, t)}{\partial t} + \xi_1 \cdot \frac{\partial P^{(1)}(x_1, \xi_1, t)}{\partial x_1} = N\sigma^2 \int_{R^3} \int_{B^-} \left[ P^{(1)}(x_1, \xi_1', t) P^{(1)}(x_1, \xi_2', t) 

-P^{(1)}(x_1, \xi_1', t) P^{(1)}(x_1, \xi_2, t) \right] |(\xi_2 - \xi_1) \cdot n| d\xi_2. \quad (1.23)$$

This dynamical equation only contains $P^{(1)}$, without any dependence on $P^{(2)}$, thanks to the chaos assumption. Readers are referred to [5] for a more detailed discussion.

The pre- and post-collision velocity relations given in equation 1.1 can also be written in the form

$$\begin{align*}
\xi_1' &= \bar{\xi} + \frac{1}{2} |\xi_1 - \xi_2| \omega \\
\xi_2' &= \bar{\xi} - \frac{1}{2} |\xi_1 - \xi_2| \omega,
\end{align*} \quad (1.24)$$

where $\bar{\xi} = \frac{1}{2} (\xi_1 + \xi_2)$ is the velocity of the center of mass, and $\omega$ is another unit vector that replaces $n$. 
For convenience in chapter 2, we write out the velocity of the center of mass in the above equations and obtain

\[ \begin{align*}
\xi'_1 &= \xi_1 - \frac{1}{2}(g - |g|\omega) \\
\xi'_2 &= \xi_1 - \frac{1}{2}(g + |g|\omega),
\end{align*} \] (1.25)

where \( g = \xi_1 - \xi_2 \).

### 1.3 Molecule model

In the last section, we derived the Boltzmann equation assuming a hard-sphere molecular model. In general, we can use many other models. This can be done by replacing the term \( \sigma^2 |(\xi_2 - \xi_1) \cdot n| \) in 1.23 by a collision kernel \( B(\theta, |(\xi_2 - \xi_1)|) \), and replacing \( dn \) by \( d\theta d\epsilon \), where \( \theta \) is the angle between vectors \( n \) and \( \xi_2 - \xi_1 \) and \( \epsilon \) is the corresponding azimuthal angle. Then we get the new, more general equation,

\[
\frac{\partial P^{(1)}(x_1, \xi_1, t)}{\partial t} + \xi_1 \cdot \frac{\partial P^{(1)}(x_1, \xi_1, t)}{\partial x_1} = N \int_{\mathbb{R}^3} \int_{B^-} \left[ P^{(1)}(x_1, \xi'_1, t) P^{(1)}(x_1, \xi'_2, t) - P^{(1)}(x_1, \xi_1, t) P^{(1)}(x_1, \xi_2, t) \right] B(\theta, |(\xi_2 - \xi_1)|) d\theta d\epsilon d\xi_2. \quad (1.26)
\]

The collision kernel \( B(\theta, |(\xi_2 - \xi_1)|) \) contains all the information about the interaction law between molecules. In the hard sphere case, we can write

\[ B(\theta, |\xi_2 - \xi_1|) = \sin \theta \cos \theta |\xi_2 - \xi_1|. \] (1.27)

In this case, the range of the force is cut off at a finite radius \( \sigma \). There is no interaction between molecules separated more than this radius. However, in a more realistic central force field, the interaction extends to infinity. There are always interactions between molecules even if they are far away, and in this case the notion of ”collision” only holds in an approximate sense when the gas is sufficiently dilute. In general, the collision kernel \( B(\theta, |\xi_2 - \xi_1|) \) can be very complex and the angular dependence and relative velocity dependence do not factor. Fortunately, for a power law potential, in which the intermolecular force decreases as the inverse power of the distance, the angular and relative
velocity dependence in the collision kernel factor as

\[ B(\theta, |\xi_2 - \xi_1|) = \beta(\theta) |\xi_2 - \xi_1|^{\frac{n-5}{n-1}}, \quad (1.28) \]

where \( \beta(\theta) \) is a non-elementary function of \( \theta \). For \( n = 5 \) we have the so-called Maxwellian molecules, for which the velocity dependence disappears. As we will see later, assuming either Maxwellian molecules or hard sphere molecules greatly simplifies the evaluation of the collision integral.

### 1.4 Collision invariants

In this section, we will investigate some general properties of solutions to the Boltzmann equation. Before doing this, we need to make a few modifications to Eqn.1.26. Instead of using a probability \( P^{(1)} \), we adopt the more widely used one-particle distribution function \( f \), and absorb the number of particles \( N \) into \( B \) to write \( B(\theta, V) \), where \( V \) is the relative velocity in Eqn.1.4. Then we get,

\[
\frac{\partial f(x_1, \xi_1, t)}{\partial t} + \xi_1 \cdot \frac{\partial f(x_1, \xi_1, t)}{\partial x_1} = \int_{R^3} \int_{B^{-}} \left[ f(x_1, \xi_1', t)f(x_1, \xi_2', t) - f(x_1, \xi_1, t)f(x_1, \xi_2, t) \right] B(\theta, V) d\theta d\epsilon d\xi_2. \quad (1.29)
\]

We change \( \xi_1 \) to \( \xi \) and \( \xi_2 \) to \( \xi_* \), and also change \( x_1 \) to \( x \), to write

\[
\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} = \int_{R^3} \int_{B^{-}} (f' f_* - f f_*) B(\theta, V) d\xi_* d\theta d\epsilon, \quad (1.30)
\]

where \( V \) is defined as \( |\xi - \xi_*| \). We hide the velocity arguments of \( f \) and change subscripts on \( \xi \) to subscripts on \( f \) for simplicity. We call the right hand side of Eqn.1.30 the collision operator. It’s quadratic in \( f \), and

\[
Q(f, f) = \int_{R^3} \int_{B^{-}} (f' f_* - f f_*) B(\theta, V) d\xi_* d\theta d\epsilon. \quad (1.31)
\]
The collision operator $Q(f, g)$ has many interesting properties. In order to better understand it, we rewrite it in a more symmetric bi-linear form,

$$Q(f, g) = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathcal{B}^-} (f'g'_* + g'f'_* - fg*)\mathcal{B}(\theta, V)d\xi_*d\theta d\epsilon.$$ (1.32)

$Q(f, g)$ is symmetric about $f$ and $g$,

$$Q(f, g) = Q(g, f),$$ (1.33)

and

$$Q(f, g)|_{f=g} = Q(f, f).$$ (1.34)

We want to study the integral of the collision operator times a general scalar function $\phi(\xi)$, assuming that the integral is well defined,

$$\int_{\mathbb{R}^3} Q(f, g)\phi(\xi)d\xi = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathcal{B}^-} (f'g'_* + g'f'_* - fg*)\mathcal{B}(\theta, V)d\xi_*d\theta d\epsilon. (1.35)$$

We will study the symmetry of the above integral under various changes of variable. First, let’s interchange the starred variables and the un-starred variables to get

$$\int_{\mathbb{R}^3} Q(f, g)\phi(\xi)d\xi = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathcal{B}^-} (f'g'_* + g'f'_* - fg*)\mathcal{B}(\theta, V)d\xi_*d\theta d\epsilon. (1.36)$$

Next, we interchange the primed and un-primed variables. We can do this because a single collision process is perfectly reversible, and interchanging the primed and un-primed variable is nothing else than interchanging the variables before collision and after collision. Note that the vector $\mathbf{n}$ is also reversed, and the minus sign is offset by the change $\mathcal{B}^-$ to
\[ \int_{\mathbb{R}^3} Q(f, g) \phi(\xi) d\xi = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{B^-} (f g_\ast + g f_\ast - f' g_\ast' - g' f_\ast') \phi(\xi') B(\theta, V) d\xi' d\xi d\theta d\epsilon. \] (1.37)

We rewrite equation 1.1 using the starred and un-starred variables as

\[ \begin{align*}
\xi' &= \xi - n(n \cdot (\xi - \xi_\ast)) \\
\xi'_\ast &= \xi_\ast + n(n \cdot (\xi - \xi_\ast)).
\end{align*} \] (1.38)

One can clearly see that the Jacobian matrix from \(\xi, \xi_\ast\) to \(\xi', \xi'_\ast\) has determinant one. Thus we can write the above equation as

\[ \int_{\mathbb{R}^3} Q(f, g) \phi(\xi) d\xi = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{B^-} (f g_\ast + g f_\ast - f' g_\ast' - g' f_\ast') \phi(\xi') B(\theta, V) d\xi' d\xi d\theta d\epsilon. \] (1.39)

We then again interchange the starred and un-starred variables in the above equation to get

\[ \int_{\mathbb{R}^3} Q(f, g) \phi(\xi) d\xi = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{B^-} (f g_\ast + g f_\ast - f' g_\ast' - g' f_\ast') \phi(\xi') B(\theta, V) d\xi' d\xi d\theta d\epsilon. \] (1.40)

Equations 1.35, 1.36, 1.39, and 1.40 are very similar to each other except for the velocity variable in the function \(\phi\). We get a new equation below by taking the sum of these four equations and dividing by 4,

\[ \int_{\mathbb{R}^3} Q(f, g) \phi(\xi) d\xi = \frac{1}{8} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{B^-} (f' g_\ast' + g' f_\ast' - f g_\ast - g f_\ast) \times (\phi(\xi) + \phi(\xi_\ast) - \phi(\xi') - \phi(\xi'_\ast)) B(\theta, V) d\xi d\xi d\theta d\epsilon. \] (1.41)
In the particular case $g = f$, the above becomes
\[
\int_{\mathbb{R}^3} Q(f, f) \phi(\xi) d\xi = \frac{1}{4} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{B^-} (f' f'_* - f f_*) \times (\phi(\xi) + \phi(\xi_*') - \phi(\xi_*) - \phi(\xi_*')) B(\theta, V) d\xi_* d\xi d\theta d\epsilon. \quad (1.42)
\]
In equation 1.42, it’s evident that if the following equation holds,
\[
\phi(\xi) + \phi(\xi_*) = \phi(\xi_1') + \phi(\xi_*') \quad (1.43)
\]
then,
\[
\int_{\mathbb{R}^3} Q(f, f) \phi(\xi) d\xi = 0. \quad (1.44)
\]
If any function $\phi(\xi)$ satisfies equation 1.43, we call it a collision invariant, since its collision average indicated by equation 1.44 vanishes. It can be shown that $\phi(\xi)$ is a collision invariant if and only if it has the following form
\[
\phi(\xi) = a + b \cdot \xi + c|\xi|^2. \quad (1.45)
\]
Here $a$ and $c$ are scalar constants, and $b$ is a constant vector. There are five collision invariants, corresponding to the conservation of mass, momentum and energy in each molecular collision: $\psi_0 = 1$, $\psi_1 = \xi_1$, $\psi_2 = \xi_2$, $\psi_3 = \xi_3$, and $\psi_4 = |\xi|^2$. In total, they span a five dimensional space. As we will see later, properly using collision invariants is a very important technique and can greatly simplify certain problems.

### 1.5 The Maxwell distribution

In the previous sections, we derived the Boltzmann equation and also found some properties of the collision kernel. In this section, we will introduce the simplest non trivial solution to the Boltzmann equation, which is called the Maxwell distribution. From equation 1.30 and 1.31, we rewrite the Boltzmann equation as
\[
\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} = Q(f, f). \quad (1.46)
\]
Chapter 1. Introduction to Boltzmann equation

A spatially uniform Boltzmann equation has the simple form

$$\frac{\partial f}{\partial t} = Q(f, f).$$  \hspace{1cm} (1.47)

A Maxwell distribution is just a solution that satisfies

$$\frac{\partial f}{\partial t} = Q(f, f) = 0.$$  \hspace{1cm} (1.48)

(There is no time change to $f$) Using equation 1.31, we have

$$Q(f, f) = \int_{R^3} \int_{B^-} (f'f_{*}' - ff_{*})B(\theta, V)d\xi_{*}d\theta d\epsilon = 0. \hspace{1cm} (1.49)$$

To solve, we multiply by $\log f$ on both sides and integrate out the $\xi$ dependence, which is just equation 1.42 in the previous collision invariant section with $\phi(\xi)$ replaced by $\log f$,

$$\int_{R^3} Q(f, f) \log f d\xi = \frac{1}{4} \int_{R^3} \int_{R^3} \int_{B^-} (f'f_{*}' - ff_{*})$$

$$\times (\log f + \log f_{*} - \log f' - \log f'_{*})B(\theta, V)d\xi_{*}d\xi d\theta d\epsilon$$

$$= \frac{1}{4} \int_{R^3} \int_{R^3} \int_{B^-} (f'f_{*}' - ff_{*})$$

$$\times \log(ff_{*}/f'f'_{*})B(\theta, V)d\xi_{*}d\xi d\theta d\epsilon. \hspace{1cm} (1.50)$$

The distribution function $f$ is certainly a positive quantity, and one can easily verify that for two positive variables $y$ and $z$,

$$(z - y) \log(y/z) \leq 0.$$  \hspace{1cm} (1.51)

Thus we have

$$\int_{R^3} Q(f, f) \log f d\xi \leq 0.$$  \hspace{1cm} (1.51)

For equality in 1.50 to hold for arbitrary $B(\theta, V)$, one needs

$$f'f_{*}' = ff_{*}. \hspace{1cm} (1.52)$$

Taking the log we get

$$\log f' + \log f_{*}' = \log f + \log f_{*}. \hspace{1cm} (1.53)$$
Comparing with equation 1.43, one finally gets the expression for Maxwellian distribution function $f$,

$$f = \exp(a + b \cdot \xi + c|\xi|^2). \quad (1.54)$$

The constant $c$ above has to be negative for integrability. One can always make a velocity shift and write the above in the more familiar form

$$f = \exp(-\beta|\xi - v|^2). \quad (1.55)$$

### 1.6 The H-Theorem

The H-Theorem reveals a feature of irreversibility of the Boltzmann equation, i.e., a time arrow in the evolution of the system. Let’s start again from the equation,

$$\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial \mathbf{x}} = Q(f, f). \quad (1.56)$$

We multiply by $\log f$ on both sides to get

$$\log f \frac{\partial f}{\partial t} + \xi \cdot \log f \frac{\partial f}{\partial \mathbf{x}} = \log f \, Q(f, f). \quad (1.57)$$

Then add the above two equations to get

$$\frac{\partial f \log f}{\partial t} + \xi \cdot \frac{\partial f \log f}{\partial \mathbf{x}} = (\log f + 1)Q(f, f). \quad (1.58)$$

Next, we integrate out the velocity dependence,

$$\frac{\partial}{\partial t} \int_{R^3} f \log f d\xi + \int_{R^3} \xi f \log f d\xi = \int_{R^3} \log f \, Q(f, f) d\xi + \int_{R^3} Q(f, f) d\xi. \quad (1.59)$$

One immediately finds that

$$\int_{R^3} Q(f, f) d\xi = 0, \quad (1.60)$$
because it’s a collision invariant. If one defines
\[
\mathcal{H} = \int_{\mathbb{R}^3} f \log f \, d\xi, \quad (1.61)
\]
\[
\mathbf{J} = \int_{\mathbb{R}^3} \xi f \log f \, d\xi, \quad (1.62)
\]
and
\[
S = \int_{\mathbb{R}^3} \log f \, Q(f, f) \, d\xi, \quad (1.63)
\]
then equation 1.59 can be expressed as
\[
\frac{\partial \mathcal{H}}{\partial t} + \frac{\partial}{\partial x} \cdot \mathbf{J} = S. \quad (1.64)
\]
From the previous section, we know that
\[
S \leq 0, \quad (1.65)
\]
where the equal sign holds only when \( f \) is a Maxwellian distribution function
\[
f = \exp(-\beta |\xi - v|^2). \quad (1.66)
\]
To better understand the meaning of equation 1.64, we rewrite it in the spatially homogeneous case,
\[
\frac{\partial \mathcal{H}}{\partial t} = S \leq 0. \quad (1.67)
\]
This is the Boltzmann’s H-Theorem. The quantity \( \mathcal{H} \) is always decreasing, but decreases much more slowly when \( f \) approaches a Maxwellian, and \( \mathcal{H} \) no longer changes when \( f \) is a Maxwellian. \(-\mathcal{H}\) here is analogous to entropy in the second law of thermodynamics, and is always increasing. In the non-homogeneous case, the situation is more complex, but we can integrate equation 1.64 with respect to \( x \) to get
\[
\frac{\partial}{\partial t} \int_{\mathbb{R}^3} \mathcal{H} \, dx + \int_{\mathbb{R}^3} (\frac{\partial}{\partial x} \cdot \mathbf{J}) \, dx = \int_{\mathbb{R}^3} S \, dx \leq 0. \quad (1.68)
\]
One can think of $-\int_{\mathbb{R}^3} \mathcal{H} d\mathbf{x}$ as the entropy for the entire system, and the second term can be written as a surface term,

$$\int_{\mathbb{R}^3} \left( \frac{\partial}{\partial \mathbf{x}} \cdot \mathbf{J} \right) d\mathbf{x} = \int_{\partial \Sigma} \mathbf{J} \cdot \mathbf{n} d\sigma. \quad (1.69)$$

The above surface term clearly is related to the boundary conditions in the specific problem. Let’s consider a simple case (readers can find other cases in \cite{5}), when the gas system is in a bounded box with specular reflection. Then the boundary term disappears (because the integrand of $\mathbf{J} \cdot \mathbf{n}$ is odd on the surface), and we get the same result as in the spatially homogeneous case.

### 1.7 The macroscopic equations

We have derived the Boltzmann equation for the distribution function $f(x, \xi, t)$. In this section, we want to connect $f$ to the macroscopic quantities of continuous gas dynamics, starting with $\rho(x, t)$, the density at space coordinate $x$ and at time $t$. We have

$$\rho(x, t) = \int_{\mathbb{R}^3} f d\xi. \quad (1.70)$$

The next is the bulk velocity $\mathbf{v}(x, t)$ of the gas,

$$\mathbf{v}(x, t) = \frac{\int_{\mathbb{R}^3} \xi f d\xi}{\int_{\mathbb{R}^3} f d\xi}. \quad (1.71)$$

One can think of the denominator just as a normalization factor. We can also move the denominator to the left and write

$$\rho \mathbf{v} = \int_{\mathbb{R}^3} \xi f d\xi. \quad (1.72)$$
Chapter 1. *Introduction to Boltzmann equation*

where \( \rho v \) is the momentum density, alternatively called mass flow. One can write it more explicitly component-wise,

\[
\begin{align*}
\rho v_x &= \int_{R^3} \xi_x f \, d\xi, \\
\rho v_y &= \int_{R^3} \xi_y f \, d\xi, \\
\rho v_z &= \int_{R^3} \xi_z f \, d\xi.
\end{align*}
\] (1.73)

One can also introduce higher-order quantities higher w.r.t velocity, such as

\[
\begin{align*}
m_{ij} &= \int_{R^3} \xi_i \xi_j f \, d\xi \quad (i, j = 1, 2, 3),
\end{align*}
\] (1.74)

which is a second order symmetric tensor and is called the momentum flow. The next is the familiar energy density

\[
w = \frac{1}{2} \int_{R^3} |\xi|^2 f \, d\xi
\] (1.75)

(the total energy per unit volume). Similarly to the mass flow and the momentum flow, we can also define the energy flow,

\[
r_i = \frac{1}{2} \int_{R^3} \xi_i |\xi|^2 f \, d\xi \quad (i = 1, 2, 3),
\] (1.76)

The bulk velocity in Eqn.1.71 is the macroscopic velocity observed in the fluid as a whole. It is zero for a gas system in equilibrium inside a box at rest. Beside the bulk velocity, we also consider the relative velocity of each molecule with respect to the bulk velocity, called the random velocity or peculiar velocity. It is given by

\[c = \xi - v.\] (1.77)
Then equation 1.74 can be written as

\[ m_{ij} = \int_{R^3} (c_i + v_i)(c_j + v_j) f d\xi \]
\[ = \rho v_i v_j + \int_{R^3} c_i c_j d\xi + v_i \int_{R^3} c_j d\xi + v_j \int_{R^3} c_i d\xi \]
\[ = \rho v_i v_j + \int_{R^3} c_i c_j d\xi \]
\[ = \rho v_i v_j + p_{ij}. \quad (1.78) \]

In the second line, the last two terms are zero, and in the last line, we have defined the pressure tensor \( p_{ij} \)

\[ p_{ij} = \int_{R^3} c_i c_j d\xi. \quad (1.79) \]

The pressure is simply the average trace of the pressure tensor, given by

\[ p = \frac{1}{3} \int_{R^3} |c|^2 f d\xi. \quad (1.80) \]

Similarly, we also rewrite equation 1.75 as

\[ w = \frac{1}{2} \int_{R^3} |\xi|^2 f d\xi \]
\[ = \frac{1}{2} \int_{R^3} |c + v|^2 f d\xi \]
\[ = \frac{1}{2} \int_{R^3} v^2 f d\xi + \frac{1}{2} \int_{R^3} c^2 f d\xi + \int_{R^3} cv f d\xi \]
\[ = \frac{1}{2} \rho v^2 + \rho e. \quad (1.81) \]

In the third line, the last term goes zero, and in the last line, we have defined the internal energy per unit volume to be

\[ \rho e = \frac{1}{2} \int_{R^3} c^2 f d\xi. \quad (1.82) \]

The definition of internal energy involves only the random velocity as expected. It describes the energy due to relative motion of the molecules with respect to the macroscopic bulk velocity of the gas system. Even if the bulk velocity of the gas system is zero, its internal energy is always a non zero quantity.
The internal energy is related to the temperature of the system. Comparing equation 1.80 and 1.82, we find

\[ p = \frac{2}{3} \rho e. \quad (1.83) \]

which suggests that we define the temperature as \( \frac{2e}{3R} \), where R is the gas constant. Thus

\[ T = \frac{1}{3\rho R} \int_{R^3} c^2 f \, d\xi. \quad (1.84) \]

Next, we also rewrite the energy flow in equation 1.76,

\[
  r_i = \frac{1}{2} \int_{R^3} \xi_i |\xi|^2 f \, d\xi \\
  = \frac{1}{2} \int_{R^3} v_i |v + c|^2 f \, d\xi + \frac{1}{2} \int_{R^3} c_i |v + c|^2 f \, d\xi \\
  = \rho v_i (\frac{1}{2} |v|^2 + e) + v_j \int_{R^3} c_i c_j f \, d\xi + \frac{1}{2} \int_{R^3} c_i |c|^2 f \, d\xi \\
  = \rho v_i (\frac{1}{2} |v|^2 + e) + v_j p_{ij} + q_i \quad (i = 1, 2, 3), \quad (1.85)
\]

where the last term in the third line and the first term in the fourth line both go zero, and in the fifth line the repeated index \( j \) means summation over \( j \), and in the last line we have defined the heat flow vector

\[ q_i = \frac{1}{2} \int_{R^3} c_i |c|^2 f \, d\xi. \quad (1.86) \]

Eqn.1.85 shows that the energy flow is composed by a macroscopic energy flow (including both kinetic and internal energies), by the stress tensor, and by the heat flow.

From the definition of the mass density in equation 1.70, we obtain the total mass as

\[ M = \int_{\Omega} \rho \, dx, \quad (1.87) \]

where the integral takes place on the whole domain \( \Omega \) containing the gas. Similarly, we write the total momentum from equation 1.72 as

\[ Q = \int_{\Omega} \rho v \, dx. \quad (1.88) \]
We also have the total energy

\[ E = \int_{\Omega} \left( \frac{1}{2} \rho v^2 + \rho e \right) d\mathbf{x}. \]  

(1.89)

Having defined the various macroscopic quantities, we can find equations connecting them. This is not difficult if we take advantage of the collision invariants. Let us go back to the Boltzmann equation,

\[ \frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial \mathbf{x}} = Q(f, f). \]  

(1.90)

We have five collision invariants, \( \psi_0 = 1, \psi_1 = \xi_1, \psi_2 = \xi_2, \psi_3 = \xi_3, \) and \( \psi_4 = |\xi|^2. \) If we multiply them by the Boltzmann equation, and integrate with respect to velocity \( \xi, \) we obtain five equations, all of them with vanishing collision operator integration since

\[ \int_{R^3} Q(f, f) \psi_i d\xi = 0, \quad (i = 0, 1, 2, 3, 4). \]  

(1.91)

Multiplying \( \psi_0 = 1 \) times the Boltzmann equation, the first equation is

\[ \frac{\partial}{\partial t} \int_{R^3} f d\xi + \frac{\partial}{\partial \mathbf{x}} \cdot \int_{R^3} \xi f d\xi = 0. \]  

(1.92)

Recalling equation 1.70 and equation 1.72, the above equation is just the mass conservation equation,

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (\rho \mathbf{v}) = 0. \]  

(1.93)

Multiplying \( \psi_i = \xi_i \) (i=1,2,3) times the Boltzmann equation, the second to fourth equations are

\[ \frac{\partial}{\partial t} \int_{R^3} \xi_i f d\xi + \frac{\partial}{\partial \mathbf{x}} \cdot \int_{R^3} \xi_i \xi f d\xi = 0. \]  

(1.94)

The second term can be written as

\[ \frac{\partial}{\partial \mathbf{x}} \cdot \int_{R^3} \xi_i \xi f d\xi = \frac{\partial}{\partial \mathbf{x}} \cdot \int_{R^3} (v_i + c_i)(\mathbf{v} + \mathbf{c}) f d\xi \]

\[ = \frac{\partial}{\partial \mathbf{x}} \cdot \int_{R^3} v_i \mathbf{v} d\xi + \frac{\partial}{\partial \mathbf{x}} \cdot \int_{R^3} c_i \mathbf{c} d\xi \]

\[ = \frac{\partial}{\partial \mathbf{x}} \cdot \rho \mathbf{v} \cdot \mathbf{v} + \frac{\partial}{\partial x_j} p_{ij}, \]  

(1.95)
where the index \( j \) in \( p_{ij} \) contracts with \( \partial x_j \). Thus, we obtain

\[
\frac{\partial}{\partial t} (\rho v_i) + \sum_{j=1}^{3} \frac{\partial}{\partial x_j} (\rho v_i v_j + p_{ij}) = 0 \quad (i = 1, 2, 3).
\] (1.96)

Multiplying \( \psi_4 = |\xi|^2 \) times the Boltzmann equation, the fifth equation is

\[
\frac{\partial}{\partial t} \int_{\mathbb{R}^3} |\xi|^2 f \, d\xi + \frac{\partial}{\partial x} \cdot \int_{\mathbb{R}^3} \xi |\xi|^2 f \, d\xi = 0.
\] (1.97)

The first integral is just the energy density, up to a constant, and the second integral is the energy flow, up to a constant. Recalling equations 1.75, 1.76 we obtain

\[
\frac{\partial}{\partial t} \left( \frac{1}{2} \rho v^2 + \rho e \right) + \sum_{j=1}^{3} \frac{\partial}{\partial x_j} \left[ \rho v_j \left( \frac{1}{2} |v|^2 + e \right) + v_i p_{ij} + q_j \right] = 0.
\] (1.98)

Equations 1.93, 1.96, and 1.98 are five equations in total, and are called conservation equations. They tell us the time change of a certain quantity in a certain region induced by the divergence of another quantity, i.e. the net flux across the surface surrounding this region. If the net flux across the surface is zero, then the quantity inside the time derivative is conserved in this region.

### 1.8 Model equations

When solving the Boltzmann equation, especially in numerical simulations, the most difficult part is the evaluation of the collision integral. Thus many alternative, simpler expressions have been devised to replace the collision integral and simplify the problem. These alternative collision terms are called model equations or kinetic models.

The original multi-fold collision integral contains detailed mechanical information about two-body collision, and it also incorporates the information about the force between molecules. The idea of model equations is to build phenomenological models which only reflect the qualitative and average properties of the full collision term.
In this section we will describe the most widely known collision model, the Bhatnagar, Gross and Krook (BGK \[2\]) model. The BGK model uses a different quantity \( J(f) \) to replace the collision operator \( Q(f, f) \). Since the collision operator has to satisfy equation 1.44 and 1.51, we expect the following equation to hold,

\[
\int_{\mathbb{R}^3} J(f) \psi(\xi) d\xi = 0, \tag{1.99}
\]

for any \( f \), where \( \psi \) are the familiar five collision invariants, \( \psi_0 = 1, \psi_1 = \xi_1, \psi_2 = \xi_2, \psi_3 = \xi_3, \) and \( \psi_4 = |\xi|^2 \).

We also expect

\[
\int_{\mathbb{R}^3} J(f) \log f d\xi \leq 0, \tag{1.100}
\]

with the equal sign holding if and only if \( f \) is a Maxwellian.

The BGK model takes \( J(f) \) of the form

\[
J(f) = \nu [\Phi(\xi) - f(\xi)], \tag{1.101}
\]

where \( \Phi(\xi) \) is a Maxwellian, and is defined by five parameters, e.g. density, velocity, and temperature, and \( \nu \) is a constant. \( J(f) \) has a form similar to Hooke’s law, and the Maxwellian \( \Phi(\xi) \) is the ”base” state, while the deviation from ”current” state to ”base” state is characterized by \( \Phi(\xi) - f(\xi) \) and proportional to the ”stiffness” coefficient \( \nu \), called the collision frequency. Whenever \( f(\xi) \) is away from Maxwellian \( \Phi(\xi) \), \( J(f) \) will drag it to approach the Maxwellian \( \Phi(\xi) \).

The five parameters in \( J(f) \) can be determined by Eqn.1.99,

\[
\int_{\mathbb{R}^3} \Phi(\xi) \psi(\xi) d\xi = \int_{\mathbb{R}^3} f(\xi) \psi(\xi) d\xi, \tag{1.102}
\]

for the five collision invariants.
\(J(f)\) still has to satisfy property 1.100,
\[
\int_{R^3} J(f) \log f d\xi = \int_{R^3} J(f) (\log f - \log \Phi) d\xi + \int_{R^3} J(f) \log \Phi d\xi \\
= \int_{R^3} \nu \Phi (1 - \frac{f}{\Phi}) \log \frac{f}{\Phi} d\xi \\
\leq 0,
\] (1.103)

where in the first line, the second term goes zero because \(\log \Phi\) is a combination of collision invariants, and from the second to third line we have applied 1.51. The equality sign only holds when \(f = \Phi\), i.e. \(f\) is a local Maxwellian.

In the BGK model the collision frequency \(\nu\) is constant. This can be modified by letting \(\nu\) depend on \(\xi\). The form and all properties of \(J(f)\) still hold, except the five coefficient of \(\Phi\) have to be determined by the following relation,
\[
\int_{R^3} \nu(\xi) \Phi(\xi) \psi(\xi) d\xi = \int_{R^3} \nu(\xi) f(\xi) \psi(\xi) d\xi,
\] (1.104)

and \(\rho, \nu, \text{ and } T\) are no longer the \(\rho, \nu, \text{ and } T\) for the local Maxwellian. There are also other modifications to the BGK model, see [37] for more discussion.

### 1.9 Knudsen number and dimensionless Boltzmann equation

For the purpose of approximately solving the Boltzmann equation, we will use a dimensionless version of Boltzmann equation [24]. Let \(L_0\) be a typical length scale, \(t_0\) a typical time scale and \(V_0 \equiv L_0/t_0\). Since \(f(t, x, v)\) has dimension \(\rho_0 V_0^{-3}\), where \(\rho_0\) is a typical density, we write
\[
f(t, x, v) = \frac{\rho_0}{V_0^3} \tilde{f}(\tilde{t}, \tilde{x}, \tilde{v}),
\] (1.105)

where \(\tilde{t} \equiv t/t_0, \tilde{x} \equiv x/L_0\) and \(\tilde{v} \equiv v/V_0\). Substituting into the Boltzmann equation for hard-sphere molecules [5], we obtain
\[
\frac{\partial \tilde{f}}{\partial \tilde{t}} + \tilde{v} \cdot \frac{\partial \tilde{f}}{\partial \tilde{x}} = \left( \frac{\rho_0 L_0 d^2}{4} \right) \int_{R^3} \int_{S^2} [\tilde{v} - \tilde{w}] [\tilde{f}(\tilde{v}') \tilde{f}(\tilde{w}') - \tilde{f}(\tilde{v}) \tilde{f}(\tilde{w})] d\tilde{e} d\tilde{w}.
\] (1.106)
We define the mean free path $\lambda_0$ as

$$\lambda_0 = \frac{1}{\sqrt{2\pi} d^2 \rho_0}$$

and the Knudsen number as

$$Kn = \frac{\lambda_0}{L_0} = \frac{\text{mean free path}}{\text{typical length scale}}.$$ 

Using these definitions, and removing the tildes, we get the dimensionless Boltzmann equation

$$\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} = \frac{1}{4\sqrt{2\pi} Kn} Q(f, f).$$  \hspace{1cm} (1.107)$$

Follow the conventions, we absorb the constant factor $4\sqrt{2\pi}$ into the definition of the Knudsen number, and write the above equation as

$$\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} = \frac{1}{Kn} Q(f, f).$$ \hspace{1cm} (1.108)$$

When solving Boltzmann equation by perturbation methods, one always looks for some "small" quantity or parameter based on which to expand the equation order by order. The Knudsen number serves an excellent role for this purpose. We have two kinds of perturbation methods to consider, one is $Kn \to 0$, corresponding to extremely small mean free path (frequent collisions between molecules), another is $Kn \to \infty$ corresponding to extremely large mean free path (molecules are almost free to move without any collisions).

1.10 The linearized collision operator

Due to the complex nonlinear nature of the collision operator, in most cases, except in the equilibrium state which has the simple Maxwellian solution, perturbation methods are the only analytical methods that can can provide some insight about solutions to the Boltzmann equation for either large or small Knudsen numbers. The idea is to expand $f$ into a series, and also expand the more complex $Q(f, f)$ into a series, and solve the
equation order by order. We first expand $f$ as

$$f = \sum_{n=0}^{\infty} \epsilon^n f_n. \quad (1.109)$$

We insert the above into $Q(f, f)$ to obtain

$$Q(f, f) = \sum_{n=0}^{\infty} \epsilon^n \sum_{k=0}^{n} Q(f_k, f_{n-k}), \quad (1.110)$$

where $Q(f_k, f_{n-k})$ is the bi-linear operator defined in equation 1.32. We denote the collision operator at $n$-th order as $Q_n$,

$$Q_n = \sum_{k=0}^{n} Q(f_k, f_{n-k}). \quad (1.111)$$

At zero order, $f_0$ is just a Maxwellian, since for a Maxwellian $M$ the left hand side of the Boltzmann equation goes zero and

$$Q_0 = Q(M, M) = 0. \quad (1.112)$$

We will use $f_0$ and $M$ alternatively to denote the Maxwellian distribution function. From equation 1.111, we can also separate terms involving $f_0$ and higher order terms to write

$$Q_n = 2Q(f_0, f_n) + \sum_{k=1}^{n-1} Q(f_k, f_{n-k}), \quad (1.113)$$

for $n > 0$. In the next step, we introduce the so-called linearized operator $Lh$ which is related to the bi-linear operator defined in Eqn.1.32, by

$$Lh = 2M^{-1}Q(Mh, M). \quad (1.114)$$

A more explicit form is obtained as follows,

$$Lh = M^{-1} \int_{R^3} \int_{B^-} (Mh' M'_* + M' Mh'_* - MhM_* - MMh_*) \mathcal{B}(\theta, V) d\xi_*, d\theta de$$

$$= \int_{R^3} \int_{B^-} M_*(h' + h'_* - h - h_*) \mathcal{B}(\theta, V) d\xi_*, d\theta de, \quad (1.115)$$
where in the first line we replaced $f$ and $g$ in equation 1.32 by $Mh$ and $M$ respectively, and from the second line to third line we have used the fact $M'M'_* = MM_*$ for a Maxwellian.

Now, using the definition of the linearized operator, we rewrite equation 1.113 as

$$Q_n = f_0 L h_n + f_0 S_n.$$  \hfill (1.116)

To understand the above expression, we could think $f_n = f_0 h_n$ while $h_n$ is unknown. In the first term above, the operator $L$ is acting on the unknown $h_n$ and the second term $f_0 S_n$ represents a source term.

Using equation 1.41, we can define an integral of the linearized collision operator as

$$\int_{R^3} Q(Mh, M) \phi(\xi) d\xi = \frac{1}{8} \int_{R^3} \int_{R^3} \int_{B^-} MM_*(h' + h'_* - h - h_*)$$

$$\times (\phi(\xi) + \phi(\xi_*) - \phi(\xi') - \phi(\xi'_*)) B(\theta, V) d\xi_* d\xi d\theta d\epsilon.$$  \hfill (1.117)

We substitute Eqn.1.32 into the left side and replace $\phi$ by $g$ to write as

$$\int_{R^3} MgL hd\xi = \frac{1}{4} \int_{R^3} \int_{R^3} \int_{B^-} MM_*(h' + h'_* - h - h_*)$$

$$\times (g + g_* - g'_* - g'_*) B(\theta, V) d\xi_* d\xi d\theta d\epsilon.$$  \hfill (1.118)

The above expression can be interpreted as an inner product of $g$ and $h$ weighted by $M$.

Note that by symmetry, we can also write

$$\int_{R^3} MhL gd\xi = \frac{1}{4} \int_{R^3} \int_{R^3} \int_{B^-} MM_*(g' + g'_* - g - g_*)$$

$$\times (h + h_* - h' - h'_*) B(\theta, V) d\xi_* d\xi d\theta d\epsilon.$$  \hfill (1.119)

Further when $g = h$, we have

$$\int_{R^3} MhLhd\xi = -\frac{1}{4} \int_{R^3} \int_{R^3} \int_{B^-} MM_*(h' + h'_* - h - h_*)^2 B(\theta, V) d\xi_* d\xi d\theta d\epsilon$$

$$\leq 0.$$  \hfill (1.120)

And the equal sign holds if and only if

$$h' + h'_* - h - h_* = 0,$$  \hfill (1.121)
that is to say. \( h \) is a collision invariant.

We can write the left side of equation 1.118 in inner-product form,

\[
(g, Lh) = \int_{R^3} MgLhd\xi. \tag{1.122}
\]

Clearly we also have

\[
(g, Lh) = (Lg, h). \tag{1.123}
\]

And from equation 1.120, we have

\[
(h, Lh) \leq 0. \tag{1.124}
\]

Also we have a trivial result from equation 1.115,

\[
L\psi_i = 0 \quad i = 0, 1, 2, 3, 4. \tag{1.125}
\]

Thus, \( \psi_i \) is an eigenvector of \( L \), and its eigenvalue is zero. In equation 1.118, the integral is zero when either \( h \) or \( g \) is a collision invariant, so we have

\[
(\psi_i, Lh) = 0. \tag{1.126}
\]

### 1.11 Linearized Boltzmann equation

In Eqn.1.109, we have expanded \( f \) into series, and in Eqn.1.110 we have also expanded \( Q(f, f) \) into series. Now insert them into the Boltzmann equation,

\[
\frac{\partial f}{\partial t} + \xi \cdot \frac{\partial f}{\partial x} = Q(f, f), \tag{1.127}
\]

and match the two sides at each order of \( \epsilon \). At zero order we have

\[
\frac{\partial f_0}{\partial t} + \xi \cdot \frac{\partial f_0}{\partial x} = Q(f_0, f_0) = 0. \tag{1.128}
\]
Clearly at zero order the solution is Maxwellian with a constant density, velocity, and temperature. At higher order we have

\[ \frac{\partial f_n}{\partial t} + \xi \cdot \frac{\partial f_n}{\partial x} = Q_n(f, f). \]  

(1.129)

In the discussion following Eqn.1.113, we wrote \( f_n = f_0 h_n \), because \( h_n \) is a small unknown, and we expect the full solution will be something like

\[ f \sim f_0 (1 + \sum_{n=1}^{N} h_n), \]

(1.130)

where \( N \) is some large number. In this approximation the gas system is assumed not far from the equilibrium status represented by Maxwellian \( f_0 \). Using \( f_n = f_0 h_n \) and equation 1.113 we have

\[ \frac{\partial h_n}{\partial t} + \xi \cdot \frac{\partial h_n}{\partial x} = L h_n + S_n, \]

(1.131)

and by comparing equation 1.111 and 1.113 we have

\[ S_1 = 0, \quad S_n = f_0^{-1} \sum_{k=1}^{n-1} Q(f_0 h_k, f_0 h_{n-k}). \]

(1.132)

Noticing the source term \( S_n \) is only dependent on lower order solutions, one can solve the equations iteratively from zeroth order. In most cases, we are interested in the perturbation equations without the source term,

\[ \frac{\partial h_n}{\partial t} + \xi \cdot \frac{\partial h_n}{\partial x} = L h_n. \]

(1.133)

Whenever the system is very near to the equilibrium status, the higher order term for \( n = 1 \) can be neglected (under certain conditions) and one obtains the so-called linearized Boltzmann equation, which can be used to approximate the solutions to the full nonlinear Boltzmann equation. For details we refer the reader to the detailed discussion in Ref. [37].
Chapter 2

Calculating the Collision Operator

2.1 Background

In chapter 1 we reviewed some basic analytic properties of the Boltzmann equation. In later chapters they will assist us in simplifying the calculation. These analytic properties help us understand the asymptotic behavior of the Boltzmann equation in both small Knudsen and large Knudsen number limit. However, analytic solutions to the Boltzmann equation in most non-trivial problems are impossible. Thus obtaining accurate numerical solutions to the nonlinear Boltzmann Equation is crucial in order to understand the complexities of almost any non-trivial rarefied gas flow, especially because so few analytic solutions are known. The task is made very difficult by the high dimension of the problem. Even for spatially one-dimensional problems, the distribution function depends on 5 variables (time, space and three velocities) and the collision integral involves an integration over three extra velocity variables. Two or three dimensional problems are even more demanding. For this reason, for many years authors in the field did not attempt direct, deterministic solutions of Bultmann’s integro-differential equation; instead, they focused their efforts on Monte Carlo-type methods, in which the gas is represented as a collection of random quasi-particles which evolve according to a suitable stochastic process designed to reproduce the Boltzmann dynamics. Among such probabilistic methods, the best known is probably the DSMC method by Bird [3], and its variants by Nanbu [19] and Babovsky and Neunzert [1]. Among more recent efforts in this direction, we should mention the Stochastic Weighted Particle Method (SWPM) by Rjasanov and
Wagner (see [24] and references therein), and also the time-relaxed Monte Carlo method by Pareschi, Lorenzo, and Russo [23]. Overall, these methods have been quite successful in simulating gas flows at relatively large Mach numbers. They have also been able to handle two or three-dimensional situations because of their reduced computational complexity, which is basically proportional to the number of cells $N$ in the simulation domain. On the downside, probabilistic methods display significant fluctuations, which decay rather slowly with respect to $N$. Conversely, deterministic methods – meaning methods that solve Boltzmann’s equation directly – have the potential to produce much more accurate, fluctuation-free simulations at small and medium Mach number, but are numerically challenging. For a review see [20].

The most significant computational bottleneck in any deterministic method is the evaluation of the Boltzmann collision operator. Such evaluation requires the computation of a three-dimensional integral at each grid point in a three-dimensional (velocity) space, and was for many years out of reach even of the fastest computers. This is why in older works the Boltzmann collision kernel was often replaced, with some success, by the Bhatnagar-Gross-Krook (BGK) [2] model or by similar approximate models, which are numerically simpler and still capture significant physical features. As faster processors became available, researchers were able to calculate more realistic approximations to the complete Boltzmann collision operator, starting with the so-called discrete velocity models (DVM) [18]. Finally, starting in the 1990’s full-fledged calculations of the Boltzmann kernel have become practically feasible. In particular, the last 15 years have seen the successful development of faster and faster spectral methods, which have the advantage of spectral accuracy and less computational complexity than a DVM or finite difference method. Among many contributions, we will mention the work by Bobylev-Rjasanow [4], who were among the first to observe that in Fourier space the collision integral takes a simpler and more compact expression. Pareschi and Russo [22] proposed a spectral treatment of the space homogeneous Boltzmann equation with reduced computational complexity $O(N^6)$. More recently, Filbet, Mouhot and Pareschi [7] developed a spectral method with only $O(N^3 \log N)$ computational complexity, by cleverly recasting the collision operator in a convolution form that can be summed using Fast Fourier transforms. To our knowledge, this is the fastest available way to calculate the collision integral. Unfortunately, it only applies to hard-sphere molecules.

In this chapter, we will explore the fast spectral method in [7]. As we will see in chapter
Chapter 2. Calculating the Collision Operator

4, it is one of the building blocks for our accurate numerical simulation of the Boltzmann equation. At the end of this chapter we will give various numerical simulation examples for the homogeneous Boltzmann equation, using this highly accurate spectral method.

2.2 Transforming from velocity space to the spectral space

The key idea behind [4] and [7] is to transform the velocity dependence of the distribution function \( f(t, x, v) \) (with fixed \( x \) and \( t \)) to Fourier space. We consider the truncated Fourier series representation of \( f(v) \),

\[
f_N(v) = \sum_{k=-N}^{N} \hat{f}_k e^{i\pi T k \cdot v} \tag{2.1}
\]

where

\[
\hat{f}_k = \frac{1}{(2T)^3} \int f(v) e^{-i\pi T k \cdot v} dv.
\]

Clearly \( f(v) \) is not a periodic function, but it is close to a Gaussian function and decays very rapidly for large velocities. Thus we can construct a series of replications of \( f(v) \) distributed periodically along the velocity axis, as illustrated in figure 2.1. As long as they are separated enough, the Fourier frequency components will not be polluted by neighboring distribution.

In order to get the "correct" separation between these replications, we need a careful analysis of the range of the various parameters inside the collision integral. First let us rewrite the collision operator in equation 1.29 as

\[
Q(f, f) = \int_{R^3} \int_{B^-} \left[ f(x_1, \xi_1', t)f(x_1, \xi_2', t) - f(x_1, \xi_1, t)f(x_1, \xi_2, t) \right] B(\theta, V) d\theta d\xi_2.
\]

\[
\xi_1' = \xi_1 - \frac{1}{2}(g - |g| \omega)
\]

\[
\xi_2' = \xi_1 - \frac{1}{2}(g + |g| \omega), \tag{2.2}
\]
where \( g = \xi_1 - \xi_2 \). Suppose \( f(v) \) has a support of radius \( R \), which means \( f(v) \) is zero for \( |v| > R \), then \( Q(f, f)(v) \) has a support of radius \( \sqrt{2}R \) (due to conservation of energy and momentum), and with \( \xi_1, \xi_2, \) and \( g \) belonging to \((0, (2 + \sqrt{2})R)\)(see [7]).

So we need to use a domain \([-T, T]^3\) with \( T \geq (2 + \sqrt{2})R \) to avoid interference at the boundary. And from the geometric illustration below, it is actually enough to take \( T \geq ((2 + \sqrt{2})R + R)/2 = (3 + \sqrt{2})R/2 \).

![Figure 2.1: Periodic distribution in the phase space](image)

**2.3 Evaluating the collision operator**

In this section, we outline the fast \( n \log n \) method to evaluate the collision integral by Pareschi et al. [7] (see also [4]). Consider the spatially homogeneous Boltzmann equation in Eq. (3.3); the five-fold integral in the definition of \( Q(f, f) \), Eq. (3.2), can be transformed to a six fold integral by a mathematical technique, see [4], leading to

\[
Q(f, f)(v) = \int_{S^2} \int_{S^2} \delta(e_1 \cdot e_2) (\Phi(v, e_1)\Phi(v, e_2) - f(v)\Psi(v, e_1, e_2)) \, de_1 \, de_2,
\]  

(2.3)
where
\[ \Phi(v, e) = \int_{-\infty}^{\infty} |\rho| f(v + \rho e) d\rho \] (2.4)
and
\[ \Psi(v, e_1, e_2) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\rho_1| |\rho_2| f(v + \rho_1 e_1 + \rho_2 e_2) d\rho_1 d\rho_2. \] (2.5)

Now using the Fourier series expansion of \( f(v) \) in 2.1, we can expand \( f(v + \rho e_1) \) inside \( \Phi(v, e_1) \) in 2.3 as
\[ f(v + \rho e_1) = \sum_{l=-N}^{N} \hat{f}_l e^{i\frac{\pi}{T} l \cdot v} e^{i\frac{\pi}{T} \rho l \cdot e_1}, \] (2.6)
\( f(v + \rho e_2) \) inside \( \Phi(v, e_2) \) as
\[ f(v + \rho e_2) = \sum_{m=-N}^{N} \hat{f}_m e^{i\frac{\pi}{T} m \cdot v} e^{i\frac{\pi}{T} \rho m \cdot e_2}, \] (2.7)
and \( f(v + \rho_1 e_1 + \rho_2 e_2) \) inside \( \Phi(v, e_1, e_2) \) as
\[ f(v + \rho_1 e_1 + \rho_2 e_2) = \sum_{m=-N}^{N} \hat{f}_m e^{i\frac{\pi}{T} m \cdot v} e^{i\frac{\pi}{T} (\rho_1 m \cdot e_1 + \rho_2 m \cdot e_2)}. \] (2.8)

Recall that
\[ f(v) = \sum_{l=-N}^{N} \hat{f}_l e^{i\frac{\pi}{T} l \cdot v}. \] (2.9)

Substituting the above four expressions into equation 2.3, extracting all Fourier components to the front and moving all components containing \( \rho \) inside the radial integral, the first term in 2.3 can be simplified to
\[ \int_{S^2} \int_{S^2} \delta(e_1 \cdot e_2) \Phi(v, e_1) \Phi(v, e_2) de_1 de_2 \]
\[ = \sum_{l} \sum_{m} e^{i\frac{\pi}{T} (l+m) \cdot v} \hat{f}_l \hat{f}_m \]
\[ \times \int_{S^2} \int_{S^2} \delta(e_1 \cdot e_2) \left( \int_{-\infty}^{\infty} |\rho_1| e^{i\frac{\pi}{T} \rho_1 e_1 \cdot l} d\rho_1 \right) \left( \int_{-\infty}^{\infty} |\rho_2| e^{i\frac{\pi}{T} \rho_2 e_2 \cdot m} d\rho_2 \right) de_1 de_2. \] (2.10)
Similarly the second term in 2.3 is simplified to

\[
\int_{S^2} \int_{S^2} \delta(e_1 \cdot e_2) f(v) \Psi(v, e_1, e_2) d e_1 d e_2 = \sum_l \sum_m e^{i \pi (l+m) \cdot v} \hat{f}_l \hat{f}_m \times \int_{S^2} \delta(e_1 \cdot e_2) \left( \int_{-\infty}^{\infty} |\rho_1| e^{i \pi \rho_1 e_1 \cdot m} d \rho_1 \right) \left( \int_{-\infty}^{\infty} |\rho_2| e^{i \pi \rho_2 e_2 \cdot m} d \rho_2 \right) d e_1 d e_2. \tag{2.11}
\]

The radial integral

\[
\int_{-\infty}^{\infty} |\rho| e^{i \pi \rho e \cdot l} d \rho, \tag{2.12}
\]

is divergent and a cutoff is necessary. We use \( R \) to denote the velocity cutoff, and it can be shown (see the illustration in figure 2.1, and also references [4], [22]) that \( T \geq (3 + \sqrt{2}) R / 2 \).

Then the radial integral becomes

\[
\phi_R(e \cdot l) \equiv \int_{-R}^{R} |\rho| e^{i \pi \rho e \cdot l} d \rho \equiv \int_{-R}^{0} -\rho e^{i \pi \rho e \cdot l} d \rho + \int_{0}^{R} \rho e^{i \pi \rho e \cdot l} d \rho \equiv \left( \frac{\pi}{T} e \cdot l \right)^{-2} \left( - \int_{-\frac{\pi}{T} e \cdot l}^{0} \rho' e^{i \rho' \cdot l'} d \rho' + \int_{0}^{\frac{\pi}{T} e \cdot l} \rho' e^{i \rho' \cdot l'} d \rho' \right) = R^2 \left( 2 \text{Sinc} \left( \frac{\pi}{T} R e \cdot l \right) - \text{Sinc}^2 \left( \frac{\pi}{2T} R e \cdot l \right) \right).
\]

Then, 2.10 can be written as

\[
\int_{S^2} \int_{S^2} \delta(e_1 \cdot e_2) \Phi(v, e_1) \Phi(v, e_2) d e_1 d e_2 = \sum_l \sum_m e^{i \pi (l+m) \cdot v} \hat{f}_l \hat{f}_m \int_{S^2} \Phi_R(e_1 \cdot l) d e_1 \int_{S^2} \delta(e_1 \cdot e_2) \Phi_R(e_2 \cdot m) d e_2. \tag{2.14}
\]

Similarly, 2.11 can be written as

\[
\int_{S^2} \int_{S^2} \delta(e_1 \cdot e_2) f(v) \Psi(v, e_1, e_2) d e_1 d e_2 = \sum_l \sum_m e^{i \pi (l+m) \cdot v} \hat{f}_l \hat{f}_m \int_{S^2} \Phi_R(e_1 \cdot m) d e_1 \int_{S^2} \delta(e_1 \cdot e_2) \Phi_R(e_2 \cdot m) d e_2. \tag{2.15}
\]

The most serious hurdle in order to obtain a \( n \) log \( n \) method is the fact that the integrals
Chapter 2. Calculating the Collision Operator

with respect to \( e_1 \) and \( e_2 \) do not factorize (i.e. the Fourier component \( l \) and \( m \) do not factorize). To circumvent this problem we discretize the \( de_1 \) integral on the unit sphere as a finite sum and rewrite the above as

\[
\sum_l \sum_m e^{i\frac{\pi}{T}(l+m) \cdot v} \int_{\theta_{p,\phi}}^m \frac{4\pi^2}{M_1 M_2} \sin \theta \phi_R(e_{p,q} \cdot l) \int_{e_2 \in S^2 \cap (\theta_{p,\phi})^\perp} \phi_R(e_2 \cdot m) de_2.
\]

In this expression, \((\theta_{p,\phi}) = (p\pi/M_1, q2\pi/M_2)\) is a ”uniform” grid on the unit sphere.

We define

\[
\alpha_{p,q}(l) = \sin \theta \phi_R(e_{p,q} \cdot l), \quad \beta_{p,q}(m) = \int_{e_2 \in S^2 \cap (\theta_{p,\phi})^\perp} \phi_R(e_2 \cdot m) de_2.
\]

Finally, 2.14 can be written as

\[
\int_{S^2} \int_{S^2} \delta(e_1, e_2) \Phi(v, e_1) \Phi(v, e_2) de_1 de_2 = \sum_l \sum_m e^{i\frac{\pi}{T}(l+m) \cdot v} \int_{\theta_{p,\phi}}^m \frac{4\pi^2}{M_1 M_2} \alpha_{p,q}(l) \beta_{p,q}(m).
\]

(2.16)

Following the same procedure, 2.15 is shown to be

\[
\int_{S^2} \int_{S^2} \delta(e_1, e_2) f(v) \Psi(v, e_1, e_2) de_1 de_2 = \sum_l \sum_m e^{i\frac{\pi}{T}(l+m) \cdot v} \int_{\theta_{p,\phi}}^m \frac{4\pi^2}{M_1 M_2} \alpha_{p,q}(m) \beta_{p,q}(m).
\]

(2.17)

Combining the above two expressions, 2.3 is finally expressed as

\[
Q(f, f)(v) = \sum_l \sum_m e^{i\frac{\pi}{T}(l+m) \cdot v} \int_{\theta_{p,\phi}}^m \frac{4\pi^2}{M_1 M_2} (\alpha_{p,q}(l) \beta_{p,q}(m) - \alpha_{p,q}(m) \beta_{p,q}(m)),
\]

(2.18)

in which the right-hand side has a convolution structure and can be calculated using Fast Fourier Transforms with cost \( n \log n \). Note that the discretization of \( e_1 = (\theta, \phi) \) has to be a symmetric cover of the unit sphere. In the next section, we will solve the spatially homogeneous Boltzmann equation using the Fourier spectral method to evaluate the collision integral.
Alternatively one could take the Fourier transform of \( f(v) \) in the left side of the above equation and substituting \( Q(f, f) \), to get

\[
\sum_{k=-N}^{N} e^{i\frac{\pi}{T}k\cdot v} \frac{\partial \hat{f}_k}{\partial t} = \sum_{l} \sum_{m} e^{i\frac{\pi}{T}(l+m)\cdot v} \hat{f}_l \hat{f}_m \sum_{p,q=0}^{M_1,M_2} \frac{4\pi^2}{M_1 M_2} (\alpha_{p,q}(l)\beta_{p,q}(m) - \alpha_{p,q}(m)\beta_{p,q}(m)).
\]

(2.19)

By orthogonality we arrive at the set of ODE’s

\[
\frac{\partial \hat{f}_k}{\partial t} = \sum_{p,q=0}^{M_1,M_2} \frac{4\pi^2}{M_1 M_2} \sum_{m} \hat{f}_{k-m} (\alpha_{p,q}(k-m)\beta_{p,q}(m) - \alpha_{p,q}(m)\beta_{p,q}(m)) \hat{f}_m.
\]

(2.20)

In this way, we solve the spatially homogeneous Boltzmann equation

\[
\frac{\partial f}{\partial t} = Q(f, f).
\]

(2.21)

in Fourier space.

We present the algorithm in the flow chart in Fig.(2.2).

### 2.4 Time relaxation process in the spatially homogeneous case

In this section, we will simulate numerically the relaxation process for the spatially uniform Boltzmann equation. The time stepping is carried out with a straightforward third-order Runge-Kutta method. The initial condition is an even mix of two Maxwellian distributions, 

\[
f_d = \rho_d (\pi T_d)^{-3/2} \exp[-((v_x - u_u)^2 + (v_y - u_u)^2 + (v_z - u_u)^2)/T_d]
+ \rho_d (\pi T_d)^{-3/2} \exp[-((v_x + u_u)^2 + (v_y + u_u)^2 + (v_z + u_u)^2)/T_d],
\]
where

\[ \rho_d = \frac{4M^2}{(M^2 + 3)}, \]

\[ T_d = \frac{(5M^2 - 1)(M^2 + 3)/16M^2}{16}, \]

\[ u_u = \sqrt{5/6}M, \]

(2.22)

\[ \rho_d = 4M^2/(M^2 + 3), \]

\[ T_d = (5M^2 - 1)(M^2 + 3)/16M^2, \]

\[ u_u = \sqrt{5/6}M, \]

and \( M = 2.0 \). In the simulation, the time step is taken to be \( \Delta t = 0.0025 \), and three different phase space resolutions \( n = 64, n = 81, \) and \( n = 100 \) are used. In figure 2.3, the initial distribution is plotted in a phase space grid \( 64 \times 64 \times 64 \). Figure 2.4 is the evolution after 50 time steps, and we can see that the two Maxwellian that were separated diagonally at the beginning started to merge. After 200 time steps, in figure 2.5, the initial distribution has fully evolved to a single Maxwellian. We also simulated the evolution on a finer grid of \( 81 \times 81 \times 81 \) in figures 2.6, 2.6, and 2.6. Compared with previous coarse grid, the surface becomes smoother. Finally, we carried out the simulation at our finest grid of \( 100 \times 100 \times 100 \) in figures 2.9, 2.10, and 2.11. In figure 2.12, we present a cross section view in X-Y plane at time step 250, from which one can tell the evolved distribution is X-Y symmetric, and further in figure 2.13 one can clearly see that the distribution is isotropic.
Chapter 2. Calculating the Collision Operator

39

initialize \( f(v) \)

FFT transform: \( \hat{f}_k \)

arrange \( \hat{f}_k \) to put zero frequency component in the center

\( \hat{f}_{l\alpha p,q}(l) \)
padding zeros

\( \hat{f}_{m\beta p,q}(m) \)
padding zeros

\( FFT(\hat{f}_{l\alpha p,q}(l)) \)

\( FFT(\hat{f}_{m\beta p,q}(m)) \)

sum angular parameter \( \alpha, \beta \)

\( FFT^{-1}(\hat{f}_{l\alpha p,q}(l)) \cdot \)

\( FFT(\hat{f}_{m\beta p,q}(m)) \)

cutoff from \( 2N - 1 \) to \( N \)

arrange to put zero frequency component in the beginning.

\( FFT^{-1} \)

sum to \( \hat{Q}(f,f) \)

\( FFT^{-1} \) to give \( Q(f,f) \)

Figure 2.2: Collision algorithm flow chart
Chapter 2. Calculating the Collision Operator

Figure 2.3: $n=64$ time step=0

Figure 2.4: $n=64$ time step=50
Chapter 2. Calculating the Collision Operator

Figure 2.5: n=64 time step=200

Figure 2.6: n=81 time step=0
Chapter 2. *Calculating the Collision Operator*

Figure 2.7: $n=81$ time step=50

Figure 2.8: $n=81$ time step=200
Figure 2.9: $n=100$ time step=0

Figure 2.10: $n=100$ time step=50
Figure 2.11: n=100 time step=200

Figure 2.12: n=100 time step=250, X-Y intersection at Z=50
Figure 2.13: n=250 time step=250, intersection at the center
Chapter 2. Calculating the Collision Operator

2.5 GPU acceleration

The evaluation of collision operator is usually the most time consuming part. Although we have adopted a $n\log n$ fast method, we still need to sum over the angular variable. Moreover, in the evaluation of the convolution structure in Eq. (2.18), we have to pad zeros after $\hat{f}_k$, which further brings down the efficiency especially for large phase space grids. For example, if $n$ is the dimension of $f(v)$, we need to do FFT on a bigger $N$ in the phase space to avoid pollution during convolution. Usually $N$ is twice as large as $n$; fortunately, because $f(v)$ has a compact support, in practice we found a $N = 1.5n$ is sufficient. We have also developed a GPU (graphics processing unit) CUDA ([42]) code (a parallel computing platform and programming model invented by NVIDIA) to take advantage of massive parallel implementation of Fast Fourier transformation. This greatly reduced the computation time. In Fig. (2.14) (data listed in table. (2.1)), we compared the CPU time and GPU time for the evaluation $Q(f, f)$ one single time. We use FFTW ([41]) to compute FFT on CPU, and CUFFT ([43]) as a CUDA library to compute FFT on GPU. The CPU is a 2.6 GHz Intel Core i7, and GPU is NVIDIA GEFORCE GT 650M with 384 CUDA cores.

![Figure 2.14: Compare CPU and GPU time (in seconds)](image-url)
Table 2.1: Compare CPU and GPU time (in seconds)

<table>
<thead>
<tr>
<th>n</th>
<th>15</th>
<th>21</th>
<th>27</th>
<th>35</th>
<th>42</th>
<th>45</th>
<th>64</th>
<th>81</th>
<th>100</th>
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<tr>
<td>CPU Time</td>
<td>0.068</td>
<td>0.57</td>
<td>0.34</td>
<td>0.87</td>
<td>1.04</td>
<td>1.97</td>
<td>4.75</td>
<td>9.23</td>
<td>22.88</td>
</tr>
<tr>
<td>GPU Time</td>
<td>0.027</td>
<td>0.049</td>
<td>0.12</td>
<td>0.26</td>
<td>0.24</td>
<td>0.38</td>
<td>0.74</td>
<td>0.91</td>
<td>1.38</td>
</tr>
</tbody>
</table>
Chapter 3

Solving the transport equation

3.1 Background

In the previous chapter, we introduced a fast spectral method to evaluate the collision operator ([7]). We then solved a relatively simple problem, spatially homogeneous time relaxation to a Maxwellian equilibrium. Of course, being able to calculate the collision integral is not sufficient in order to solve the full Boltzmann equation. One also needs an appropriate scheme in order to handle the advective terms in the equation, and ensure that they cancel out with the collision term. As a general strategy, the splitting method [27], which solves the transport process and collision process in an alternating fashion, is easy to implement and usually ensures second-order accuracy. In order to implement the splitting method, however, one needs a high order hyperbolic conservation-law solver for the ”advection step”, which is the topic in this chapter. In principle, many methods are available: one could consider finite-difference, finite-volume, finite-element, spectral methods etc. In kinetic theory, however, the positivity of the distribution function should be preserved. Some positivity-preserving methods have been presented in the vast literature about numerical solutions to the Vlasov-Poisson equation, where splitting schemes are ubiquitous and involve to same free-flow advection equation as in the Boltzmann case; we refer to [9] for a review. For instance, in [8], Filbet and Russo applied to the Boltzmann equation the PFC method which they had first developed in the Vlasov context [10]. It is essentially a third order Semi-Lagrangian (SL) scheme [26] with a flux limiter which preserves positivity and global maximum. One should not assume, however,
that Vlasov-optimized advection methods are necessarily the best choice for rarefied gas flows. In many practical applications of the Boltzmann equation one deals with steep, shock-type solutions, which often require dealing with discontinuities in the initialization data. This limits seriously the applicability of spectral methods, which are very vulnerable to the effects of Gibbs phenomena near points of discontinuity (so that suitable filtering schemes are necessary in order to keep the method stable, see [13],[12]). An attractive option, which will be explored here, is to use non-oscillatory, positivity preserving, shock-capturing finite-difference schemes. In the Vlasov case such schemes would be prohibitively expensive because of the well-known filamentation effects, which would require finer and finer grids as the simulation progresses. Conversely, no such problem arises for the Boltzmann equation, due to its good dissipation properties at physically relevant Knudsen numbers.

Historically, a second-order accurate Essentially Non-Oscillatory (ENO) method for hyperbolic conservation laws was first proposed in [15]; see also [25] for a higher order version. Other authors [17], [16] proposed a fifth order Weighted Essentially Non-Oscillatory method combined with a Total Variation Diminishing [14] integrator in time. The philosophy of all these methods is to use a high order polynomial in each cell to reconstruct the values of the unknown function on the cell’s boundaries starting from grid values at the centers of the cells. Because the polynomials are different in each cell, at each boundary between cells there is a ”left” value and a ”right” value. Since this is essentially a Riemann problem, one can then choose an appropriate scheme to ”mix” the left flux and right flux and obtain the flux across the cell. An ENO method plus a flux scheme and a Runge-Kutta time-stepping scheme form a complete method to solve the advection equation. In this section we do not intend to give a comprehensive introduction of various methods in solving the transport equation, instead, we will emphasize on the WENO methods with appropriate flux limiter, and the PFC method.

3.2 The splitting method

After choosing suitable reference scales (see Section. (1.9)), the dimensionless Boltzmann equation is

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

(3.1)
Chapter 3. Solving the transport equation

\( Q(f, f) \) is the collision term. We recall that for a gas of hard spheres, \( Q(f, f) \) is given by

\[
Q(f, f)(v) = \int_{\mathbb{R}^3} \int_{S^2} |v - w|[f(v')f(w') - f(v)f(w)]de dw,
\]

where \( w' \) and \( v' \) are given in terms of \( w \) and \( v \) by

\[
v' = \frac{1}{2}(v + w + |v - w|e), \quad w' = \frac{1}{2}(v + w - |v - w|e)
\]

and \( e \) is a unit vector.

In the splitting method [39], instead of solving the whole Boltzmann equation, we solve two separate equations, namely the advection equation,

\[
\frac{\partial f}{\partial t} + v \cdot \frac{\partial f}{\partial x} = 0,
\]

and the collision equation,

\[
\frac{\partial f}{\partial t} = Q(f, f).
\]

We denote the action of the advection step on the distribution function \( f(v) \) as an operator \( S^\Delta t_A \), and the action of the collision step on \( f(v) \) as an operator \( S^\Delta t_B \) where \( \Delta t = t^{n+1} - t^n \) is one time step. In a first order splitting method, we approximate \( f(v) \) at \( t^{n+1} \) as

\[
f(t^{n+1}, v) = S^\Delta t_B S^\Delta t_A f(t^n, v).
\]

In a second order splitting method, which we will use in this paper,

\[
f(t^{n+1}, v) = S^\Delta t_A S^\Delta t_B S^\Delta t_A f(t^n, v).
\]

We will concentrate on the case when the spatial dependence of \( f \) is one-dimensional, so that Eq. (3.2) reduces to

\[
\frac{\partial f}{\partial t} + v_1 \frac{\partial f}{\partial x_1} = 0,
\]

where \( x_1 \) and \( v_1 \) indicate, respectively, the first component of \( x \) and the corresponding component of \( v \). In order to simplify the notation, in what follows we will just write \( x \) for \( x_1 \) and \( v_x \) for \( v_1 \). The splitting algorithm is shown in Fig.(3.1).
3.3 Solving the 1-d transport equation

In this section, we will introduce the general framework of finite volume method in solving the transport equation. The formula is expressed in 1-d case, but no generality is lost as it can be applied to the 3-d case in the same manner. We want solve the following 1-d transport equation,

\[
\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} = 0,
\]  

(3.5)

where \( f \) is the distribution function as usual. In order to conform to the prevalent notation in the literature on hyperbolic conservation laws, we instead use \( q(x, t) \) to denote the unknown function, and \( f(q) \) to denote a generic function of \( q \). In the case of Eq. (3.4),
Chapter 3. *Solving the transport equation* 52

\[ q(x,t) \equiv f(x,v,t) \text{ (for each fixed } v) \text{ and } f(q) \equiv v_x q. \] We discretize

\[ \frac{\partial q}{\partial t} + \frac{\partial f(q)}{\partial x} = 0, \quad (3.6) \]

on an even spatial grid with spacing \( \Delta x = x_{i+1} - x_i \) (so that for each choice of \( v \) the CFL number will be \( \frac{v \Delta t}{\Delta x} \)). The spatial discretization uses a finite volume approach, in which each node value \( q_i \) represents the average value of \( q \) in the cell \( C_i \equiv [x_{i-1/2}, x_{i+1/2}] \). The grid system is illustrated in Fig. (3.2).

<table>
<thead>
<tr>
<th>( i-4 )</th>
<th>( i-3 )</th>
<th>( i-2 )</th>
<th>( i-1 )</th>
<th>( i )</th>
<th>( i+1 )</th>
<th>( i+2 )</th>
<th>( i+3 )</th>
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</thead>
<tbody>
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<td>( x_{i-\frac{5}{2}} )</td>
<td>( x_{i-\frac{3}{2}} )</td>
<td>( x_{i-\frac{1}{2}} )</td>
<td>( x_{i+\frac{1}{2}} )</td>
<td>( x_{i+\frac{3}{2}} )</td>
<td>( x_{i+\frac{5}{2}} )</td>
<td>...</td>
<td></td>
</tr>
</tbody>
</table>

**Figure 3.2:** Finite volume grid

Eq. (3.6) can be rewritten as

\[ \frac{\partial q}{\partial t} = L, \quad (3.7) \]

and \( L \) is the net flux crossing the cell \( C_i \) expressed as

\[ L = -\frac{1}{\Delta x} (f_{i+1/2} - f_{i-1/2}). \quad (3.8) \]

Since we only know the cell average value \( f_i \), the values at the cell boundary have to be approximated, as discussed below in the section about reconstruction in the WENO method. The reconstruction process usually involve several grid points depending on the approximation order. At the space domain boundary, we have to extrapolate a few "ghost" points. The strategy is described in Ref. [28]. Specifically, at the right-most grid point \( x_N \), for positive velocities we extrapolate the next ghost point as \( q_{N+1} = q_N \). For negative velocities, we extrapolate the next ghost point using a third order Lagrangian extrapolation formula,

\[ q_{N+1} = 3q_N - 3q_{N-1} + q_{N-2}. \]

The left boundary is handled in a similar fashion. These boundary conditions are consistent with a choice of the reference frame in which the shock travels from left to right.
3.4 WENO method

3.4.1 Time Advance

The WENO is a high order finite volume method, specially designed for solutions that contain steep gradient or discontinuities. It is typically carried at a fifth order, but higher order methods are also available. The general framework of the WENO methods is semi-discrete, in the sense that one discretizes Eq. (3.6) in space and then uses a separate high-order Runge-Kutta integrator in time [16]. The calculation consists of several steps described in subsequent subsections step by step.

Suppose that in Eq.(3.7) the fluxes $L(q)$ have been calculated, we then proceed with a standard third-order Runge-Kutta time step of the form

$$
q_i^{(1)} = q_i^n + \Delta t L(q_i^n)
$$

$$
q_i^{(2)} = \frac{3}{4} q_i^n + \frac{1}{4} q_i^{(1)} + \frac{1}{4} \Delta t L(q_i^{(1)})
$$

$$
q_i^{n+1} = \frac{1}{3} q_i^n + \frac{2}{3} q_i^{(2)} + \frac{2}{3} \Delta t L(q_i^{(2)})
$$

where $q_i^n$ is the value of $q_i$ at time step $n$ and $L(q_i)$ is spatial flux operator, and we rewrite Eq.(3.8) as

$$
L(q_i) = \frac{1}{\Delta x} (F_{i-1/2} - F_{i+1/2}). \quad (3.9)
$$

Here, we use $F_{i-1/2}$ and $F_{i+1/2}$ instead of those in Eq.(3.8), representing the flux scheme described in the flux calculation subsection.

3.4.2 WENO Reconstruction

At each time step, following the general WENO procedure [16], we use high order polynomials involving the $q$-values from several neighboring cells in order to reconstruct, for each cell $C_i$ centered at the grid point $x_i$, the values $q_{i-1/2}^R$ at the left boundary approached from the right side, and $q_{i+1/2}^L$ at the right boundary approached from left side (see Fig. 3.3).
In a cell $C_i$, the formulas in [16] are used to approximate the value of $q_{i-1/2}^R$ and $q_{i+1/2}^L$. While the value of $q_{i-1/2}^L$ can be obtained by using the formulas in cell $C_{i-1}$, and $q_{i+1/2}^R$ is obtained by using it in cell $C_{i+1}$. The formulas below introduce three different stencils $\hat{q}_j^i$ with index $j$, $j = 0, 1, 2$, that approximate $q_{i+1/2}^L$ at the cell’s right boundary. For positive velocities $v \geq 0$, they are

\[
\begin{align*}
\hat{q}_0^i &= \frac{1}{3} q_{i-2} - \frac{7}{6} q_{i-1} + \frac{11}{6} q_i \\
\hat{q}_1^i &= -\frac{1}{6} q_{i-1} + \frac{5}{6} q_i + \frac{1}{3} q_{i+1} \\
\hat{q}_2^i &= \frac{1}{3} q_i + \frac{5}{6} q_{i+1} - \frac{1}{6} q_{i+2}.
\end{align*}
\tag{3.10}
\]

The value of $q_{i+1/2}^L$ is given by the weighted combination

\[
q_{i+1/2}^L = \omega_0 \hat{q}_0^i + \omega_1 \hat{q}_1^i + \omega_2 \hat{q}_2^i,
\tag{3.11}
\]

where $\omega_k = \alpha_k / \sum \alpha_l$, and

\[
\begin{align*}
\alpha_0 &= \frac{1}{10(IS_0 + 10^{-6})^2} \\
\alpha_1 &= \frac{6}{10(IS_1 + 10^{-6})^2} \\
\alpha_2 &= \frac{3}{10(IS_2 + 10^{-6})^2}.
\end{align*}
\tag{3.12}
\]
Chapter 3. Solving the transport equation

The smoothness indicators $IS_k$ are

\[
IS_0 = \frac{13}{12} (q_{i-2} - 2q_{i-1} + q_i)^2 + \frac{1}{4} (q_{i-2} - 4q_{i-1} + 3q_i)^2
\]

\[
IS_1 = \frac{13}{12} (q_{i-1} - 2q_i + q_{i+1})^2 + \frac{1}{4} (q_{i-1} - q_{i+1})^2
\]

\[
IS_2 = \frac{13}{12} (q_i - 2q_{i+1} + q_{i+2})^2 + \frac{1}{4} (3q_i - 4q_{i+1} + 3q_{i+2})^2.
\]  

(3.13)

In the negative velocity case, $q_{i+1/2}^L$ is still expressed by Eq. (3.11) and Eq. (3.12), but the stencils in Eq. (3.10) are reflected around $x_{i+1/2}$,

\[
\hat{q}_i^0 = \frac{1}{6} q_{i-1} - \frac{5}{6} q_i + \frac{1}{3} q_{i+1}
\]

\[
\hat{q}_i^1 = \frac{1}{3} q_i + \frac{5}{6} q_{i+1} - \frac{1}{6} q_{i+2}
\]

\[
\hat{q}_i^2 = \frac{11}{6} q_{i+1} - \frac{7}{6} q_{i+2} + \frac{1}{3} q_{i+3}
\]

(3.14)

and the smoothness indicators in Eq. (3.13) also have to be reflected around $x_{i+1/2}$,

\[
IS_0 = \frac{13}{12} (q_{i+1} - 2q_i + q_{i-1})^2 + \frac{1}{4} (3q_{i+1} - 4q_i + 3q_{i-1})^2
\]

\[
IS_1 = \frac{13}{12} (q_{i+2} - 2q_{i+1} + q_i)^2 + \frac{1}{4} (q_{i+2} - q_i)^2
\]

\[
IS_2 = \frac{13}{12} (q_{i+3} - 2q_{i+2} + q_{i+1})^2 + \frac{1}{4} (q_{i+3} - 4q_{i+2} + 3q_{i+1})^2.
\]  

(3.15)

In the above equations, to facilitate comparison, we have reversed the order of list of stencils and $IS_k$.

So far we have $q_{i+1/2}^L$ for both positive and negative velocity. For $q_{i-1/2}^R$ it is convenient to consider the negative velocity case first, which can be obtained by reflecting Eq.(3.10) around $x_i$ (or by reflecting about $x_{i+1/2}$ and then shifting the index to the left by 1), because the original equation remains unchanged by reflecting both $x$ and the velocity,

\[
\hat{q}_i^2 = \frac{1}{6} q_{i-2} + \frac{5}{6} q_{i-1} + \frac{1}{3} q_i
\]

\[
\hat{q}_i^1 = \frac{1}{3} q_{i-1} + \frac{5}{6} q_i - \frac{1}{6} q_{i+1}
\]

\[
\hat{q}_i^0 = \frac{11}{6} q_i - \frac{7}{6} q_{i+1} + \frac{1}{3} q_{i+2}.
\]  

(3.16)
Chapter 3. Solving the transport equation

The smoothness indicators $I_{S_k}$ in Eq. (3.13) is also reflected about $x_i$, and is given by

$$I_{S_0} = \frac{13}{12} (q_{i-2} - 2q_{i-1} + q_i)^2 + \frac{1}{4} (3q_{i-2} - 4q_{i-1} + 3q_i)^2$$

$$I_{S_1} = \frac{13}{12} (q_{i-1} - 2q_i + q_{i+1})^2 + \frac{1}{4} (q_{i-1} - q_{i+1})^2$$

$$I_{S_2} = \frac{13}{12} (q_i - 2q_{i+1} + q_{i+2})^2 + \frac{1}{4} (3q_i - 4q_{i+1} + q_{i+2})^2. \tag{3.17}$$

In the above two equations, we also have reversed the order of the list of stencils and $I_{S_k}$. Then $q_{i-1/2}^R$ is given by the weighted combination

$$q_{i-1/2}^R = \omega_0 \hat{q}_0^i + \omega_1 \hat{q}_1^i + \omega_2 \hat{q}_2^i. \tag{3.18}$$

To get the positive velocity case of $q_{i-1/2}^R$, one needs to reflect Eq. (3.16) about $x_{i-1/2}$,

$$\hat{q}_0^i = \frac{1}{3} q_{i-3} - \frac{7}{6} q_{i-2} + \frac{11}{6} q_{i-1}$$

$$\hat{q}_1^i = -\frac{1}{6} q_{i-2} + \frac{5}{6} q_{i-1} + \frac{1}{3} q_i$$

$$\hat{q}_2^i = \frac{1}{3} q_{i-1} + \frac{5}{6} q_i - \frac{1}{6} q_{i+1}. \tag{3.19}$$

The smoothness indicators $I_{S_k}$ in Eq. (3.17) are also reflected about $x_i$,

$$I_{S_0} = \frac{13}{12} (q_{i-3} - 2q_{i-2} + q_{i-1})^2 + \frac{1}{4} (q_{i-3} - 4q_{i-2} + 3q_{i-1})^2$$

$$I_{S_1} = \frac{13}{12} (q_{i-2} - 2q_{i-1} + q_i)^2 + \frac{1}{4} (q_{i-2} - q_i)^2$$

$$I_{S_2} = \frac{13}{12} (q_{i-1} - 2q_i + q_{i+1})^2 + \frac{1}{4} (3q_{i-1} - 4q_i + 3q_{i+1})^2. \tag{3.20}$$

Eq. (3.18) and Eq. (3.12) remains the same.

### 3.4.3 Flux Calculation

Since the WENO polynomials vary from cell to cell, at each boundary between two cells we have a "left" value and a "right" value, for example, at $x_{i+1/2}$ we have $q_{i+1/2}^L$ and $q_{i+1/2}^R$ which can be calculated by procedures described in last section. In order to produce an accurate overall value for the flux across the given boundary, we must choose
an appropriate flux scheme to "mix" these two different values. Among many candidates we will consider three possibilities:

In the first case, Godunov flux is an upwind flux, which was originally proposed as the exact solution of the piece-wise Riemann problem [11].

\[
F_{i+1/2}^{GOD} = f(q_{i+1/2}^L) \quad v > 0. \\
F_{i+1/2}^{GOD} = f(q_{i+1/2}^R) \quad v < 0.
\]

The idea behind the Godunov flux is rather straightforward, for example, if the velocity is positive, then the information is always flowing into the cell from the left side, that’s why we simply choose the "left" value in a cell boundary. Being an upwind flux, it has the great advantage of respecting the physics of a wave front traveling in a specific direction.

Another popular choice is the Rusanov flux,

\[
F_{i+1/2}^{RUS}(q_{i+1/2}^L, q_{i+1/2}^R) = \frac{1}{2}(f(q_{i+1/2}^L) + f(q_{i+1/2}^R)) - \frac{1}{2}S_{i+1/2}^+(q_{i+1/2}^R - q_{i+1/2}^L),
\]

where \(S_{i+1/2}^+\) is the maximum signal speed across the boundary, which in our case is simply the constant velocity \(v_x\).

In the limiting case \(S_{i+1/2}^+ = \Delta x/\Delta t\) the Rusanov flux reduces to the widely used Lax-Friedrichs (LF) flux,

\[
F_{i+1/2}^{LF}(q_{i+1/2}^L, q_{i+1/2}^R) = \frac{1}{2}(f(q_{i+1/2}^L) + f(q_{i+1/2}^R)) - \frac{1}{2}\Delta x \frac{\Delta t}{\Delta x}(q_{i+1/2}^R - q_{i+1/2}^L).
\]

To help understanding, let’s take LF flux as an example. Starting from Eq.(3.6), using a forward scheme in time and a centered scheme in space, we rewrite the equation as

\[
\frac{q_{i+1}^n - 1}{2}(q_{i+1}^n + q_{i-1}^n) - \frac{\Delta t}{2\Delta x}(f(q_{i+1}^n) - f(q_{i-1}^n)) = 0,
\]

so we can express \(q_{i+1}^n\) as

\[
q_{i+1}^n = \frac{1}{2}(q_{i+1}^n + q_{i-1}^n) - \frac{\Delta t}{2\Delta x}(f(q_{i+1}^n) - f(q_{i-1}^n)).
\]
The above expression can be further written in finite volume form,

$$q_{i}^{n+1} = q_{i}^{n} - \frac{\Delta t}{\Delta x}(f(q_{i+1/2}^{n}) - f(q_{i-1/2}^{n})),$$  \hspace{2cm} (3.25)

where $f(q_{i+1/2}^{n})$ and $f(q_{i-1/2}^{n})$ are just the LF flux defined in Eq.(3.22).

Since the solutions are expected to remain positive and bounded, one should consider the possibility of adding a limiter to the flux to ensure positivity and to preserve the global maximum. In our simulations we used a Maximum-principle-satisfying flux limiter described in next section in combination with the Godunov, Rusanov and Lax-Friedrichs fluxes.

### 3.4.4 Maximum-principle-satisfying flux limiter

A flux limiter operates by modifying $q_{i-1/2}^{R}$ and $q_{i+1/2}^{L}$ to new values $\tilde{q}_{i-1/2}^{R}$ and $\tilde{q}_{i+1/2}^{L}$ for each cell $C_{i}$. The modified values can be proved to lie between the required maximum and minimum. The tilde values are then substituted into the flux schemes described in the previous section. We briefly describe the procedure; for details and proofs we refer to [29] [30]. First, we construct a fifth order polynomial $P_{i}(x)$ which interpolates $q$ at five points, $q_{i-1}, q_{i-1/2}^{R}, q_{i}^{L}, q_{i+1/2}^{L}$ and $q_{i+1}$.

$$P_{i}(x) = a_{4}(x - x_{i})^{4} + a_{3}(x - x_{i})^{3} + a_{2}(x - x_{i})^{2} + a_{1}(x - x_{i}) + a_{0},$$ \hspace{2cm} (3.26)

where the coefficients are given by

$$a_{0} = \frac{q_{i-1} + 298q_{i} + q_{i+1} - 54(q_{i-1/2}^{R} + q_{i+1/2}^{L})}{192},$$

$$a_{1} = \frac{q_{i-1} - q_{i+1} - 10(q_{i-1/2}^{R} - q_{i+1/2}^{L})}{8\Delta x},$$

$$a_{2} = \frac{-(q_{i-1} + 58q_{i} + q_{i+1}) + 30(q_{i-1/2}^{R} + q_{i+1/2}^{L})}{8\Delta x^{2}},$$

$$a_{3} = \frac{q_{i+1} - q_{i-1} + 2(q_{i-1/2}^{R} - q_{i+1/2}^{L})}{\Delta x^{3}},$$

$$a_{4} = \frac{5q_{i-1} + 50q_{i} + 5q_{i+1} - 30(q_{i-1/2}^{R} + q_{i+1/2}^{L})}{12\Delta x^{4}}.$$
Next, we identify the local minimum $m_i$ and the local maximum $M_i$ of the values taken by the polynomial at the quadrature points in $C_i$ mapped from the Gauss-Lobatto quadrature points on $[-\frac{1}{2}, \frac{1}{2}]$.

We modify the polynomial $p_i$ to

$$
\tilde{p}_i(x) = \theta (p_i(x) - q_i) + q_i, \quad \theta = \min \left\{ \frac{M_i - q_i}{M - q_i}, \frac{M - q_i}{m_i - q_i}, 1 \right\},
$$

(3.27)

where $M$ and $m$ are the global maximum and minimum respectively. Lastly, we evaluate $\tilde{p}_i(x)$ at cell boundaries, and get

$$
\tilde{q}^{R}_{i-1/2} = \tilde{p}_i(x_{i-\frac{1}{2}}), \quad \tilde{q}^{L}_{i+1/2} = \tilde{p}_i(x_{i+\frac{1}{2}}).
$$

(3.28)

All of the above is valid only for CFL numbers smaller than 1/12.

### 3.5 PFC

In this section we briefly describe the PFC method, which we have also implemented as a comparison to test the WENO method. For more details, see reference [10], where it is also shown that the method preserves positivity and the global maximum. The idea is to track back the value of $f$ along the characteristics. We know the transport equation has the exact solution

$$
q(t^{n+1}, x) = q(t^n, x - vt),
$$

(3.29)

which can be integrated on both sides, giving

$$
q^{n+1} = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q(t^{n+1}, x) dx = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}} - v\Delta t}^{x_{i+\frac{1}{2}} - v\Delta t} q(t^n, x) dx
$$

$$
= q^n_i - \frac{1}{\Delta x} \left( \int_{x_{i+\frac{1}{2}} - v\Delta t}^{x_{i+\frac{1}{2}}} q(t^n, x) dx - \int_{x_{i-\frac{1}{2}} - v\Delta t}^{x_{i-\frac{1}{2}}} q(t^n, x) dx \right).
$$

(3.30)

Define

$$
\Phi_{i+1/2}(t^n) = \int_{x_{i+\frac{1}{2}} - v\Delta t}^{x_{i+\frac{1}{2}}} q(t^n, x)
$$

(3.31)
Chapter 3. Solving the transport equation

and

\[ \Phi_{i-1/2}(t^n) = \int_{x_{i-1/2}^n}^{x_i-1/2} q(t^n, x) \, dx; \quad (3.32) \]

then, Eq. (3.30) becomes a finite volume form

\[ q^{n+1} = q^n - \frac{1}{\Delta x} \left( \Phi_{i+1/2}(t^n) - \Phi_{i-1/2}(t^n) \right). \quad (3.33) \]

To carry out the integration in Eq. (3.31) and Eq. (3.32) we use a third order polynomial \( q_h(t^n, x) \) to represent \( q(t^n, x) \) within the cell \( C_i \),

\[ q_h(t^n, x) = q^n_i + \frac{1}{6\Delta x^2} \left[ 2(x-x_i)(x-x_{i-3/2}) + (x-x_{i-1/2})(x-x_{i+1/2}) \right] (q^n_{i+1} - q^n_i) - \frac{1}{6\Delta x^2} \left[ 2(x-x_i)(x-x_{i+3/2}) + (x-x_{i-1/2})(x-x_{i+1/2}) \right] (q^n_i - q^n_{i-1}). \quad (3.34) \]

Note that \( q_h(t^n, x) \) has the property

\[ \frac{1}{\Delta x} \int_{x_{i-1/2}^n}^{x_{i+1/2}^n} q_h(t^n, x) \, dx = q_i. \quad (3.35) \]

To preserve positivity and satisfy a maximum principle, \( q_h(t^n, x) \) needs to be modified to

\[ q_h(t^n, x) = q^n_i + \frac{\epsilon^+_i}{6\Delta x^2} \left[ 2(x-x_i)(x-x_{i-3/2}) + (x-x_{i-1/2})(x-x_{i+1/2}) \right] (q^n_{i+1} - q^n_i) - \frac{\epsilon^-_i}{6\Delta x^2} \left[ 2(x-x_i)(x-x_{i+3/2}) + (x-x_{i-1/2})(x-x_{i+1/2}) \right] (q^n_i - q^n_{i-1}) \quad (3.36) \]

where, \( \epsilon^+_i \) and \( \epsilon^-_i \) are the limiters, defined by

\[ \epsilon^+_i = \begin{cases} 
\min \left( \frac{1}{1; \frac{2q^n_i}{q^n_{i+1} - q^n_i}}, f^n_{i+1} - f^n_i \right) & f^n_{i+1} - f^n_i > 0 \\
\min \left( \frac{1}{1; \frac{-2(q^n_{i-1} - q^n_i)}{q^n_{i-1} - q^n_i}}, f^n_{i+1} - f^n_i \right) & f^n_{i+1} - f^n_i < 0 
\end{cases} \quad (3.37) \]

and

\[ \epsilon^-_i = \begin{cases} 
\min \left( \frac{1}{1; \frac{2q^n_i}{q^n_{i-1} - q^n_i}}, f^n_{i-1} - f^n_i \right) & f^n_{i-1} - f^n_i > 0 \\
\min \left( \frac{1}{1; \frac{-2(q^n_{i+1} - q^n_i)}{q^n_{i+1} - q^n_i}}, f^n_{i-1} - f^n_i \right) & f^n_{i-1} - f^n_i < 0 
\end{cases} \quad (3.38) \]
Chapter 3. Solving the transport equation

Now, we can substitute $q_h(t^n, x)$ in 3.31. We use superscript $+$ on $\Phi$ represents positive $v$’s (and superscript $-$ for negative velocity case later),

$$
\Phi_{i+1/2}^+(t^n) = \int_{x_{i+1/2}}^{x_{i+3/2}} q_h(t^n, x) dx
= v \Delta t [q_{i+1}^n - \epsilon_+^6 (1 - \lambda)(2 - \lambda)(q_{i+2}^n - q_i^n) \\
+ \epsilon_-^6 (1 + \lambda)(1 + \lambda)(q_{i+1}^n - q_{i-1}^n)].
$$

(3.39)

The integration is illustrated by the shaded area in Fig.(3.4). We start to integrate from a distance of $v \Delta t$ to the left of the cell right boundary. $\Phi_{i-1/2}^+(t^n)$ is obtained by changing $i$ to $i - 1$.

Because $q_h(t^n, x)$ is the approximation within cell $i$, while the negative velocity case is evaluated at the boundary $x_{i+1/2}$ and this involves tracking the flux from cell $i + 1$, it is more convenient to compute negative case at boundary $x_{i-1/2}$ first, and then use symmetry to get the expression at boundary $x_{i+1/2}$. In the negative velocity case $x_{i-1/2} - v \Delta t > x_{i-1/2}$ and the expression for $q_h(t^n, x)$ is valid within the shaded area in Fig.(3.5). We find

$$
\Phi_{i-1/2}^-(t^n) = \int_{x_{i-1/2}}^{x_{i-3/2}} q_h(t^n, x) dx \\
= - \int_{x_{i-1/2}}^{x_{i-3/2}} q_h(t^n, x) dx \\
= v \Delta t [q_i^n - \epsilon_+^6 (1 - \lambda)(1 + \lambda)(q_{i+1}^n - q_i^n) \\
- \epsilon_-^6 (1 + \lambda)(2 + \lambda)(q_{i+1}^n - q_{i-1}^n)].
$$

(3.40)
$v < 0 \quad \rightarrow$

<table>
<thead>
<tr>
<th>$i - 4$</th>
<th>$i - 3$</th>
<th>$i - 2$</th>
<th>$i - 1$</th>
<th>$i$</th>
<th>$i + 1$</th>
<th>$i + 2$</th>
<th>$i + 3$</th>
<th>$i + 4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_i - \frac{5}{2}$</td>
<td>$x_i - \frac{3}{2}$</td>
<td>$x_i - \frac{1}{2}$</td>
<td>$x_i + \frac{1}{2}$</td>
<td>$x_i + \frac{3}{2}$</td>
<td>$x_i + \frac{5}{2}$</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 3.5: PFC: Integral at the left boundary for a negative velocity

$\Phi_{i+1/2}(t^n)$ is obtained by changing $i$ to $i + 1$.

Finally, we get the complete equation, for positive $v$'s,

$$q_i^{n+1} = q_i^n - \lambda \left\{ \left[ q_i^n + \frac{\epsilon_i^+}{6} (1 - \lambda) (2 - \lambda) (q_{i+1}^{n} - q_i^n) + \frac{\epsilon_i^-}{6} (1 - \lambda) (1 + \lambda) (q_i^n - q_{i-1}^{n}) \right] - \left[ i \rightarrow i - 1 \right] \right\}$$  \hspace{1cm} (3.41)

For a negative $v$'s

$$q_i^{n+1} = q_i^n - \lambda \left\{ \left[ q_i^{n+1} - \frac{\epsilon_i^+}{6} (1 - \lambda) (1 + \lambda) (q_{i+2}^{n} - q_{i+1}^{n}) - \frac{\epsilon_i^-}{6} (1 + \lambda) (2 + \lambda) (q_{i+1}^{n} - q_{i}^{n}) \right] - \left[ i \rightarrow i - 1 \right] \right\}$$  \hspace{1cm} (3.42)

where $\lambda$ is the CFL number.
Chapter 4

Shock waves in the Boltzmann equation

4.1 Shock waves

In this section, we apply our deterministic Boltzmann solver to a classical problem of kinetic theory, the study of the Boltzmann shock structure. The shock wave problem is the simplest problem that fully reflects the nonlinearity in the Boltzmann equation, in the sense that it cannot be studied using perturbative methods, inasmuch as the flow is not close to any Maxwellian equilibrium but rather involves connecting two different equilibria at plus and minus spatial infinity.

We will consider traveling shock wave solutions of the form of $f = f(x - ct, \xi)$, where $c$ is the constant traveling speed. The traveling wave satisfies

$$(\xi_1 - c)f' = Q(f, f), \quad (4.1)$$

where $f'$ exclusively denotes the derivative taking with respect to $x - ct$. The boundary conditions are

$$f(x - ct, \xi)|_{x \to \pm \infty} = M_{\pm \infty}, \quad (4.2)$$
where \( M_{\pm \infty} \) are two Maxwellians,
\[
M_{\pm \infty} = \rho_{\pm \infty} (2\pi RT_{\pm \infty})^{-3/2} \exp \left( -\frac{\vert \xi - u_{\pm \infty} i \vert^2}{2RT_{\pm \infty}} \right). \tag{4.3}
\]
The \( u_{\pm \infty} \) in the above is the bulk velocity. A positive bulk velocity means the molecules flow from left (minus infinity) boundary to right (positive infinity) boundary. The solution is called a traveling wave because the wave travels at a constant speed without changing its shape. It is quite obvious that the constant \( c \) in Eqn.4.1 plays no significant role. Since we can always change the frame of reference to set \( c \) to zero, we can rewrite Eqn.4.1 as
\[
\xi_1 \frac{\partial f}{\partial x} = Q(f, f). \tag{4.4}
\]
The fluid parameters in Eqn.4.3 can not be chosen arbitrarily. The conservation of mass, momentum and energy has to be imposed, and particularly must hold at infinity. We then have,
\[
\begin{align*}
\rho_{\pm} u_{\pm} &= \rho_{-} u_{-} \\
\rho_{+}(u_{+}^2 + RT_{+}) &= \rho_{-}(u_{-}^2 + RT_{-}) \\
\rho_{+} u_{+}(\frac{1}{2}u_{+}^2 + \frac{5}{2}RT_{+}) &= \rho_{-} u_{-}(\frac{1}{2}u_{-}^2 + \frac{5}{2}RT_{-}). \tag{4.5}
\end{align*}
\]
The above relations are the well-known Rankine-Hugoniot conditions, which connect the density, bulk velocity and temperature values in the upstream and in the downstream.

4.2 Analytical study

In this section, we investigate analytically the static shock solution for Boltzmann equation, which satisfies
\[
v_x \frac{\partial f}{\partial x} = Q(f, f). \tag{4.6}
\]
Due to the nonlinearity of the Boltzmann equation, it’s very hard, if at all possible, to find the shock wave solution analytically. The simplest and most important approximate solution is the Mott-Smith bi-modal approximation, proposed by H. M. Mott-Smith in 1954 ([34]). The model assumes that the distribution function is a linear combination of the upstream and downstream Maxwellians with \( x \)-dependent coefficients \( a_{\pm}(x) \). Then
the conservation of mass, momentum and energy can be written as

\[
\begin{align*}
    a_+(x)\rho_+ u_+ + a_-(x)\rho_- u_- &= \rho_\pm u_\pm \\
    a_+(x)\rho_+(u_+^2 + RT_+) + a_-(x)\rho_-(u_-^2 + RT_-) &= \rho_\pm(u_\pm^2 + RT_\pm) \\
    a_+(x)\rho_+ u_+ \left(\frac{1}{2}u_+^2 + \frac{5}{2}RT_+\right) + a_-(x)\rho_- u_- \left(\frac{1}{2}u_-^2 + \frac{5}{2}RT_-\right) &= \rho_\pm u_\pm \left(\frac{1}{2}u_\pm^2 + \frac{5}{2}RT_\pm\right).
\end{align*}
\]

(4.7)

It follows that \( a_+(x) \) and \( a_-(x) \) are not independent and related by \( a_+(x) + a_-(x) = 1 \) [5]. One usually adopts the convention of \( a_+(x) = a(x) \), where \( a(x) \) turns out to have the form of

\[
a(x) = \frac{e^{\beta x}}{e^{\beta x} + 1}.
\]

(4.8)

Under the bi-modal assumption, the constant \( \beta \) can be calculated using a moment equation (for example Mott-Smith multiplied the Boltzmann equation by \( \xi^2_1 \) before integrating out the \( \xi \) dependence in order to find \( \beta \)). However, the value of \( \beta \) changes significantly with the choice of moment.

An interesting question is what is the best possible \( \beta \) in the bi-modal solution in Eqn.4.8 This was already investigated by R.Narasimha and S.M.Deshpande (ND) in [38]. There the authors found the best beta by minimizing the \( L^2 \) norm of the “residual” for the bi-modal approximation. Here we will compare their value of \( \beta \) with that obtained by minimizing the (physically more natural) \( L^1 \) norm of the error of the residual. While in the \( L^2 \) case most (but not all) of the calculation can be done analytically, in the \( L^1 \) case optimizing \( \beta \) requires that several integrals be calculated numerically. Our results will show that the \( L^1 \) and \( L^2 \) norms give almost identical \( \beta \) values with respect to the Mach number.

Let us then consider the bi-modal solution for a 1-d static shock

\[
f_B(x, v) = \frac{M^+}{1 + e^{-\beta x}} + \frac{M^-}{1 + e^{\beta x}},
\]

(4.9)

where \( M^- \), \( M^+ \) are the upstream and downstream Maxwellian, respectively. Then, we define the residual as

\[
R_\beta(x, v) = v_x \frac{\partial f_B}{\partial x} - Q(f_B, f_B).
\]

(4.10)

The task is to find the best \( \beta \) that minimizes this residual is a suitable integral norm.
From the definition of bi-modal solution in Eqn.4.9, we can directly calculate

\[ \frac{v_x}{x} \frac{\partial f_B}{\partial x} = v_x \left( \frac{\beta M^+ e^{-\beta x}}{(1 + e^{-\beta x})^2} - \frac{\beta M^- e^{\beta x}}{(1 + e^{\beta x})^2} \right) \]

\[ = \frac{v_x \beta}{(1 + e^{-\beta x})(1 + e^{\beta x})} (M^+ - M^-). \]  \hspace{1cm} (4.11)

We also directly calculate the collision operator as

\[ Q(f_B, f_B) = \frac{1}{(1 + e^{-\beta x})^2} Q(M^+, M^+) + \frac{1}{(1 + e^{\beta x})^2} Q(M^-, M^-) \]

\[ + \frac{2}{(1 + e^{-\beta x})(1 + e^{\beta x})} Q(M^+, M^-) \]

\[ = \frac{2}{(1 + e^{-\beta x})(1 + e^{\beta x})} Q(M^+, M^-), \]  \hspace{1cm} (4.12)

where the two terms in the first line disappear because of collision invariance. Luckily Eqn.4.10 and Eqn.4.12 share a common factor. Combining the two, we rewrite the residue as

\[ R_\beta(x, v) = \frac{1}{(1 + e^{-\beta x})(1 + e^{\beta x})} \left( v_x \beta (M^+ - M^-) - 2Q(M^+, M^-) \right). \]  \hspace{1cm} (4.13)

If we take the \( L^2 \) norm of the residual we obtain

\[ R_\beta^2 = \int \frac{dx}{(1 + e^{-\beta x})^2(1 + e^{\beta x})^2} \int dv \left[ v_x \beta (M^+ - M^-) - 2Q(M^+, M^-) \right]^2, \]  \hspace{1cm} (4.14)

and we have

\[ \int \frac{dx}{(1 + e^{-\beta x})(1 + e^{\beta x})} = \frac{1}{\beta}, \]  \hspace{1cm} (4.15)

Hence, we can further write the 2-norm of the residue as

\[ R_\beta^2 = \beta \int dv \ v_x^2 (M^+ - M^-)^2 + \frac{4}{\beta} \int dv \ Q^2(M^+, M^-) \]

\[ - 4 \int dv \ v_x (M^+ - M^-)Q(M^+, M^-). \]  \hspace{1cm} (4.16)
Chapter 4. Shock waves in the Boltzmann equation

The follow quantities must evaluated numerically,

\[ X = \int d\mathbf{v} \, v_x^2 (M^+ - M^-)^2 \]
\[ Y = 4 \int d\mathbf{v} \, Q^2 (M^+, M^-) \]
\[ Z = 4 \int d\mathbf{v} \, v_x (M^+ - M^-)Q(M^+, M^-). \]

(4.17)

Finally we simplify \( R_\beta^2 \) as

\[ R_\beta^2 = \beta X + \frac{1}{\beta^2} Y - Z. \]

(4.18)

Taking the derivative according to \( \beta \),

\[ \frac{dR_\beta^2}{d\beta} = X - \frac{Y}{\beta^2} = 0. \]

(4.19)

we find the “best” \( \beta \) as

\[ \beta = \sqrt{\frac{Y}{X}}. \]

(4.20)

One thing worth noting is that minimizing the 2-norm is not the only possible choice. Starting from Eqn.4.13, one can also minimize the \( L^1 \) of the residual,

\[ R_\beta = \int \frac{dx}{(1 + e^{-\beta x})(1 + e^{\beta x})} \int d\mathbf{v} \left| v_x \beta (M^+ - M^-) - 2Q(M^+, M^-) \right| \]
\[ = \int d\mathbf{v} \left| v_x (M^+ - M^-) - \frac{2Q(M^+, M^-)}{\beta} \right|. \]

(4.21)

Unfortunately, one cannot go very far analytically starting from this expression, and a numerical method must be used.

In [38], the authors adopted a different notation for the bi-modal approximation, as

\[ f_B(x, \mathbf{v}) = (1 - \nu(x))M^+ + \nu(x)M^-, \]

(4.22)

where \( \nu(x) \) is defined as

\[ \nu(x) = \frac{1}{2} \left( 1 + \tanh(2x/\delta) \right), \]

(4.23)
and $\delta$ is the shock thickness. It turns out the conventions we used and theirs can be connected by the following relation,

$$\beta l_- = 4 \left( \frac{l_-}{\delta} \right). \quad (4.24)$$

Here $\beta$ is what we used in our previous analysis, $\frac{l_-}{\delta}$ is the one used by ND, and $l_-$ is the hot-side mean free path

$$l_- = (\sqrt{2\pi}\sigma^2 n)^{-1}. \quad (4.25)$$

An alternative definition called the local hot-side mean free path is

$$l_- = \frac{u_0}{\rho_- T_-} \sqrt{\frac{\pi RT_-}{2}}. \quad (4.26)$$

In a shock, the hot-side macroscopic quantities can be expressed in terms of the Mach number $M$,

$$u_- = \sqrt{\frac{5}{96}} \frac{M^2 + 3}{M}$$

$$\rho_- = \frac{4M^2}{M^2 + 3}$$

$$T_- = \frac{(5M^2 - 1)(M^2 + 3)}{16M^2} \quad (4.27)$$

so that also $l_-$ in 4.26 involves only the Mach number.

In the table below, we have listed the hot-side mean free path for various Mach numbers for later use.

<table>
<thead>
<tr>
<th>Mach number</th>
<th>1.2</th>
<th>1.4</th>
<th>1.59</th>
<th>2.0</th>
<th>2.5</th>
<th>3.0</th>
<th>4.0</th>
<th>8.0</th>
<th>16.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l_-$</td>
<td>0.527</td>
<td>0.384</td>
<td>0.305</td>
<td>0.210</td>
<td>0.166</td>
<td>0.141</td>
<td>0.117</td>
<td>0.100</td>
<td>0.092</td>
</tr>
</tbody>
</table>

In table 4.2 below, we compare the $L^2$ results from [38] with our $L^1$ results.

Using $L^1$ norm data in table refcomparing 1-norm and 2-norm, the hot-side mean free path values in table 4.1, and the relation 4.24, we get the best $\beta$ for various Mach numbers:
Table 4.2: comparing 1-norm and 2-norm

<table>
<thead>
<tr>
<th>Mach number</th>
<th>1.2</th>
<th>1.4</th>
<th>1.59</th>
<th>2.0</th>
<th>2.5</th>
<th>3.0</th>
<th>4.0</th>
<th>8.0</th>
<th>16.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-norm $L_-/\delta$</td>
<td>0.049</td>
<td>0.078</td>
<td>0.098</td>
<td>0.117</td>
<td>0.130</td>
<td>0.137</td>
<td>0.146</td>
<td>0.159</td>
<td>0.169</td>
</tr>
<tr>
<td>2-norm $L_-/\delta$</td>
<td>0.046</td>
<td>0.075</td>
<td>-</td>
<td>0.117</td>
<td>0.132</td>
<td>0.142</td>
<td>0.150</td>
<td>0.166</td>
<td>0.173</td>
</tr>
</tbody>
</table>

Table 4.3: Best $\beta$

<table>
<thead>
<tr>
<th>Mach number</th>
<th>1.2</th>
<th>1.4</th>
<th>1.59</th>
<th>2.0</th>
<th>2.5</th>
<th>3.0</th>
<th>4.0</th>
<th>8.0</th>
<th>16.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta$ 1-norm</td>
<td>0.372</td>
<td>0.813</td>
<td>1.285</td>
<td>2.229</td>
<td>3.133</td>
<td>3.887</td>
<td>4.991</td>
<td>6.360</td>
<td>7.348</td>
</tr>
<tr>
<td>$\beta$ Ohwada</td>
<td>0.350</td>
<td>-</td>
<td>1.280</td>
<td>2.300</td>
<td>3.390</td>
<td>4.180</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Ohwada’s paper ([21]) provides accurate static shock profile data, and is very suitable as an independent source for verification purpose. I used them in order to estimate the best $\beta$ by minimizing the error between the bi-modal approximation and their numerical results. Ohwada used $\sqrt{\pi}l_+/2$ as the spatial unit, and $l_+$ for the cold-side MFP. I transformed the spatial unit to $L_-$, the hot-side value. The calculated $\beta$ values are listed in the second line of table 4.3. The $\beta$ values from two different methods are quite close to each other.

We plotted the shock profile below using data in [21]. For example, Figure 4.1 is the density profile for a Mach 1.2 shock with hot-side MFP as the spatial unit, and Table 4.4 is the original data after transformed to proper reference scale. I also did the same for other Mach numbers.
Chapter 4. *Shock waves in the Boltzmann equation*

**Figure 4.1:** Mach 1.2 density profile

**Table 4.4:** Mach 1.2 density: estimated best $\beta = 0.35$

<table>
<thead>
<tr>
<th></th>
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<th></th>
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</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>1.297</td>
<td>1.297</td>
<td>1.295</td>
<td>1.288</td>
<td>1.276</td>
<td>1.261</td>
<td>1.246</td>
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<th>-1.641</th>
<th>-1.093</th>
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<th>0.546</th>
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<td>$\rho$</td>
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<tbody>
<tr>
<td>$\rho$</td>
<td>1.089</td>
<td>1.075</td>
<td>1.060</td>
<td>1.042</td>
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<td>1.009</td>
<td>1.002</td>
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Figure 4.2: Mach 1.59 density profile

Table 4.5: Mach 1.59 density: estimated best $\beta = 1.28$

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<td>$\rho$</td>
<td>$1.829$</td>
<td>$1.831$</td>
<td>$1.830$</td>
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<td>$1.812$</td>
<td>$1.781$</td>
<td>$1.743$</td>
<td>$1.705$</td>
<td>$1.670$</td>
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</table>

<table>
<thead>
<tr>
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<th>$-2.196$</th>
<th>$-1.641$</th>
<th>$-1.093$</th>
<th>$-0.546$</th>
<th>$0$</th>
<th>$0.546$</th>
<th>$1.093$</th>
<th>$1.641$</th>
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<tr>
<td>$\rho$</td>
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<td>$1.018$</td>
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Table 4.6: Mach 2.0 density: estimated best $\beta = 2.30$

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<tr>
<th>$X$</th>
<th>-9.687</th>
<th>-6.760</th>
<th>-4.916</th>
<th>-3.422</th>
<th>-2.358</th>
<th>-1.674</th>
<th>-1.255</th>
<th>-0.988</th>
<th>-0.792</th>
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<td>$\rho$</td>
<td>2.287</td>
<td>2.287</td>
<td>2.287</td>
<td>2.286</td>
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<th>0.310</th>
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<td>2.098</td>
<td>2.032</td>
<td>1.952</td>
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<th>1.255</th>
<th>1.674</th>
<th>2.358</th>
<th>3.422</th>
<th>4.916</th>
<th>6.760</th>
<th>9.687</th>
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<tbody>
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<td>$\rho$</td>
<td>1.230</td>
<td>1.155</td>
<td>1.088</td>
<td>1.034</td>
<td>1.007</td>
<td>1.001</td>
<td>1.000</td>
<td>1.000</td>
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</table>
Figure 4.4: Mach 2.5 density profile

Table 4.7: Mach 2.5 density: estimated best $\beta = 3.39$

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<tr>
<th>$X$</th>
<th>-9.687</th>
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<th>-4.916</th>
<th>-3.422</th>
<th>-2.358</th>
<th>-1.674</th>
<th>-1.255</th>
<th>-0.988</th>
<th>-0.792</th>
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<tr>
<td>$\rho$</td>
<td>2.703</td>
<td>2.703</td>
<td>2.703</td>
<td>2.703</td>
<td>2.701</td>
<td>2.693</td>
<td>2.672</td>
<td>2.639</td>
<td>2.595</td>
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<th>-0.155</th>
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<tbody>
<tr>
<td>$\rho$</td>
<td>2.535</td>
<td>2.453</td>
<td>2.341</td>
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<td>1.834</td>
<td>1.647</td>
<td>1.480</td>
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<th>3.422</th>
<th>4.916</th>
<th>6.760</th>
<th>9.687</th>
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<tbody>
<tr>
<td>$\rho$</td>
<td>1.230</td>
<td>1.142</td>
<td>1.072</td>
<td>1.024</td>
<td>1.004</td>
<td>1.000</td>
<td>1.000</td>
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</table>
Chapter 4. *Shock waves in the Boltzmann equation*

Figure 4.5: Mach 3.0 density profile

Table 4.8: Mach 3.0 density: estimated best $\beta = 4.18$

<table>
<thead>
<tr>
<th>X</th>
<th>-9.687</th>
<th>-6.760</th>
<th>-4.916</th>
<th>-3.422</th>
<th>-2.358</th>
<th>-1.674</th>
<th>-1.255</th>
<th>-0.988</th>
<th>-0.792</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>3.001</td>
<td>3.001</td>
<td>3.001</td>
<td>3.000</td>
<td>2.999</td>
<td>2.994</td>
<td>2.978</td>
<td>2.949</td>
<td>2.907</td>
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<tr>
<th>X</th>
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<th>-0.155</th>
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<th>0.310</th>
<th>0.466</th>
<th>0.624</th>
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<tbody>
<tr>
<td>$\rho$</td>
<td>2.845</td>
<td>2.752</td>
<td>2.618</td>
<td>2.435</td>
<td>2.207</td>
<td>1.957</td>
<td>1.715</td>
<td>1.507</td>
<td>1.345</td>
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<table>
<thead>
<tr>
<th>X</th>
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<th>0.988</th>
<th>1.255</th>
<th>1.674</th>
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<th>6.760</th>
<th>9.687</th>
</tr>
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<tbody>
<tr>
<td>$\rho$</td>
<td>1.223</td>
<td>1.131</td>
<td>1.063</td>
<td>1.020</td>
<td>1.003</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
<td>1.000</td>
</tr>
</tbody>
</table>

To conclude this discussion of “best” bimodal approximations to the shock profile, we have found that minimizing the $L^1$ and $L^2$ norm of the error between the true solution and the bi-modal approximation gave identical ”best $\beta$”. The $L^1$ method is the most common way to minimize the error, however, the $L^2$ method is physically more natural. We are now ready to move on and solve the problem numerically.
4.3 Numerical study

In Chapter (3) we used various Weighted Essentially Non-Oscillatory (WENO) schemes to calculate the advection (free-transport) step of a splitting-method solver for the Boltzmann equation. For the advection step we considered three different WENO schemes for the purpose of spatial discretization, and used a Total Variation Diminishing (TVD) Runge-Kutta method for time-stepping. The WENO schemes differ only in terms of the underlying flux scheme (Godunov, Lax-Friedrichs or Rusanov). In Chapter (2) we calculated the space homogeneous collision equation with a hard-sphere molecule model. There the collision integral is calculated using a fast spectral method recently proposed by Filbet et al. in [7].

In this section we study the general one dimensional shock problem numerically by comparing the WENO methods among themselves, and also with a Positive Flux Conservation (PFC) method [8] and with Bird’s well-known Direct Simulation Monte Carlo (DSMC) method. Our results ([36]) show that WENO-Godunov method produces accurate and stable shock solutions in good agreement with the Monte Carlo results, whereas solutions obtained with the other two WENO methods and the PFC method display some nonphysical features such as density undershoots near the shock front and excessive downstream temperature.

We use as a test problem a one-dimensional shock front traveling from left to right. In order to compare our results to the shock profile obtained with Bird’s well-known DSMC program [3], we take as a reference a gas of hard spheres, each with mass \( m = 5.0 \times 10^{-26} \) kg and diameter \( d = 4.0 \times 10^{-10} \) m. We also adopt a reference temperature \( T_0 = 273 \) °K and a number density \( 1.4 \times 10^{19} \), so the reference density is \( \rho_0 = 7.0 \times 10^{-7} \) kg/m³. Then, the reference velocity \( V_0 \) is defined by \( \sqrt{2k_B T_0/m} \). The reference length \( L_0 \) is one mean free path, which turns out to be about 0.1 m. Therefore, a computational domain [-5 m, 5 m] corresponds roughly to 100 times of the mean free path. If we start the simulation from a step function that connects two Maxwellian.

\[
\begin{align*}
  f_u &= \rho_u (\pi T_u)^{-3/2} \exp[-((v_x - u_u)^2 + v_y^2 + v_z^2)/T_u], \\
  f_d &= \rho_d (\pi T_d)^{-3/2} \exp[-((v_x - u_d)^2 + v_y^2 + v_z^2)/T_d].
\end{align*}
\]
and run the computation up to 10 mean free times (MFT), we can expect the shock to be fully formed. Without loss of generality we take $\rho_u = 1$ and $T_u = 1$, and set $u_u = \sqrt{5/6} M$ where $M$ is the Mach number. Then, the downstream quantities are given in terms of $M$ by the Rankine-Hugoniot conditions [21],

$$\begin{align*}
\rho_d &= 4M^2/(M^2 + 3), \\
u_d &= \sqrt{5/96} (M^2 + 3)/M, \\
T_d &= (5M^2 − 1)(M^2 + 3)/16M^2.
\end{align*}$$

We track the following macroscopic quantities: density, bulk velocity, longitudinal temperature, transverse temperature and temperature, defined as

$$\begin{align*}
\rho &= \int f(v) dv, \\
u &= \frac{1}{\rho} \int v_x f(v) dv, \\
T_\parallel &= \frac{1}{3\rho} \int (v_x - u)^2 f(v) dv, \\
T_\perp &= \frac{1}{6\rho} \int (v_y^2 + v_z^2) f(v) dv, \\
T &= T_\parallel + 2T_\perp
\end{align*}$$

In the plots the values of these macroscopic quantities have been shifted and re-scaled so that the origin of the $y$ axis coincides with the upstream values, and the downstream values are equal to one. The origin of the $x$ axis corresponds to the center of density. In general, density, bulk velocity and temperature are centered at different positions.

Figures 4.6 and 4.7 show the density and temperature profiles for the shock front with $M = 2$, for all five methods under consideration: WENO with Godunov, LF and Rusanov fluxes, PFC and Bird’s DSMC method [3]. The deterministic methods were run on 100 spatial grid points with 64 Fourier modes for each velocity component. The time step was chosen so as to have CFL number 0.01. In the DSMC code we set IMEG=100 [3], which implies $10^6$ “molecules.” The most immediate observation is that the results divide in two distinct groups. The LF, Rusanov and PFC results are all very similar, whereas
the profiles obtained using the Godunov flux resemble more closely the Monte Carlo simulation. Let us discuss these two groups separately.

As far as the gas density is concerned, the LF, Rusanov and PFC methods produce sharp, well-defined shock profiles with widths that match closely the Godunov and DSMC values. However, the plots show two problematic features:

a) In all three cases, by the end of the simulation the density profile developed an up-stream "undershoot" just to the right of the shock front. This is clearly nonphysical phenomenon.

b) The temperature profiles are significantly less steep than in the Godunov and DSMC cases, and seem to suggest a wider shock, which would be inconsistent with the width obtained from the gas density values.

In order to assess the situation more precisely, in Figures 4.8 through 4.13 we magnify the details of the shock layer by suitably re-scaling the $x$ axis. We plot separately the density, bulk velocity and temperature for each method, including, in figure 4.10, a slightly modified LF method in which the Godunov flux formulas are used in a few computational cells to the right of the shock front. Generally speaking, the bulk velocity profiles are smooth and very close to an odd function. However, the LF, Rusanov and PFC temperature
curves are “lifted” on the upstream side, so much so that by the end of the simulations the first derivative of the temperature is no longer monotonic. This suggests that excessive numerical diffusion is distorting the heat flux across the shock front. One may wonder if this could also be the cause of the upstream density undershoot produced by these three methods. Our modified LF method, Figure 4.10, suggests that this is not the case. Just using a few Godunov cells immediately to the upstream of the shock front is sufficient to cure the density undershoot, while the excess in the upstream temperature remains significant. This suggest that the density undershoot is a separate phenomenon that reflects how these methods handle the transport of information, not numerical diffusion. One possible reason is that, unlike the Godunov scheme, they are not strictly upwind methods because the flux formulas use information from both sides of each computational cell, which is not consistent with the physics of collision-less transport.

The simulation using the using Godunov upwind flux, Figure 4.13, produces a sharp, smooth shock profile without any nonphysical effects, and in excellent agreement with the DSMC calculation. For example, in both methods the intersection of the density and bulk velocity curves takes place at \( y = 0.4 \), which is also the value obtained by Ohwada [21] using a finite-difference solver for the stationary Boltzmann equation. In the other three methods this intersection point lies closer to 0.5 on the y axis due to the temperature lift-up. In order to carry out a more detailed comparison of the WENO-Godunov and DSMC methods, in Figure 4.14 we plot various quantities for these two methods only, separating the longitudinal and transversal parts of the temperature. Whereas, the density and bulk velocity values are in excellent agreement, some interesting differences can be observed in the temperature plots. For the total temperature, the DSMC curve displays a slight negative slope downstream from the shock; the WENO-Godunov curve, on the contrary remains nice and flat all the way to the shock front and then displays a small overshoot. When the longitudinal and transversal temperatures are plotted separately, we observe that the two deterministic curves are very similar, and that the greater contribution to the overshoot comes from the transversal part. The opposite is true for the DSMC curves: the longitudinal temperature overshoots very visibly, whereas the transversal temperature does not (we recall that all these graphs are normalized to one). Both methods show (see 4.15 and 4.16) that the longitudinal temperature is larger than transversal temperature, whereas the opposite is true for the WENO-LF, WENO-Rusanov and PFC methods.
However, the two temperatures are farther apart in the DSMC case than in the WENO-Godunov case. This discrepancy suggests that the Monte Carlo simulation is somehow less efficient at transferring kinetic energy from the longitudinal to the transversal degrees of freedom. Why this is the case, and which scenario is physically more accurate are two interesting open questions. We should mention that the deterministic simulations are somewhat sensitive to the choice of the velocity cutoff used in the computation of the cross section. The DSMC method, on the other hand, is sensitive to the choice of various parameters that appear in the definition of the stochastic quasi-particles.

To sum up, the results in this chapter show that a WENO method combined with a Godunov flux scheme provides a viable, accurate method to carry out the advection step in a splitting-method Boltzmann solver. The method produced a smooth and monotonic density shock profile without any nonphysical downstream undershoot and no nonphysical excess diffusion across the shock front. The solution displayed a slight total temperature overshoot, in agreement with the DSMC method, even though the deterministic calculation showed less separation between the longitudinal and transversal temperatures. WENO methods that use other flux schemes, however, proved less accurate. The WENO-Godunov method also gave better results than the Semi-Lagrangian PFC method. Generally speaking, our results suggest that in the Boltzmann context it is possible to use advanced non-oscillatory hyperbolic solvers that would be computationally very expensive, for instance, in a (collision-less, non-dissipative) Vlasov context.
Chapter 4. Shock waves in the Boltzmann equation

Figure 4.8: DSMC

Figure 4.9: WENO-LF

Figure 4.10: WENO-LF with fix

Figure 4.11: WENO-Rusanov

Figure 4.12: PFC

Figure 4.13: WENO-Godunov
Chapter 4. *Shock waves in the Boltzmann equation*  

Figure 4.14: WENO-Godunov vs. DSMC comparison

Figure 4.15: DSMC

Figure 4.16: WENO-Godunov
Chapter 5

Shock curvature correction

5.1 Background

An interesting problem in rarefied gas dynamics is to establish appropriate “jump conditions” across a shock front, which relate the values of density, temperature and bulk velocity on the two sides of the shock. Typically, such relations can be used as boundary conditions for numerical solutions of the motion of the gas outside of the shock. In the in-viscid case they are given by the well-known Rankine-Hugoniot conditions, but in a viscous gas they must be modified to account for the details of the shock structure and also for its curvature. Whenever the thickness of the shock is comparable with the mean free path, this requires using kinetic theory, e.g. a suitable Boltzmann equation. Several years ago, Carlo Cercignani and Carlo Lancellotti performed a general analysis of curvature corrections to the Rankine-Hugoniot condition for a curved shock, using singular perturbation methods in order to "connect" the solutions to the the Boltzmann equation inside and outside the shock layer. It turned out that the corrections due to curvature can be obtained at leading order by integrating appropriately the Boltzmann shock profile for a planar (one-dimensional in space) shock wave. However, such corrections are entirely due to the spatially asymmetry of the shock, and they vanish if the shock is described using a simple bi-modal ansatz like the well-know Mott-Smith model. In the present work, we use the highly-accurate deterministic (spectral) method developed in the previous chapters in order to solve numerically the Boltzmann equation for a gas of hard-spheres and compute the non-bi-modal part of the shock structure. We then use
these results and the results form perturbation theory in order to obtain the values of the curvature-induced corrections to the Rankine-Hugoniot conditions. Finally, we discuss in detail how such corrections depend on the Mach number and on the shock’s curvature.

This chapter is based on our published paper ”Corrections to the Rankine-Hugoniot Conditions for Curved Shock Waves” by Carlo Lancellotti and Yubei Yue ([40]).

5.2 Introduction

An important problem in gas dynamics is to establish appropriate ”jump conditions” across a shock front, which relate the values of density, temperature and bulk velocity on the two sides of the shock. Typically, such relations can be used as boundary conditions for numerical solutions of the motion of the gas outside of the shock. In the in-viscid case they are given by the well-known Rankine-Hugoniot conditions, but in a viscous gas they must be modified to account for the details of the shock structure and also for its curvature. Whereas one can calculate such corrections in the framework of compressible fluid dynamics [31–33], in many practical situations a continuum approach cannot be expected to give truly accurate results because the thickness of the shock is comparable to the mean free path. In these cases, the corrections to the Rankine-Hugoniot conditions should be calculated using kinetic theory, e.g. a suitable Boltzmann equation.

How to do so was the subject of a study by Cercignani and Lancellotti some years ago [6]. At that time, singular perturbation theory was used in order to obtain the desired corrections for a two-dimensional curved shock; they were given by integrals across the shock of certain second-order moments of the distribution function for the planar, one-dimensional shock profile (as determined by the zeroth-order values of the density, bulk velocity and temperature on the two sides). As a consequence, the corrections are entirely due to the spatially even part of the shock profile, since the spatially odd part integrates to zero. This means that no corrections can be found by using the simplest bi-modal (Mott-Smith) approximation [34] to the Boltzmann shock profile. In order to circumvent this problem one could use a more sophisticated Ansatz for the one-dimensional shock profile, like the tri-modal one due to Salwen et. al. [35]. However, given that the tri-modal approximation requires a considerable amount of numerical work, and given the dramatic growth in computing power over the last quarter of a century, one could just
as well go ahead and use an accurate numerical solution for the one-dimensional shock profile in order to obtain the corrections to the Rankine-Hugoniot conditions for a curved shock front. This is the main subject of the present chapter.

This chapter is divided into two parts. In the first part we revisit the perturbation calculation in Ref. [6] and extend it to the more general situation of a three-dimensional (non necessarily cylindrical) stationary shock front; we also show that the formulas can be considerably simplified by exploiting the conservation of the flows of mass, momentum and density across the shock. In the second part we present detailed numerical results for the jump conditions for the longitudinal flux of longitudinal momentum for a gas of hard spheres. For this purpose, we use a recently developed deterministic Boltzmann solver [36] in order to calculate the even part of the one-dimensional shock profile.

5.3 Jump conditions

In this section we review the results in Ref. [6], and extend them to any stationary (not necessarily two-dimensional) curved shock. At any point $P$ on the shock front we use the local reference frame determined by the normal and tangent vectors to the shock, as depicted schematically in Fig. (5.1). We denote the spatial coordinates by $x_1, x_2$ and $x_3$, and the corresponding velocities by $v_1, v_2$ and $v_3$. Assuming that in a neighborhood of $P$ the shock front satisfies an equation of the form $x_1 = g(x_2, x_3)$ (with $g$ twice differentiable), we have $\partial_{x_2} g(0,0) = \partial_{x_2} g(0,0) = 0$. Without loss of generality we can also choose the $x_2$ and $x_3$ axes to coincide with the (orthogonal) eigen-vectors of the Hessian of $g$, so that $\partial_{x_i x_j} g(0,0) = 0$ and $\partial_{x_i x_i} g(0,0) = \kappa_i$ (for $i, j = 2, 3$ and $i \neq j$), where $\kappa_2$ and $\kappa_3$ are the principal curvatures of $g$ at $P$. Then, a standard calculation recasts the dimensionless Boltzmann equation in terms of the local variables. At $x_2 = x_3 = 0$ we find

$$v_1 \frac{\partial f}{\partial x_1} + \sum_{i=2,3} \left[ v_i \left(1 + \kappa_i x_1\right) \frac{\partial f}{\partial x_i} - \kappa_i v_i^2 \frac{\partial f}{\partial v_1} + \kappa_i v_1 v_i \frac{\partial f}{\partial v_i} \right] = \frac{1}{\epsilon} Q(f, f)$$

(5.1)

where $Q$ is the Boltzmann collision operator and $\epsilon$ is the Knudsen number for the gas, which in our case will be defined as

$$\epsilon = \kappa \ell$$
where $\ell$ is the mean free path and $\kappa = \kappa_2 + \kappa_3$ is the average curvature at $P$.

In order to find the desired jump conditions, [6], Eq. (5.1) is supplemented by the equation obtained by re-scaling $x_1$ to $X = x_1/\epsilon$,

$$v_1 \frac{\partial \tilde{f}}{\partial X} + \epsilon \sum_{i=2,3} v_i (1 + \epsilon \kappa_i x_1) \frac{\partial \tilde{f}}{\partial x_i} - \kappa_i v_i^2 \frac{\partial \tilde{f}}{\partial v_1} + \kappa_i v_1 v_i \frac{\partial \tilde{f}}{\partial v_i} = Q(\tilde{f}, \tilde{f})$$  (5.2)

where $\tilde{f}(X, x_2, x_3, \vec{v}) = f(\epsilon X, x_2, x_3, \vec{v})$ and again $x_2$ and $x_3$ are set equal to zero. Then, one considers separately $\tilde{f}$ (the ”inner” distribution) and $f^\pm$, the solutions to Eq. (5.1) on the two sides of the shock (the upstream and downstream ”outer” distributions). The strategy is to expand all three in powers of $\epsilon$

$$\tilde{f} = \tilde{f}_0 + \epsilon \tilde{f}_1 + \epsilon^2 \tilde{f}_2 + \ldots$$

$$f^\pm = f^\pm_0 + \epsilon f^\pm_1 + \epsilon^2 f^\pm_2 + \ldots$$

and then use matched asymptotics in order to relate the values of $f^\pm$ as $x_1 \to 0$ to the values of $\tilde{f}$ as $X \to \pm\infty$.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{local_coordinates.png}
\caption{Local coordinate system at a point on the shock}
\end{figure}
5.3.1 Zero-order conditions

At order zero the outer distributions satisfy \( Q(f_0^±, f_0^±) \) and therefore must be Maxwellian

\[
f_0^± = \frac{ρ_0^±}{(2πRT_0^±)^{3/2}} \exp \left[ -\frac{|v - u_0^±|^2}{2RT_0^±} \right]
\]

(5.3)
determined by the zero-th order densities \( ρ_0^± \), bulk velocities \( u_0^± \) and temperatures \( T_0^± \) on each side of the shock (all functions of \( x_1 \)). The inner distribution satisfies the one-dimensional Boltzmann equation

\[
v_1 \frac{∂f_0}{∂X} = Q(\tilde{f}_0, \tilde{f}_0),
\]

(5.4)
and a standard matched-asymptotic analysis leads to the relations

\[
f_0^± \bigg|_{x_1=0} = \tilde{f}_0 \bigg|_{X=±∞}.
\]

(5.5)

Equation (5.4) implies that the flows of density, bulk velocity and kinetic energy are constant through the shock. This fact combined with Eq. (5.5) yields immediately the classical Rankine-Hugoniot conditions

\[
[ρu_1]^+ = 0
\]

(5.6)
\[
[ρu_1^2 + p_0]^+ = 0
\]

(5.7)
\[
[ρu_1 u_2]^+ = 0
\]

(5.8)
\[
[ρu_1 u_3]^+ = 0
\]

(5.9)
\[
[ρu_1 \left( \frac{u_2^2}{2} + \frac{5}{2} RT \right)]^+ = 0
\]

(5.10)

where we follow the notation in Ref. [5] for the various hydrodynamic variables. We do not write out explicitly the indexes that refer to the order of approximation and we use the notation \([h]^± = h^+|_{x_1=0} - h^-|_{x_1=0} \). We also exploited the fact that a Maxwellian has a diagonal stress tensor and no heat flow. Note that the first condition can be used to simplify the third, fourth and fifth conditions. In particular, \( u_2^+ = u_2^- \) and \( u_3^+ = u_3^- \), i.e. there is no slip in the transversal velocities at zero-th order. Hence, the fifth condition reduces immediately to the familiar one-dimensional form involving only \( u_1 \). Finally,
$f_0^\pm$ supplemented by the Rankine-Hugoniot conditions provide the boundary values at $X \to \pm \infty$ for the inner equation, Eq. (5.4). Therefore, at zero-th order the “inner” problem coincides with the classical problem of calculating the one dimensional (planar) shock structure.

### 5.3.2 First-order conditions

At first order, the outer distribution functions $f_1^\pm$ satisfy two linearized equations, see Eq. (10) in Ref. [6]. The outer expansion is just an example of the well-known Hilbert perturbation method to solve the Boltzmann equation in “normal” regions ([37] section V.2). Accordingly, these equations can be handled by standard techniques in order to obtain $f_1^\pm$ in terms of $f_0^\pm$ and its derivatives. The details of this derivation will be omitted; in Ref. [6] it was shown that for Maxwellian molecules they lead to some standard fluid-dynamical terms identical to those that would be obtained in the Navier-Stokes context [32]. Our goal here is to obtain first-order corrections to the Rankine-Hugoniot conditions, Eqs. (5.10), that can be used as boundary conditions for any numerical or analytical study of the flow on the two sides of the shock, not just Hilbert-type solutions to the Boltzmann equation. For this purpose, the solutions for $f_1^\pm$ are not necessary, because all we need is the inner equation

$$v_1 \frac{\partial \tilde{f}_1}{\partial X} + \sum_{i=2,3} v_i \left[ \frac{\partial \tilde{f}_0}{\partial x_i} - \kappa_i v_i^2 \frac{\partial \tilde{f}_0}{\partial v_1} + \kappa_i v_1 v_i \frac{\partial \tilde{f}_0}{\partial v_i} \right] = 2 Q(\tilde{f}_0, \tilde{f}_1). \quad (5.11)$$

combined with the matching relations [6]

$$f_1^\pm |_{x_1=0} = \tilde{f}_1 |_{X=\pm \infty} \quad \frac{\partial f_0^\pm}{\partial x_1} |_{x_1=0} = 0. \quad (5.12)$$

in order to express the the boundary values of $f_1^\pm$ to in terms of $\tilde{f}_0$. To do so, we first integrate Eq. (5.11) in $d\vec{v}$ against the collision invariants $\{\psi_\alpha, \alpha = 1, 2, 3, 4, 5\} \equiv \{1, v_1, v_2, v_3, |\vec{v}|^2\}$. We would like to integrate also in $dX$ from $-\infty$ to $+\infty$, in order to


get an equation of the form
\[
\int d\vec{v} \psi_\alpha v_1 \left[ f_1 \right]_{-\infty}^{+\infty} + \sum_{i=2,3} \int_{-\infty}^{+\infty} dX \int d\vec{v} \psi_\alpha \left( v_i \frac{\partial \tilde{f}_0}{\partial x_i} - \kappa_i v_i^2 \frac{\partial \tilde{f}_0}{\partial v_1} + \kappa_i v_1 v_i \frac{\partial \tilde{f}_0}{\partial v_i} \right) = 0.
\]
(5.13)

However, the integrals with respect to \(X\) are not well-defined, since \(\tilde{f}_0\) does not go to zero at infinity. This difficulty can be overcome by observing [6] that the integral in question would be exactly equal to zero if \(\tilde{f}_0\) were a bi-modal distribution that decays rapidly to the Maxwellian \(f_0^\pm \big|_{x_1=0} \) at \(\pm \infty\), of the form
\[
\hat{f} = \frac{f_0^+ \big|_{x_1=0}}{1 + e^{-\beta(x_2,x_3) X}} + \frac{f_0^- \big|_{x_1=0}}{1 + e^{+\beta(x_2,x_3) X}}
\]
(5.14)
(as is the case, for example, for the well-known Mott-Smith solution). This suggests the following renormalization procedure: before sending the extremes of \(X\)-integration to \(\pm \infty\) we add and subtract \(\hat{f}\) from each \(\tilde{f}_0\). Then, as the domain of integration in \(X\) approaches infinity, one recovers Eq. (5.13) with \(\tilde{f}_0\) replaced by \(\tilde{f}_0 - \hat{f}\), and the integral is certainly well-defined. Note that the choice of the function \(\beta(x_2,x_3)\) is irrelevant (one can just take \(\beta \equiv 1\)); all that matters is the particular structure of \(\hat{f}\). Finally, using the matching relations in Eq. (5.12) on the left-hand side of Eq. (5.13), and integrating by parts on the right-hand side, we obtain
\[
\int d\vec{v} \psi_\alpha v_1 \left[ f_1 \right]_{-\infty}^{+\infty} = -\sum_{i=2,3} \left[ \frac{\partial}{\partial x_i} \int d\vec{v} v_i \psi_\alpha \tilde{f}_0^* - \kappa_i \int d\vec{v} \phi_{\alpha,i} \tilde{f}_0^* \right]
\]
(5.15)
where
\[
\{\phi_{\alpha,i}, \alpha = 1, 2, 3, 4, 5\} \equiv \{v_1, v_1^2 - v_i^2, (1 + \delta_{2,i}) v_1 v_2, (1 + \delta_{3,i}) v_1 v_3, v_1 |\vec{v}|^2\}
\]
and
\[
\tilde{f}_0^* = \int_{-\infty}^{+\infty} (\tilde{f}_0 - \hat{f}) dX.
\]
We recall that \(\tilde{f}_0\) and \(\hat{f}\) have the same, constant flows of mass, momentum and energy across the shock layer. Therefore, the integrals \(\int d\vec{v} \phi_{\alpha,i} \tilde{f}_0^*\) vanish except for \(\alpha = 2\);
conversely, the integrals \( \int d\vec{v} v_\alpha \tilde{f}_0 \) vanish (in general) only for \( \alpha = 2 \), and the first-order corrections reduce to

\[
\begin{align*}
[\rho u_1]_+ & = -\epsilon \sum_{i=2,3} \frac{\partial}{\partial x_i} [\tilde{\rho}^* \tilde{u}_i^*] \\
[\rho u_1^2 + p_{11}]_+ & = -\epsilon \sum_{i=2,3} \kappa_i [\tilde{\rho}^* \tilde{u}_i^{*2} + \tilde{p}_{ii}] \\
[\rho u_1 u_2 + p_{12}]_+ & = -\epsilon \sum_{i=2,3} \frac{\partial}{\partial x_i} [\tilde{\rho}^* \tilde{u}_i^* \tilde{u}_i^* + \tilde{p}_{2i}] \\
[\rho u_1 u_3 + p_{13}]_+ & = -\epsilon \sum_{i=2,3} \frac{\partial}{\partial x_i} [\tilde{\rho}^* \tilde{u}_3^* \tilde{u}_i^* + \tilde{p}_{3i}] \\
[\rho u_1 (\frac{\tilde{u}_1^2}{2} + \frac{3}{2} \tilde{T}) + \sum_{j=1}^2 u_j p_{1j} + q_1]_+ & = -\epsilon \sum_{i=2,3} \frac{\partial}{\partial x_i} [\tilde{\rho}^* \tilde{u}_i^* (\frac{\tilde{u}_i^*}{2} + \frac{3}{2} \tilde{T}^*) \\
& \quad + \sum_{j=1}^2 \tilde{u}_{ij}^* \tilde{p}_{ij} + \tilde{q}_i^*]
\end{align*}
\]

where the quantities on the left are now first-order accurate and the starred quantities on the right are obtained from \( \tilde{f}_0^* \) according to Eq. (5.15). By exploiting the conservation of the flows we have been able to recast these relations in a simpler form than found in both references [6] and [31, 32]. Of course, the major difference between these formulas and those found by in the Navier-Stokes context [31, 32] is that here the tilded zeroth order quantities on the right side reflect the one-dimensional Boltzmann shock profile (as opposed to its less accurate Navier-Stokes counterpart).

### 5.4 1-1 momentum flow discontinuity

Among the various corrections in Eqs. (5.16) through (5.20), Eq. (5.17) stands out because it is not the result of a transversal gradient in the zero-th order hydrodynamical variables, and also because it depends explicitly on the principal curvatures of the shock front (not just indirectly through the Knudsen number \( \epsilon \)). Whereas the other correction vanish, for instance, for a shock propagating in a uniform gas, Eq. (5.17) reveals a first order discontinuity – in the longitudinal flow of the first component of the momentum – which
is entirely due to the shock’s structure and curvature. As such, this term is especially interesting and deserves a precise evaluation, which in turn requires an accurate solution for $\tilde{f}_0^*$, since Eq. (5.17) can be written explicitly as

$$
\left[ \rho \mathbf{u}_1^2 + p_{11} \right]^- = -\epsilon \sum_{i=2,3} \kappa_i \int_{-\infty}^{+\infty} dX \int \left( \tilde{f}_0^* - \hat{f} \right) v_i^2 dv.
$$

(5.21)

For this purpose, we solve numerically Eq. (5.4) for a gas of hard spheres, using a deterministic Boltzmann solver that developed in Chapter.3. The method of solution relies on the well-known splitting approach, applied not to Eq. (5.4) directly but to the full time-dependent Boltzmann equation. Accordingly, we obtain the solution for a moving shock, and then derive the stationary shock profile simply by following the shock front as it propagates. As usual, the splitting method requires that we solve both a homogeneous Boltzmann equation (collision step) and a purely advective collision free equation (transport step). For the collision step, we use a fast spectral method which was recently introduced by Pareschi et al. [7] coupled with a third order Runge-Kutta time integrator. For the advection step, we use a semi-discrete method, meaning that we first discretize the equation in space and then use a separate high-order Runge-Kutta integrator in time [16]. The space discretization is based on a non-oscillatory WENO method [17] with Godunov flux; the reader is referred to [36] for details. In Figure 5.2 we plot the density,

![Figure 5.2: M = 2 shock profiles](image)
bulk velocity, and temperature profiles (in dimensionless units, see [36]) obtained from our numerical solution for \( \tilde{f}_0^* \) for a \( M = 2 \) shock. The curves are very smooth, and the temperature displays a slight upstream overshoot.

In order to compute the correction in Eq. (5.21), of course, we must focus on the \( v_2^2 \) and \( v_3^2 \) moments of \( \tilde{f}_0^* - \hat{f} \). In fact, since \( \tilde{f}_0^* \) and \( \hat{f} \) are isotropic with respect to the transversal velocities, we only need to calculate one of the two terms in the sum, the other being identical. The spatial dependence of \( \int v_2^2 (\tilde{f}_0^* - \hat{f}) \, dv \) is presented in Figure 5.3. Recall, however, that only the spatially even parts of \( v_2^2 (\tilde{f}_0 - \hat{f}) \) and \( v_3^2 (\tilde{f}_0 - \hat{f}) \) contribute to the \( X \)-integral in Eq. (5.21). Moreover, subtracting the Mott-Smith-like distribution \( \hat{f} \) makes the integrals well defined but does not affect the integration of the even part of \( \tilde{f}_0^* \).

Figure 5.5 shows the odd and even parts of \( v_2^2 \tilde{f}_0 \), also for \( M = 2 \). Although the peak value of the even part is small, less than 3\% of the odd part near the upstream boundary, the integration gives a (dimensionless value of 0.56, which is significant, although of course the actual correction is obtained by multiplying this number by \( \epsilon \kappa_i \), \( i = 2, 3 \) and adding the contributions from the two transversal directions.
Finally, Figure 5.6 shows the dependence of the strength of the correction on the Mach number. The amplitude of the correction coefficient grows steadily with $M$ and attains value one at about $M = 2.4$. 

$\int_{-\infty}^{\infty} dX \int v_2^2 (\tilde{f}_0^* - \tilde{f}) dv$ as a function of the Mach number
5.5 Concluding remarks

We have obtained analytical expressions for the first order corrections to the Rankine-Hugoniot conditions for a three-dimensional, stationary shock. The most interesting effect seems to be a “slip” in the flow of longitudinal momentum across the shock, which has been evaluated numerically. We remark that our method could be easily adapted to include non-stationary shocks. In the near future we would like to try and extend out calculation to higher Mach numbers, in order to determine if the slip in the longitudinal momentum flow saturates at some maximum value.
Bibliography


