Solution of time-dependent Boltzmann equation for electrons in non-thermal plasma

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Description of plasma

- **Kinetic description:**
  - most fundamental way providing $f(r, v, t)$
  - achieved by solving the **Boltzmann equation**
  - self-consistently determined the electromagnetic fields via Maxwell’s equations

- **Fluid description:**
  - description of the plasma based on macroscopic quantities
  - fluid equations obtained by taking velocity moments of the BE

- **Hybrid description:**
  - a combination of fluid and kinetic models
    - treating some components of the system as a fluid and others kinetically

- **Gyrokinetic Description:**
  - appropriate to systems with a strong background magnetic field
  - the kinetic equations are averaged over the fast circular motion of the gyroradius
What will I talk about?

- weakly ionized plasma (small fraction of the atoms are ionized)
- moderate pressure ($\sim 1$ Torr)
- non-thermal or 'cold' plasma ($T_e \gg T_{\text{ion}} = T_{\text{gas}}$)
- non-magnetized plasma ($B=0$)
- solution of linear Boltzmann equation for electrons
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Are you still interested?
The Boltzmann equation

The Boltzmann equation is an equation for the time evolution of the distribution function \( f(r, v, t) \) in phase space, where \( r \) and \( v \) are position and velocity:

\[
\frac{\partial f}{\partial t} + v \cdot \nabla_r f + a \cdot \nabla_v f = \frac{\partial f}{\partial t} \bigg|_c
\]

We will discussed the Boltzmann equation with a collision term for two-body collisions between particles of different types that are assumed to be uncorrelated prior to the collision: the linear Boltzmann equation.
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How we can solve it?
How to solve the Boltzmann equation?

There are generally two ways:

- **Monte Carlo methods (TPMC, PIC/MCC)**
  - A way how to solve it without solving it

- **Actual solution of “The Equation”**
  - difficult but in simple cases and with approximations it is feasible
Monte Carlo methods

- a way how to obtain results with minimum of approximations
- MC:
Solves a particle charge transport by the numerical simulation of large particle ensemble, collision processes are introduced by generating appropriately distributed random numbers.
Monte Carlo methods

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- **MC:** Solves a particle charge transport by the numerical simulation of large particle ensemble, collision processes are introduced by generating appropriately distributed random numbers.

How does it work?
Consider $n$-dimensional integral

$$I = \int_0^1 \cdots \int_0^1 f(x_1, \ldots, x_n) \, d^n x,$$

in $n$-cube of unit volume. It is the mean value

$$I = \langle f \rangle.$$

**MC** gives us an approximation of exact value of the mean value with statistic estimate based on a numerical experiment. The mean value is estimated on an average over $N$ trials

$$I \approx \frac{\sum_{i=1}^N f(\eta_1, \ldots, \eta_n)}{N},$$

which is exact for $N \to \infty$. 
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But why random numbers?
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$$I \sim \frac{\sum_{i=1}^N f(\eta_1, \ldots, \eta_n)}{N},$$

which is exact for $N \to \infty$.

Because a finite distribution of regular points gives a poor resolution when the dimension $n$ is high.
Propagation method

- Problem to be solved:
  - determination of distribution function $f$ of charged particles based on the initial condition $f_0$.
  - Initial condition is a sum of mathematical particles ($\delta$-functions) which are propagated in time and space to represent a solution at later times

- Consider $N$ simulated superparticles, these represent $N_{\text{real}}$ real particles

$$w = \frac{N_{\text{real}}}{N} \quad \text{weight of superparticles}$$
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How to determine the density and the energy distribution function?
• Estimation of particle density in a given cell of the mathematical mesh

\[ n = \frac{N_{\text{cell}} w}{\Delta x \Delta y \Delta z} \]

• Determination of energy distribution function by introducing a mesh on the kinetic energy axis
How to propagate particles?

- performing a numerical solution of equations of motion under the effect of Lorentz force and random force which represents collision events between charged particles and neutral particles background

\[
\frac{dr}{dt} = v
\]

\[
\frac{dv}{dt} = \frac{q}{m}E + \frac{F_{\text{coll}}}{m}
\]

- collision events are instantaneous, successions of “kicks”
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How are collision times, \( t_c \), distributed?
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\]

- collision events are instantaneous, successions of “kicks”

How are collision times, \( t_c \), distributed?

**The answer is simple for constant collision frequency!**
Distribution of collision times

- for constant collision frequency $\alpha$
  
  $$P(t_c) = \alpha \exp(-\alpha t_c)$$

- free flight time can be generated easily
  
  $$t_c = -\frac{\ln \eta}{\alpha}.$$ 

- Implementation of propagation:
  - ∀ particle collisionless equation of motion between $(t, t + t_c)$ is solved
    
    $$\frac{dr}{dt} = v$$
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Distribution of collision times

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And …
Distribution of collision times

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- Implementation of propagation:
  - $\forall$ particle collisionless equation of motion between $(t, t + t_c)$ is solved

$$\frac{dr}{dt} = v$$

$$\frac{dv}{t} = \frac{q}{m} E$$

- the collision is introduced by laws of physics, based on appropriate random distribution of impact parameters
But . . .
Collision frequency is not a constant!
Null collision technique

- A new collision frequency is introduced

\[ \alpha_{\text{max}} = \max_{r, v \leq w} \alpha(v, r). \]

\[ \alpha(v, r) = \sum_{p} n(r)v\sigma_{p}(v) \]

- \( \alpha(v, r) \) is a sum of all contributions from different collision processes “p”

- A new “null” collision process is added in order to equate \( \alpha(v, r) \) and \( \alpha_{\text{max}} \)

- Non-physical collisions are eliminated by considering “null” collision with probability

\[ 1 - \frac{\alpha(v, r)}{\alpha_{\text{max}}} \]
Null collision technique

- selection of an event with a probability $p$:
  
  Uniform $\eta \in (0, 1] : (p > \eta \, ? \, \text{accepted} : \text{rejected})$

- after the collision a new direction of velocity and its magnitude is determined
Null collision technique

- Isotropic scattering can be assumed in many cases, momentum transfer cross section is used instead of DCS.
Null collision technique

- Isotropic scattering can be assumed in many cases, momentum transfer cross section is used insted of DCS.

Is the Monte Carlo technique merely a solution on the bases of physical analogy?
Formal view of Monte Carlo technique

- Consider linear Boltzmann equation in the form

\[
\frac{df}{dt} = -\alpha_{\text{max}} f + \alpha_{\text{max}} Af
\]

$A$ is a linear combination of unit operator and a Boltzmann collision operator

- The integral form:

\[
f(t) = \exp(-\alpha_{\text{max}} t) + \alpha_{\text{max}} \int_{0}^{t} \exp(-\alpha_{\text{max}} \tau) A(\tau) f(\tau) d\tau
\]

- Monte carlo method can be derived from numerical solution of this equation. MC procedure is applied to calculate this integral.
Solving the BE by solving it

- Approximations:
  - spatially homogeneous
  - electrons collide with neutral gas particles
  - collisions are isotropic
  - ionization is taken to be conservative
  - gas particles at rest

- The Boltzmann equation solved by the expansion into the Legendre polynomials
Expansion of the BE into the LPs

- \( E \parallel z\)-axis \( \implies f(\bm{v}, t) \rightarrow f(\bm{v}, \theta, t) \) (rotational symmetry)
- BE has a form
  \[
  \frac{\partial f}{\partial t} + \frac{eE}{m} \frac{\partial f}{\partial v_z} = \left. \frac{\partial f}{\partial t} \right|_c .
  \]
- Distribution function expanded into Legendre polynomials:
  \[
  f(\bm{v}, \theta, t) = \sum_{n=0}^{\infty} f_n(\bm{v}, t) P_n(\cos \theta) .
  \]
  \[
  \sum_{n=0}^{\infty} \left[ \frac{\partial f_n}{\partial t} + \frac{eE}{m} \left( \frac{n}{2n-1} \frac{\partial f_{n-1}}{\partial v} + \frac{n+1}{2n+3} \frac{\partial f_{n+1}}{\partial v} + \right. \right.
  \]
  \[
  + \left. \frac{(n+2)(n+1)}{2n+3} \frac{f_{n+1}}{v} - \frac{n(n-1)}{2n-1} \frac{f_{n-1}}{v} \right) \right] P_n(\cos \theta) = \left. \frac{\partial f}{\partial t} \right|_c .
  \]
Expansion of BE into LPs

- Resulting hierarchy of PDEs

\[
\frac{\partial f_n(v, t)}{\partial t} = - \frac{n}{2n-1} \left[ - \frac{eE(t)}{m} v^{n-1} \frac{\partial}{\partial v} \left( \frac{f_{n-1}(v, t)}{v^{n-1}} \right) \right] - \\
- \frac{n+1}{2n+3} \left[ - \frac{eE(t)}{m} \frac{1}{v^{n+2}} \frac{\partial}{\partial v} \left( v^{n+2} f_{n+1}(v, t) \right) \right] + \\
+ vN(t) (Q_n(v) - Q_0(v)) f_n(v, t) + \\
+ \frac{m}{M} \frac{1}{v^2} \frac{\partial}{\partial v} \left[ v^4 N(t) (Q_{1n}(v) - Q_n(v)) f_n(v, t) \right] + \\
+ \sum_k \left[ \frac{(v_A^k)^2}{v} N(t) Q_n^k(v_A^k) f_n(v_A^k, t) - \\
- vN(t) Q_0^k(v) f_n(v, t) \right],
\]

\[ n \geq 0, \quad f_{-1} \equiv 0, \]

where ...
... where

\[
Q_n(v) = \int_0^{2\pi} d\phi \int_0^{\pi} \sigma^{\text{el}}(v, \theta) P_n(\cos \theta) \sin \theta \, d\theta,
\]

\[
Q_{1n}(v) = \int_0^{2\pi} d\phi \int_0^{\pi} \sigma^{\text{el}}(v, \theta) P_1(\cos \theta) P_n(\cos \theta) \sin \theta \, d\theta,
\]

\[
Q_k^n(v) = \int_0^{2\pi} d\phi \int_0^{\pi} \sigma^k(v, \theta) P_n(\cos \theta) \sin \theta \, d\theta,
\]

where \(\sigma^{\text{el}}(v)\) and \(\sigma^k(v)\) are differential collision cross sections for elastic and \(k\)-th inelastic collision process and

\[
v_A^k = \left( v^2 + \frac{2A_k}{m} \right), \quad A_k > 0
\]

\(A_k\) is excitation energy of \(k\)-th state.

- For numerical solution \textbf{kinetic energy} \(U\) used instead of velocity \(v\):

\[
U = \left( \frac{v}{\gamma} \right)^2, \quad \gamma = (2/m)^{1/2}.
\]

- \textbf{Isotropic scattering (introducing } m_t)
Different approximations of the expansion of BE

- **Two-term approximations:**
  - **conventional two-term approx.**
    \[ \frac{\partial f_1}{\partial t} = 0, \quad f_1(U, t) \sim E(t) \frac{\partial f_0(U, t)}{\partial U} \]
    you cannot choose \( f_1(U, 0) \)!
  - **strict time-dependent two-term approx.**
    \( f_2(U, t) \equiv 0 \)

- **Multi-term approximation:**
  Expansion truncated after arbitrary (> 2) number of terms

- **Effective field approximation (2-term):**
  \( E(t) = E_0 \exp j\omega t \)
  Time variation \( f_0 \) a \( f_1 \) “slow enough” compared to \( \omega \).
  Generally: \( \omega/2\pi \sim \text{GHz or higher} \)
Solution procedure

- Hierarchy of PDEs solved as a initial–boundary value problem

\[
\frac{\partial f_0}{\partial U} \bigg|_{U=0} = 0, \quad f_n(U = 0, t) = 0, \quad n \geq 1
\]

\[
f_n(U \geq U_\infty, t) = 0, \quad n \geq 0,
\]

\(U_\infty\) sufficiently large energy,

by the method of lines

- BE discretized in energy space on uniform mesh \(U \in (0, U_\infty)\)
- system of ODEs received
- ODEs integrated by Runge Kutta method of order 4(5) with step-size control
Case study: Reid ramp model


- Hypothetical gas
  - mass: 4 amu
  - cross section for elastic collisions

\[ \sigma_{el} = 6.0 \times 10^{-20} \text{ m}^2 \]

- cross section for inelastic collisions

\[ \sigma_{in} = \begin{cases} 0 & \varepsilon \leq 0.2 \text{ eV} \\ 10(\varepsilon - 0.2) \times 10^{-20} \text{ m}^2 & \varepsilon > 0.2 \text{ eV} \end{cases} \]

- All collisions assumed to be isotropic
- Thermal motion of gas particles neglected
Reid ramp model: results

- Time independent electric field
- Initial distribution of electrons: Maxwellian 300 K.
- Steady state for $E/N = 24$ Td ($1 \text{Td} = 10^{-21} \text{V m}^{-1}$)

<table>
<thead>
<tr>
<th></th>
<th>BE</th>
<th>MC</th>
<th>Reid</th>
<th>Ness</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drift velocity (10^4 m s^-1)</td>
<td>8.892</td>
<td>8.88</td>
<td>8.89</td>
<td>8.886</td>
</tr>
<tr>
<td>Mean energy (eV)</td>
<td>0.4079</td>
<td>0.408</td>
<td>0.413</td>
<td>–</td>
</tr>
</tbody>
</table>
Reid ramp model: $E/N = 24$ Td, 1 Torr
Rare gases and the effect of ‘negative mobility’

Argon:

- initial distribution: Gaussian, center 5.5 eV, width 1 eV
- gas density \(3.45 \times 10^{22} \text{ m}^{-3}\) (pressure 1 Torr, temperature 273 K)
  \(E = 2 \text{ kV m}^{-1}, \ E/N = 58 \text{Td.}\)
Xenon:

- initial distribution: Gaussian, center 15.0 eV, width 1 eV
- gas density $3.45 \times 10^{22} \text{ m}^{-3}$ (pressure 1 Torr, temperature 273 K)

$$E = 2 \text{ kV m}^{-1}, \frac{E}{N} = 58 \text{ Td}$$
Conclusions

For a solution of time-dependent Boltzmann equation

- **the Monte Carlo Method**: is easy to implement, rather straightforward method, even for complex boundary conditions, may be rather time consuming

- **Solution of the Equation**: is a challenge, it is a fun, it gives good results (multi-term), for many problems it is impossible