Numerical methods for collisional kinetic equations

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Course Outline

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Part I: Boltzmann equations

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Outline

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The Boltzmann equation

The model

The model is characterized by a density function \( f(x, v, t) \) describing the time evolution of a monoatomic rarefied gas of particles which move with velocity \( v \in \mathbb{R}^3 \) in the position \( x \in \Omega \subset \mathbb{R}^3 \) at time \( t > 0 \) which satisfies the Boltzmann equation

\[
\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f, f)
\]

The parameter \( \varepsilon > 0 \) is called the \textit{Knudsen number} and is proportional to the mean free path between collisions. The bilinear collision operator \( Q(f, f) \) describes the binary collisions of the particles

\[
Q(f, f)(v) = \int_{\mathbb{R}^3} \int_{S^2} B(v, v_*, \omega) \left[ f(v') f(v'_*) - f(v) f(v_*) \right] d\omega \, dv_*
\]

\[
= Q^+(f, f)(v) - L[f](v) f(v)
\]

\[
Q^+(f, f)(v) = \int_{\mathbb{R}^3} \int_{S^2} B(v, v_*, \omega) f(v') f(v'_*) d\omega \, dv_*
\]

\[
L[f](v) = \int_{\mathbb{R}^3} \int_{S^2} B(v, v_*, \omega) f(v_*) d\omega \, dv_*
\]
In the above expression \( \omega \) is a unit vector of the sphere \( S^2 \).
Moreover \((v', v'_*)\) represent the collisional velocities associated with \((v, v_*)\). The collisional velocities satisfy microscopic momentum and energy conservation
\[
v' + v'_* = v + v_*, \quad |v'|^2 + |v'_*|^2 = |v|^2 + |v_*|^2.
\]
The above system of algebraic equations has the following parametrized solution
\[
v' = \frac{1}{2}(v + v_* + |v - v_*| \omega), \quad v'_* = \frac{1}{2}(v + v_* - |v - v_*| \omega)
\]
where \(v - v_*\) is the relative velocity.
The **collision kernel** $B(v, v_*, \omega)$ is a nonnegative function which characterizes the details of the binary interactions and depends only on $|v - v_*|$ and the scattering angle $\theta$ between relative velocities $v - v_*$ and $v' - v'_* = |v - v_*|\omega$.

$$\cos \theta = \frac{(v - v_*) \cdot \omega}{|v - v_*|}.$$ 

The kernel has the form

$$B(v, v_*, \omega) = |v - v_*| \sigma(|v - v_*|, \cos \theta),$$

where the function $\sigma$ is the **scattering cross-section**.

**Examples:**

- In the **hard sphere model** the particles are assumed to be ideally elastic spheres of diameter $d > 0$ and thus

  $$\sigma(|v - v_*|, \cos \theta) = \frac{d^2}{4}, \quad B(v, v_*, \omega) = \frac{d^2}{4}|v - v_*|.$$

- In the case of inverse $k$-th power forces between particles the kernel has the form

  $$\sigma(|v - v_*|, \cos \theta) = b_\alpha(\cos \theta)|v - v_*|^{\alpha - 1}, \quad B(v, v_*, \omega) = b_\alpha(\cos \theta)|v - v_*|^\alpha,$$

  with $\alpha = (k - 5)/(k - 1)$. For $k > 5$ we have **hard potentials**, for $k < 5$ we have **soft potentials**.
• The special situation $k = 5$ gives the **Maxellian model** with

$$B(v, v_*, \omega) = b_0(\cos \theta).$$

• For numerical purposes, a widely used model is the **Variable Hard Sphere** (VHS) model, corresponding to take $b_\alpha(\cos \theta) = C_\alpha$ where $C_\alpha$ is a positive constant and hence

$$\sigma(|v - v_*|, \cos \theta) = C_\alpha |v - v_*|^{\alpha-1}, \quad B(v, v_*, \omega) = C_\alpha |v - v_*|^{\alpha}.$$ 

**Remark:** For the Maxwellian case the collision kernel $B(v, v_*, \omega)$ is independent of the relative velocity. This case has been widely studied theoretically, in particular exact analytic solutions can be found in the space homogeneous case ($f = f(v, t)$).
**Remark:** The collision integral $Q(f, f)$ can be written in different equivalent forms, accordingly to the parametrization used for the collisional velocities. A frequently used form is given by

$$Q(f, f)(v) = \int_{\mathbb{R}^3} \int_{S^2} \tilde{B}(v, v_*, \omega)[f(v')f(v_*') - f(v)f(v_*)]\, d\omega\, dv_*$$

with

$$v' = v - ((v - v_*) \cdot \omega)\omega, \quad v'_* = v_* + ((v - v_*) \cdot \omega)\omega,$$

and

$$\tilde{B}(v, v_*, \omega) = 2|v - v_*||\cos\theta|\sigma(|v - v_*|, 1 - 2|\cos\theta|).$$

Now the hard sphere case corresponds to

$$\tilde{B}(v, v_*, \omega) = \frac{d^2}{2}|v - v_*||\cos\theta|,$$

whereas the Maxwellian molecules case gives

$$\tilde{B}(v, v_*, \omega) = 2|\cos\theta|b_0(\cos\theta).$$
A simplified one-dimensional space homogeneous Maxwell model is given by the *Kac equation*. It reads

\[
\frac{\partial f}{\partial t} = \int_{\mathbb{R}} \int_{0}^{2\pi} \frac{1}{2\pi} [f(v')f(v') - f(v)f(v_*)] \, d\theta \, dv_*
\]

where the collisional velocities are characterized by rotations in the collisional plane

\[
v'' = v \cos \theta - v_* \sin \theta, \quad v' = v \sin \theta + v_* \cos \theta.
\]

For this model we have only microscopic conservation of energy \( (v')^2 + (v_*')^2 = v^2 + v_*^2 \).
Physical properties

During the evolution process, the collision operator preserves mass, momentum and energy, i.e.,

$$\int_{\mathbb{R}^3} Q(f, f) \phi(v) \, dv = 0, \quad \phi(v) = 1, v^x, v^y, v^z, |v|^2,$$

and in addition it satisfies Boltzmann’s well-known \textit{H}-theorem

$$\int_{\mathbb{R}^3} Q(f, f) \ln(f(v)) \, dv \leq 0.$$

The above properties are a consequence of the following identity that can be easily proved for any test function $\phi(v)$

$$\int_{\mathbb{R}^3} Q(f, f) \phi(v) \, dv = -\frac{1}{4} \int_{\mathbb{R}^6} \int_{S^2} B(v, v_*, \omega) [f'_* f'_* - f f_*] \left[ \phi' + \phi'_* - \phi - \phi_* \right] \, d\omega \, dv_* \, dv,$$

where we have omitted the explicit dependence from $v, v_*, v', v'_*$ to simplify the expression.

In order to prove this identity we used the micro-reversibility $B(v, v_*, \omega) = B(v_*, v, \omega)$ and the fact that the Jacobian of the transformation $(v, v_*) \leftrightarrow (v', v'_*)$ is equal to 1.
A function $\phi$ such that

$$\phi(v') + \phi(v'_*) - \phi(v) - \phi(v_*) = 0$$

is called a \textit{collision invariant}. It can be shown that a continuous function $\phi$ is a collision invariant if and only if $\phi \in \text{span}\{1, v, |v|^2\}$ or equivalently

$$\phi(v) = a + b \cdot v + c|v|^2, \quad a, c \in \mathbb{R}, \quad b \in \mathbb{R}^3.$$  

Assuming $f$ strictly positive, for $\phi(v) = \ln(f(v))$ we obtain

$$\int_{\mathbb{R}^3} Q(f, f) \ln(f) \, dv$$

$$= -\frac{1}{4} \int_{\mathbb{R}^6} \int_{S^2} B(v, v_*, \omega) [ff'_* - ff_*][\ln(f') + \ln(f'_*) - \ln(f) - \ln(f_*)] \, d\omega \, dv_* \, dv$$

$$= -\frac{1}{4} \int_{\mathbb{R}^6} \int_{S^2} B(v, v_*, \omega) [ff'_* - ff_*] \ln \left( \frac{ff'_*}{ff_*} \right) \, d\omega \, dv_* \, dv \leq 0,$$

since the function $z(x, y) = (x - y) \ln(x/y) \geq 0$ and $z(x, y) = 0$ only if $x = y$.

In particular the equality holds only if $\ln(f)$ is a collision invariant that is

$$f = \exp(a + b \cdot v + c|v|^2), \quad c < 0.$$
If we define the density, mean velocity and temperature of the gas by

\[ \rho = \int_{\mathbb{R}^3} f \, dv, \quad u = \frac{1}{\rho} \int_{\mathbb{R}^3} v f \, dv, \quad T = \frac{1}{3R\rho} \int_{\mathbb{R}^3} [v - u]^2 f \, dv, \]

we obtain that the distribution function has the form of a locally Maxwellian distribution

\[ f(v, t) = M(\rho, u, T)(v, t) = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(-\frac{|u-v|^2}{2RT}\right). \]

The constant \( R \) is called the gas constant and scales the temperature. Boltzmann’s \( H \)-theorem implies that any equilibrium distribution function, i.e. any function \( f \) for which \( Q(f, f) = 0 \), has the form of a locally Maxwellian distribution.

If we define the \( H \)-function

\[ H(f) = \int_{\mathbb{R}^3} f \ln(f) \, dv, \]

we obtain immediately the inequality

\[ \frac{dH(f)}{dt} = \int_{\mathbb{R}^3} Q(f, f) \ln(f) \, dv \leq 0. \]

Thus the \( H \)-function is monotonically decreasing until \( f \) reaches the equilibrium Maxwellian state for which we have

\[ H(M) = \rho \left( \ln\left(\frac{\rho}{(2\pi RT)^{3/2}}\right) - \frac{3}{2} \right). \]
**Fluid limit**

If we multiply the Boltzmann equation by its collision invariants and integrate the result in velocity space we obtain

\[
\frac{\partial}{\partial t} \int_{\mathbb{R}^3} f\phi(v) \, dv + \nabla_x \left( \int_{\mathbb{R}^3} vf\phi(v) \, dv \right) = 0, \quad \phi(v) = 1, v_1, v_2, v_3, |v|^2.
\]

These equations describe the balance of mass, momentum and energy. The system of five equations is not closed since it involves higher order moments of the distribution function \( f \).

As \( \varepsilon \to 0 \) we have formally \( Q(f, f) \to 0 \) and thus \( f \) approaches the local Maxwellian. In this case the higher order moments of the distribution function can be computed as function of \( \rho, u, \) and \( T \) and we obtain the closed system of \textit{compressible Euler equations}

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho u) & = 0 \\
\frac{\partial \rho u}{\partial t} + \nabla_x \cdot (\rho u \otimes u + p) & = 0 \\
\frac{\partial E}{\partial t} + \nabla_x \cdot (Eu + pu) & = 0
\end{align*}
\]

where \( p \) is the gas pressure.

**Remark:** Standard numerical methods will become extremely expensive near the fluid dynamic regime.
Boundary conditions

The Boltzmann equation is complemented with the boundary conditions for $v \cdot n \geq 0$ and $x \in \partial \Omega$, where $n$ denotes the unit normal, pointing inside the domain $\Omega$. Usually the boundary represents the surface of a solid object (an obstacle or a container). The particles of the gas that hit the surface interact with the atoms of the object and are reflected back into the domain $\Omega$.

Mathematically, such boundary conditions are modeled by an expression of the form

$$|v \cdot n| f(x, v, t) = \int_{v \cdot n < 0} |v_* \cdot n(x)| K(v_* \rightarrow v, x, t) f(x, v_*, t) dv_*.$$ 

This is the so-called \textit{reflective boundary condition} on $\partial \Omega$. 

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The ingoing flux is defined in terms of the outgoing flux modified by a given boundary kernel \( K \). This boundary kernel is such that positivity and mass conservation at the boundaries are guaranteed,

\[
K(v_* \to v, x, t) \geq 0, \quad \int_{v \cdot n(x) \geq 0} K(v_* \to v, x, t) \, dv = 1.
\]

Commonly used reflecting boundary conditions are the so-called Maxwell’s conditions. From a physical point of view, one assumes that a fraction \( \alpha \) of molecules is absorbed by the wall and then re-emitted with the velocities corresponding to those in a still gas at the temperature of the wall, while the remaining fraction \( (1 - \alpha) \) is specularly reflected.

This is equivalent to impose for the ingoing velocities

\[
f(x, v, t) = (1 - \alpha) Rf(x, v, t) + \alpha Mf(x, v, t),
\]

in which \( x \in \partial \Omega, \quad v \cdot n(x) \geq 0 \). The coefficient \( \alpha \), with \( 0 \leq \alpha \leq 1 \), is called the **accommodation coefficient** and

\[
Rf(x, v, t) = f(x, v - 2n(n \cdot v), t), \quad Mf(x, v, t) = \mu(x, t) M_w(v).
\]

If we denote by \( T_w \) the temperature of the solid boundary, \( M_w \) is given by

\[
M_w(v) = \exp\left(-\frac{v^2}{2T_w}\right),
\]

and the value of \( \mu \) is determined by mass conservation at the surface of the wall

\[
\mu(x, t) \int_{v \cdot n \geq 0} M_w(v) |v \cdot n| \, dv = \int_{v \cdot n < 0} f(x, v, t) |v \cdot n| \, dv.
\]
Remark: For $\alpha = 0$ (specular reflection) the re-emitted molecules have the same flow of mass, temperature and tangential momentum of the incoming molecules, while for $\alpha = 1$ (full accommodation) the re-emitted molecules have completely lost memory of the incoming molecules, except for conservation of the number of molecules.

In the case of **inflow boundary conditions**, one assumes that the distribution function of the particles entering the domain is known, i.e.

$$f(x, v, t) = g(v, t), \quad x \in \partial \Omega, \quad v \cdot n > 0,$$

A typical example of such condition is used in shock wave calculations, where one assumes that the distribution function at the boundary of the computational domain is a Maxwellian. In this case the particles that enter the domain in a time step $\Delta t$ have a distribution proportional to $v \cdot n g(v, t)$, $v \cdot n > 0$. In fact the number of particles that enter the domain in a time interval $\Delta t$ with velocity between $v$ and $v + dv$ through a small area $\Delta S$ is given by

$$dN = \Delta S \Delta t v \cdot n g(v, t) d^3v.$$
Variants

A simplified model Boltzmann equation is given by the BGK model. In this model the collision operator is replaced by a relaxation operator of the form

\[ Q_{BGK}(f, f)(v) = -\rho(f - M(f)) \]

where \( M(f) \) is a Maxwellian with the same moments of \( f \).

Conservation of mass, momentum and energy as well as Boltzmann H-theorem are readily satisfied. The equilibrium solutions are clearly Maxwellians

\[ Q_{BGK}(f, f) = 0 \iff f = M(f). \]

Remarks: Numerical computations, as well as the analytic theory, are much simpler. Main drawback: some unphysical features (wrong Prandtl number).
The **Landau model** is a common kinetic model in plasma physics characterized by the following collision operator

\[
Q_L(f, f)(v) = \nabla_v \cdot \int_{\mathbb{R}^d} A(v - v_*)[f(v_*)\nabla_v f(v) - f(v)\nabla_v f(v_*)] \, dv_*
\]

\[
A(z) = \Psi(|z|)\Pi(z): \text{ } d \times d \text{ nonnegative symmetric matrix}
\]

\[
\Pi(z) = (\pi_{ij}(z)) \text{: orthogonal projection upon the space orthogonal to } z,
\]

\[
\pi_{ij}(z) = \left( \delta_{ij} - \frac{z_i z_j}{|z|^2} \right)
\]

\[
\Psi(|z|) = \Lambda|z|^\alpha + 2: \text{ for inverse-power laws, with } \alpha \geq -3 \text{ and } \Lambda > 0.
\]

\[
\alpha = -3: \text{ Coulombian case}, \text{ of primary importance for applications.}
\]

**Remark:** Conservations and H-theorem hold. Equilibrium are Maxwellians.
Other variants

- **Enskog models**: diameter of the interacting spheres $\delta$ is finite (as opposite to Boltzmann). The collision operator is delocalized in space.

- **Quantum-Boltzmann models**: the nonlinear interactions $f'f_* - ff_*$ is replaced by
  \[ f'f'(1 \pm f)(1 \pm f_*) - ff_*(1 \pm f')(1 \pm f'_*). \]
  Sign $-$ Pauli operator, Sign $+$ Bose-Einstein operator.

- **Semiconductor-Boltzmann models**: linear Boltzmann equation for semiconductor devices
  \[ Q_S(f, f) = \int \sigma(v, v_*)\{M(v)f(v_*) - M(v_*)f(v)\} dv_*, \]
  where $M$ is the normalized Maxwellian at the temperature $\theta$ of the semiconductor.

- **Granular gas models**: particles undergo inelastic collisions. Energy is dissipated by the model.

**Remark**: Other Boltzmann-like models in vehicular traffic flows, biomathematics, ...
**Splitting approach**

The most common approach to solve the full Boltzmann equation is based on an operator splitting.

The solution in one time step $\Delta t$ may be obtained by the sequence of two steps. First integrate the space homogeneous equation for all $x \in \Omega$,

$$\frac{\partial \tilde{f}}{\partial t} = \frac{1}{\varepsilon} Q(\tilde{f}, \tilde{f}),$$

$$\tilde{f}(x, v, 0) = f_0(x, v),$$

for a time step $\Delta t$ (collision step) to obtain $\tilde{f} = C_{\Delta t}(f_0)$, and then the transport equation using the output of the previous step as initial condition,

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = 0,$$

$$f(x, v, 0) = \tilde{f}(x, v, \Delta t).$$

for a time step $\Delta t$ (transport step) to get $f = T_{\Delta t}(\tilde{f}) = T_{\Delta t}(C_{\Delta t}(f_0))$.

After computing an approximation of the solution at time $\Delta t$, the process may be iterated to obtain the numerical solution at later times. After this splitting almost all the main numerical difficulties are contained in the collision step.

**Remark** The discretization of these equations can be performed in a variety of ways (finite volume, finite difference, Monte Carlo methods and so on). The choice of the discretization mainly depends on the method that is used for the solution of the space homogeneous Boltzmann equation.
The splitting scheme (simple splitting) described above is first order accurate in space and time. Note that the order of accuracy of this simple splitting does not improve even if we solve with great accuracy both collision and convection steps. The accuracy in time may be improved by a more sophisticated splitting. For example Strang splitting is second order accurate, provided both steps are at least second order. It can be written as

\[ f = C_{\Delta t/2}(T_{\Delta t}(C_{\Delta t/2}(f_0))), \]

or equivalently as

\[ f = T_{\Delta t/2}(C_{\Delta t}(T_{\Delta t/2}(f_0))). \]

**Remark:** If a scheme is able to treat the collision step in the simple splitting for vanishingly small values of \( \varepsilon \), then the splitting scheme become a first order kinetic scheme for the underlying fluid dynamic limit. In fact the collision step becomes a projection towards the local Maxwellian \( C_{\Delta t}(f_0) = M(f_0) \) which is then transported by the transport step \( f = T_{\Delta t}(M(f_0)). \)

Unfortunately Strang splitting reduces its accuracy to first order in time in this regime. This problem seems to occur for all high order splitting methods developed in the present literature.
Numerical challenges

- **Velocity approximation**
  - Physical properties (conservations, H-theorem)
  - Computational cost
  - Bounded domain
  - Accuracy control

- **Time discretization**
  - Stiffness of the problem for small values of $\epsilon$
  - Order reduction for small values of $\epsilon$

- **Space discretization**
  - Complicated geometries
  - Large velocities
  - Shocks
Discrete velocity models

Derivation

Historically this was the first method for discretizing the Boltzmann equation in velocity space. The model is built starting from physical rather than numerical considerations. We assume the gas particles can attain only a finite set of velocities

\[ V_N = \{v_1, v_2, v_3, \ldots, v_N\}, \quad v_i \in \mathbb{R}^3. \]

Particles collide by simple elastic collisions. The collision \((v_i, v_j) \leftrightarrow (v_k, v_l)\) is admissible if \(v_i, v_j, v_k, v_l \in V_N\) and preserves momentum and energy

\[ v_i + v_j = v_k + v_l, \quad |v_i|^2 + |v_j|^2 = |v_k|^2 + |v_l|^2. \]

The set of admissible output pairs \((v_k, v_l)\) corresponding to a given input pair \((v_i, v_j)\) will be denoted by \(C_{ij}\) and its cardinality by \(q_{ij}\).
Sketch of a planar model based on a cartesian grid. For the collision \((v_i, v_j)\) in Figure we have 3 admissible output collision pairs \((v_k, v_l)\) hence \(q_{ij} = 3\). Note that in general few grid points will belong to the collision circle.
The discrete collision operator is obtained by computing first the transition probabilities $a_{ij}^{kl}$ of the collision $(v_i, v_j) \leftrightarrow (v_k, v_l)$ which must satisfy the relations

$$a_{ij}^{kl} \geq 0, \quad \sum_{k,l=1}^{N} a_{ij}^{kl} = 1, \quad \forall i, j = 1, \ldots, N.$$ 

**Example:** All output pairs are assumed to be equally probable

$$a_{ij}^{kl} = \begin{cases} 
\frac{1}{q_{ij}} & \text{if } (v_i, v_j) \leftrightarrow (v_k, v_l) \text{ admissible} \\
0 & \text{if } (v_i, v_j) \leftrightarrow (v_k, v_l) \text{ not admissible.}
\end{cases}$$

Note that $a_{ij}^{kl} = a_{kl}^{ij}$ and $a_{ij}^{kl} = a_{ji}^{kl} = a_{lk}^{ji} = a_{lk}^{ij}$ (microreversibility).

Next we introduce the transition rates $A_{ij}^{kl} = S|v_i - v_j|a_{ij}^{kl}$, where $S$ is the cross sectional area of particles, and write the discrete Boltzmann equation as

$$\frac{\partial f_i}{\partial t} + v_i \cdot \nabla_x f_i = Q_i(f, f),$$

where

$$Q_i(f, f) = \sum_{j,k,l=1}^{N} A_{ij}^{kl}(f_k f_l - f_i f_j),$$

where $f_i, f_j, f_k, f_l$ are the distribution densities of particles with velocities $v_i, v_j, v_k, v_l$. 

Properties

It is easy to check that the discrete Boltzmann equation satisfies for any test function \( \phi_i = \phi(v_i) \)

\[
\sum_{i=1}^{N} Q_i(f, f) \phi_i = -\frac{1}{4} \sum_{i,j,k,l=1}^{N} A_{ij}^{kl}(f_k f_l - f_i f_j)(\phi_k + \phi_l - \phi_i - \phi_j),
\]

and thus the **discrete collision invariants** satisfy

\[
\phi_k + \phi_l - \phi_i - \phi_j = 0.
\]

Thus we have \( \phi(v_i) = 1, v_i^x, v_i^y, v_i^z, |v_i|^2 \) as collision invariants. Note that due to the finite number of velocities we can have models with additional spurious collision invariants or models where the collision invariants are not independents. Models with the correct space of collisions invariants are called **regular**.

The main macroscopic quantities are defined as

\[
\rho = \sum_{i=1}^{N} f_i, \quad u = \frac{1}{\rho} \sum_{i=1}^{N} f_i v_i, \quad T = \frac{1}{3 R \rho} \sum_{i=1}^{N} f_i (v_i - u)^2.
\]

In addition taking \( \phi_i = \ln(f_i) \) we obtain

\[
\sum_{i=1}^{N} Q_i(f, f) \ln(f_i) = -\frac{1}{4} \sum_{i,j,k,l=1}^{N} A_{ij}^{kl}(f_k f_l - f_i f_j) \ln\left(\frac{f_k f_l}{f_i f_j}\right) \leq 0,
\]

and hence the discrete analogue of Boltzmann’s H-theorem.
By the same arguments as in the continuous case we obtain that the equilibrium states are characterized by the equation

\[ f_i = \exp(a + b \cdot v_i + c|v_i|^2), \quad c < 0. \]

However in the discrete case it is not possible to write explicitly \( a, b, c \) as functions of the macroscopic quantities \( \rho, u, T \) except in some particular cases.

In general one has to solve for \( a, b, c \) the system of nonlinear equations characterized by

\[
\begin{align*}
\rho &= \sum_{i=1}^{N} \exp(a + b \cdot v_i + c|v_i|^2) \\
u &= \frac{1}{\rho} \sum_{i=1}^{N} \exp(a + b \cdot v_i + c|v_i|^2)v_i, \\
T &= \frac{1}{3R\rho} \sum_{i=1}^{N} \exp(a + b \cdot v_i + c|v_i|^2)(v_i - u)^2.
\end{align*}
\]

**Remark:** This requires a suitable numerical method if the local Maxwellian equilibrium is needed explicitly.
Similarly we can formally write the corresponding conservation equations. Note however that since discrete Maxwellian equilibrium states differ from true Maxwellians the corresponding fluid equations will contain spurious terms due to the truncation of the Maxwellian tails.

**Remarks:** Similar arguments (necessity to solve a nonlinear system and truncation effects) apply also to discrete BGK models of the Boltzmann equation.
Drawbacks

We have seen that the discrete Boltzmann equation is a discrete model of the Boltzmann equation that has the nice property of preserving the essential physical features (conservations, H-theorem, equilibrium states). From a computational point of view the discrete Boltzmann equation unfortunately presents two main drawbacks.

- The computational cost is high in general, larger than $O(N^2)$. 

![Graph showing computational cost vs N]
The accuracy of the method is poor. Present theoretical estimates (very difficult to obtain) for regular hypercubes give an error of the order of $O(1/n^\beta)$, with $\beta \approx 6/11$ in $3D$ and $\beta \approx 1$ in $2D$ where $N = n^3$ (less then first order accuracy).

Remarks: For this reasons applications have been mainly limited to simple models with few velocities in order to have qualitative results.

However numerical convergence test shows up to first order convergence rates of the method. This can be understood if we consider that numerically the discrete Boltzmann equation corresponds to take a quadrature formula for the Boltzmann equations where

$$V_N = \{v_1, v_2, v_3, \ldots, v_N\} \quad \text{quadrature nodes}$$

$$a_{ij}^{kl} \quad \text{quadrature weights}.$$ 

Thus for a grid of regular hypercubes with all weights equals we expect a rectangular rule convergence to the Boltzmann equation for hard spheres.
Examples

Broadwell models

Here we consider a set of one dimensional Broadwell models defined by

\[ \frac{\partial f_1}{\partial t} + \frac{\partial f_1}{\partial x} = \frac{1}{\epsilon} (f_3^2 - f_1 f_2) \]
\[ \frac{\partial f_2}{\partial t} - \frac{\partial f_2}{\partial x} = \frac{1}{\epsilon} (f_3^2 - f_1 f_2) \]
\[ \frac{\partial f_3}{\partial t} = \frac{1}{\alpha \epsilon} (f_1 f_2 - f_3^2) \]

being now \( f_1, f_2, f_3 \) the density of particles with velocity \( 1, -1, 0 \) respectively. The parameter \( \alpha \geq 1 \) is proportional to the number of particle densities moving with zero velocity. In particular for \( \alpha = 1 \) we have the reduced four velocity Broadwell model, whereas for \( \alpha = 2 \) it corresponds to the reduced six velocity Broadwell model.
The space of collision invariant has dimension 2 corresponding to conservation of mass and mean velocity

\[ \rho = f_1 + f_2 + 2\alpha f_3, \quad \rho u = f_1 - f_2. \]

The Maxwellian state is characterized by two constants \( a \) and \( b \) such that

\[ M_1 = a \exp\{b\}, \quad M_2 = a \exp\{-b\}, \quad M_3 = a. \]

In particular it is possible to get the analytic expression of \( a \) and \( b \) as a function of \( \rho \) and \( u \)

\[ a = \frac{\rho(1 - e)}{2\alpha}, \quad b = \log \left[ \frac{(1 - e)}{\alpha(e - u)} \right], \]

where \( e = e(u) \) is given by

\[ e = \frac{1}{2}(1 + u^2), \quad \alpha = 1 \]

\[ e = \frac{1}{(\alpha^2 - 1)} \left( \alpha \sqrt{\alpha^2 u^2 + 1 - u^2} - 1 \right), \quad \alpha > 1. \]
A numerical example

After the splitting we need a numerical scheme for solving the transport phase for \( f_1 \) and \( f_2 \). In our numerical experiments we considered the first order upwind scheme with uniform mesh spacing \( \Delta x \) in the spatial grid points \( x_i \) given by

\[
f_{j}^{n+1/2}(x_i) = f_{j}^{n}(x_i) + \eta [f_{j}^{n}(x_{i+i}) - f_{j}^{n}(x_{i})], \quad j = 1, 2
\]

and its second order TVD (total variation diminishing) extension

\[
f_{j}^{n+1/2}(x_i) = f_{j}^{n}(x_i) + \eta [f_{j}^{n}(x_{i+i}) - f_{j}^{n}(x_{i})] - \frac{i_j \eta (1 - \eta)}{2} [F_{j}^{n}(x_{i+i}) \Delta x - F_{j}^{n}(x_{i}) \Delta x], \quad j = 1, 2
\]

where \( \eta = \Delta t / \Delta x \), \( i_j = (-1)^j \),

\[
F_{j}(x_i) = \frac{[f_{j}(x_{i-j+2}) - f_{j}(x_{i-j+1})]}{\Delta x} \phi(\theta_{j}(x_i)), \quad \theta_{j}(x_i) = \frac{[f_{j}(x_{i}) - f_{j}(x_{i-1})]}{[f_{j}(x_{i+1}) - f_{j}(x_{i})]}^{i_j},
\]

and \( \phi \) is the particular slope-limiter function.

**Examples**: The “superbee” limiter of Roe

\[
\phi_{RS}(\theta) = \max\{0, \min\{1, 2\theta\}, \min(\theta, 2)\},
\]

and Van Leer’s limiter function

\[
\phi_{VL}(\theta) = (|\theta| + \theta) / (1 + |\theta|).
\]
The initial data is characterized by two local Maxwellian with mass and velocity

\begin{align*}
\rho, \ u, \quad x \leq 0 \\
\bar{\rho}, \ \bar{u}, \quad x > 0.
\end{align*}

where the macroscopic quantities \( \bar{\rho}, \bar{u} \) are computed in terms of \( \rho, u \) from the classical Rankine-Hugoniot relations.

The test case we consider is the infinite Mach number shock wave problem for \( \alpha = 2 \) characterized by

\begin{align*}
\bar{\rho} = 4.0, \quad \bar{u} = 0; \quad \rho = 1.0, \quad u = 1.0.
\end{align*}

In this situation, corresponding to a shock wave travelling with speed \( s = 1/3 \), the problem can be solved exactly

\begin{align*}
\rho(x, t) &= \frac{4 + e^{\xi/\epsilon}}{1 + e^{\xi/\epsilon}}, \\
u(x, t) &= \frac{e^{\xi/\epsilon}}{1 + e^{\xi/\epsilon}},
\end{align*}

where \( \xi = (3x - t)/2 \).
Profiles for different Knudsen numbers $\epsilon = 0.1, 0.05, 10^{-6}$ of $\rho (\circ)$ and $u (\otimes)$ for the second order scheme with $\phi = \phi_{VL}$ and $\eta = 0.5$, $\Delta x = 0.01$ at $t = 1.5$. 
Basic References


Note: B►Boltzmann equation, D►Discrete velocity models, T►Time discretization, S►Space discretization.