

ENSEIRB-MATMECA



Solving the linear Boltzmann equation using Monte Carlo methods

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1 Introduction

1.1 Terms and definitions

The transport equation plays a crucial role in describing the behavior of particles in various physical systems. One of its important derivatives, the linear Boltzmann equation, is governed by the evolution of particle distribution in phase space. In this project, a numerical solution for the linear Boltzmann equation is developed utilizing the Monte Carlo method. The report is structured as follows:

- Transport Equation:** The fundamental transport equation is introduced, providing a basis for understanding the derivation of the linear Boltzmann equation.
- Linear Boltzmann Equation:** Building upon the transport equation, the linear Boltzmann equation is explored, emphasizing its significance in characterizing particle transport phenomena.
- Monte Carlo Method for Linear Boltzmann Equation:** The approach to solving the linear Boltzmann equation using the Monte Carlo method is presented, along with a discussion of the advantages and challenges associated with this numerical technique.
- Semi-Analog Monte Carlo Scheme:** A semi-analog Monte Carlo scheme is introduced as an innovative strategy to enhance the efficiency and accuracy of simulations.

1.2 Context and Applications

The linear Boltzmann equation finds applications in a wide range of industrial and research contexts. Notable examples include its use in nuclear reactor physics, radiation shielding design, medical imaging, and astrophysics. Applications extend to industries such as nuclear energy, healthcare, and aerospace, where accurate simulations of particle transport are crucial for optimizing designs and ensuring safety protocols.

In the realm of academic research, the linear Boltzmann equation serves as a cornerstone in the study of rarefied gas dynamics, plasma physics, and neutron transport. Collaborations between universities, research institutions, and companies contribute to advancements in understanding and solving complex problems associated with particle transport phenomena.

Leading companies in the field, such as [Company1], [Company2], and [Company3], actively engage in research and development related to the linear Boltzmann equation. Their work encompasses both theoretical advancements and practical applications, demonstrating the equation's significance in addressing real-world challenges.

This project aims to contribute to the broader understanding and application of the linear Boltzmann equation, with a focus on developing efficient numerical methods for solving this intricate problem.

Note Here is a brief summary of the various existences and uniqueness of solutions based on different cases of equations to be solved. The primary source used is the transport and diffusion document.

2 Transport Equation

In this section, we will examine the solutions of the transport equation, a particular case of the Boltzmann equation, defined below:

Let's $v \in \mathbb{R}^N$

$$\frac{\partial f}{\partial t}(t, x) + v \cdot \nabla_x f(t, x) + a(t, x)f(t, x) = S(t, x), \quad x \in \mathbb{R}^N, \quad t > 0. \quad (1)$$

f is the unknown function, a is the given damping or amplification rate, and S is the given source term.

2.1 Cauchy Problem

2.1.1 Special Case without Absorption or Source Term

Let's consider the following Cauchy problem:

$$\begin{cases} \frac{\partial f}{\partial t}(t, x) + v \cdot \nabla_x f(t, x) = 0, & x \in \mathbb{R}^N, \quad t > 0. \\ f(0, x) = f^{in}(x) \end{cases}$$

If $f^{in} \in \mathcal{C}^1(\mathbb{R}^n)$, then using the method of characteristics, we can easily demonstrate that the Cauchy problem has a unique solution $f \in \mathcal{C}^1(\mathbb{R}_+ \times \mathbb{R}^n)$. This solution is given as follows:

$$f(t, x) = f^{in}(x - tv) \quad \forall (t, x) \in \mathbb{R}_+ \times \mathbb{R}^n$$

2.1.2 With Absorption and Source Term

This time, we consider damping and the source term, assuming they belong to $\mathcal{C}^1(\mathbb{R}_+ \times \mathbb{R}^n)$. The considered Cauchy problem is as follows:

$$\begin{cases} \frac{\partial f}{\partial t}(t, x) + v \cdot \nabla_x f(t, x) + a(t, x)f(t, x) = S(t, x), & x \in \mathbb{R}^N, \quad t > 0. \\ f(0, x) = f^{in}(x) \end{cases}$$

In this case, if $f^{in} \in \mathcal{C}^1(\mathbb{R}^n)$, then using the method of characteristics, we can still demonstrate that the Cauchy problem has a unique solution $f \in \mathcal{C}^1(\mathbb{R}_+ \times \mathbb{R}^n)$. This solution is given as follows:

$$f(t, x) = f^{in}(x - tv)e^{-\int_0^t a(\tau, x + (t-\tau)v) d\tau} + \int_0^t e^{-\int_0^s a(\tau, x + (t-\tau)v) d\tau} S(s, x + (s-t)v) ds \quad \forall (t, x) \in \mathbb{R}_+ \times \mathbb{R}^n$$

2.2 Boundary Value Problems

In the previous section, we presented results applicable when considering complete freedom for the spatial variable in \mathbb{R}^n . However, for a significant portion of physical problems, this may not be the case. That is why we are more interested in a problem of the boundary value type. In this section, we will consider the set Ω , which is an open set with a \mathcal{C}^1 boundary in \mathbb{R}^n . Additionally, we take $v \in \mathbb{R}^n \setminus \{0\}$.

2.2.1 Special Case without Absorption or Source Term

If, moreover, Ω is convex, and let $f_b^- \in \mathcal{C}^1(\mathbb{R}_+ \times \partial\Omega^-)$ and $f^{in} \in \mathcal{C}^1(\overline{\Omega})$, where $\partial\Omega^- = \{x \in \partial\Omega \mid v \cdot n_x < 0\}$, then the problem:

$$\begin{cases} \frac{\partial f}{\partial t}(t, x) + v \cdot \nabla_x f(t, x) = 0, & x \in \mathbb{R}^N, \quad t > 0. \\ \upharpoonright f \partial\Omega = f_b^- \\ \upharpoonright ft = 0 = f^{in}(x) \end{cases}$$

has a unique solution $f \in \mathcal{C}^1(\mathbb{R}_+ \times \Omega)$ and $f \in \mathcal{C}^0(\mathbb{R}_+ \times \overline{\Omega})$ if and only if $\forall y \in \partial\Omega^-$,

$$f_b^-(0, y) = f^{in}(y), \quad \frac{\partial f_b^-}{\partial t}(t, y) + v \cdot \nabla f^{in}(y) = 0.$$

The expression of the solution is then given by:

$$f(t, x) = \begin{cases} f^{in}(x - tv) & \text{si } t \leq \tau_x, \\ f_b^-(t - \tau_x, x - \tau_x v) & \text{si } t > \tau_x, \end{cases}$$

With $\tau_x = \inf\{t \geq 0 \mid x - tv \notin \overline{\Omega}\}$

2.2.2 With Absorption and Source Term

We still consider Ω to be convex, with $f_b^- \in \mathcal{C}^1(\mathbb{R}_+ \times \partial\Omega^-)$, $f^{in} \in \mathcal{C}^1(\overline{\Omega})$, a , and $S \in \mathcal{C}^1(\mathbb{R}_+ \times \overline{\Omega})$. If we assume that $\forall y \in \partial\Omega^-$,

$$f_b^-(0, y) = f^{in}(y),$$

$$\frac{\partial f_b^-}{\partial t}(0, y) + v \cdot \nabla_x f^{in}(y) + a(0, y) f^{in}(y) = S(0, y)$$

In this case, the problem becomes:

$$\begin{cases} \frac{\partial f}{\partial t}(t, x) + v \cdot \nabla_x f(t, x) + a(t, x) f(t, x) = S(t, x), & x \in \mathbb{R}^N, \quad t > 0. \\ \upharpoonright f \partial\Omega = f_b^- \\ \upharpoonright ft = 0 = f^{in}(x) \end{cases}$$

has a unique solution $f \in \mathcal{C}^1(\mathbb{R}_+ \times \Omega)$ and $f \in \mathcal{C}^0(\mathbb{R}_+ \times \overline{\Omega})$. The expression for f is then:

$$\begin{aligned} f(t, x) = & \mathbf{1}_{t \leq \tau_x} f^{in}(x - tv) \exp \left(- \int_0^t a(s, x + (s - t)v) ds \right) \\ & + \mathbf{1}_{t > \tau_x} f_b^-(t - \tau_x, x - \tau_x v) \exp \left(- \int_{t - \tau_x}^t a(s, x + (s - t)v) ds \right) \\ & + \int_{t - \tau_x}^t \exp \left(- \int_s^t a(\tau, x + (\tau - t)v) d\tau \right) S(s, x + (s - t)v) ds \end{aligned}$$

2.3 Generalized Solutions

In this section, Ω is not necessarily convex. This implies that the continuity of potential solutions is not guaranteed. However, in practice, these cases must be addressed. Below, we define the concept of generalized solutions, which allows us to handle this issue without resorting to the theory of distributions.

Definition Let Ω be an open set with a \mathcal{C}^1 boundary in \mathbb{R}^n , and let a and S be continuous on $\mathbb{R}_+ \times \Omega$. We say that f is a generalized solution of the problem

$$\frac{\partial f}{\partial t}(t, x) + v \cdot \nabla_x f(t, x) + a(t, x) f(t, x) = S(t, x), \quad x \in \mathbb{R}^N, \quad t > 0.$$

if and only if the function

$s \mapsto f(t + s, x + sv)$ is of class \mathcal{C}^1 almost everywhere in $(t, x) \in \mathbb{R}_+ \times \Omega$ and satisfies

$$\frac{d}{ds} f(t + s, x + sv) + a(t + s, x + sv) f(t + s, x + sv) = S(t + s, x + sv) \quad (t + s, x + sv) \in \mathbb{R}_+^* \times \Omega.$$

Let Ω be an open set with a \mathcal{C}^1 boundary in \mathbb{R}^n , and let a and S be continuous on $\mathbb{R}_+ \times \Omega$. Let $f_b^- \in \mathbf{L}_{loc}^\infty(\mathbb{R}_+ \times \partial\Omega^-)$ and $f^{in} \in \mathbf{L}_{loc}^\infty(\overline{\Omega})$.

In this case, the problem:

$$\begin{cases} \frac{\partial f}{\partial t}(t, x) + v \cdot \nabla_x f(t, x) + a(t, x) f(t, x) = S(t, x), & x \in \mathbb{R}^N, \quad t > 0. \\ \upharpoonright f \partial\Omega = f_b^- \\ \upharpoonright ft = 0 = f^{in}(x) \end{cases}$$

has a unique generalized solution. The formula for this solution is the same as in the previous case, i.e., almost everywhere in $(t, x) \in \mathbb{R}_+ \times \Omega$, we have:

$$\begin{aligned}
f(t, x) = & \mathbf{1}_{t \leq \tau_x} f^{in}(x - tv) \exp \left(- \int_0^t a(s, x + (s - t)v) ds \right) \\
& + \mathbf{1}_{t > \tau_x} f_b^-(t - \tau_x, x - \tau_x v) \exp \left(- \int_{t - \tau_x}^t a(s, x + (s - t)v) ds \right) \\
& + \int_{t - \tau_x}^t \exp \left(- \int_s^t a(\tau, x + (\tau - t)v) d\tau \right) S(s, x + (s - t)v) ds
\end{aligned}$$

3 Linear Boltzmann Equation

In this section, we will focus on the actual Boltzmann equation. This integro-differential equation is described in 2.

$$\frac{\partial f}{\partial t}(t, x, v) + v \cdot \nabla_x f(t, x, v) + a(t, x) f(t, x, v) = \int_{\mathbb{R}^n} k(t, x, v, w) f(t, x, w) d\mu(w) + Q(t, x, v). \quad (2)$$

To simplify notations, this equation will be written as:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + af = \mathcal{K}f + Q$$

Here, v and k are given continuous functions. The range of possibilities for the velocity v is very diverse due to the variety of physical problems that can be considered. Therefore, the notation $d\mu(w)$ encompasses all these possibilities by incorporating a weight function. The major difference from the transport equation is that, this time, we consider exchange phenomena, and thus, v cannot be seen as a simple parameter.

In this section, we cannot highlight the exact expression of the solutions because the method of characteristics yields another integral equation involving the solution.

Definition Let Q be continuous on $]0, T[\times \Omega \times \mathbb{R}^n$. We say that f is a generalized solution of the problem, continuous on $]0, T[\times \Omega \times \mathbb{R}^n$,

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + af = \mathcal{K}f + Q$$

if and only if, for all $(t, x, v) \in]0, T[\times \Omega \times \mathbb{R}^n$, the function

$$s \mapsto f(t + s, x + sv, v)$$

is of class \mathcal{C}^1 for all $x + sv \in \Omega$ and satisfies, for all $s \in \mathbb{R}$ such that $x + sv \in \Omega$,
 $\frac{d}{ds} f(t + s, x + sv, v) + a(t + s, x + sv, v) f(t + s, x + sv, v) = (\mathcal{K}f + Q)(t + s, x + sv, v).$

3.1 Cauchy Problem

Let $f^{in} \in \mathbf{C}_b(\mathbb{R}^n \times \mathbb{R}^n)$ and $Q \in \mathbf{C}_b(]0, T[\times \mathbb{R}^n \times \mathbb{R}^n)$. Also, let $0 \leq a \in \mathbf{C}_b(]0, T[\times \mathbb{R}_x^n \times \mathbb{R}_v^n)$ and $0 \leq k \in \mathbf{C}_b(]0, T[\times \mathbb{R}_x^n \times \mathbb{R}_v^n \times \mathbb{R}_w^n)$. The notation $\mathbf{C}_b(X)$ denotes the set of bounded continuous functions on X with values in \mathbb{R} .

We assume that:

$$\sup_{(t, x, v) \in]0, T[\times \mathbb{R}^n \times \mathbb{R}^n} \int_{\mathbb{R}^n} k(t, x, v, w) d\mu(w) < +\infty$$

Then the problem is:

$$\begin{cases} \frac{\partial f}{\partial t} + v \cdot \nabla_x f + af = \mathcal{K}f + Q & (t, x, v) \in]0, T[\times \mathbb{R}^n \times \mathbb{R}^n \\ \upharpoonright f t = 0 = f^{in} \end{cases}$$

has a unique generalized solution $f \in \mathbf{C}_b([0, T[\times \mathbb{R}^n \times \mathbb{R}^n)$.

3.2 Boundary Value Problem

We define the set Γ_- as $\Gamma_- = \{(x, v) \in \partial\Omega \times \mathbb{R}^n \mid v \cdot n_x < 0\}$

Let $f^{in} \in \mathbf{C}_b(\overline{\Omega} \times \mathbb{R}^n)$, $f_b^- \in \mathbf{C}_b([0, T] \times \Gamma_-)$ such that $f_b^-(0, y, v) = f^{in}(y, v) \quad \forall (y, v) \in \Gamma_-$

Let $Q \in \mathbf{C}_b([0, T] \times \overline{\Omega} \times \mathbb{R}^n)$.

Let $0 \leq a \in \mathbf{C}_b(\mathbb{R}_+ \times \Omega_x \times \mathbb{R}_v^n)$ and $0 \leq k \in \mathbf{C}_b(\mathbb{R}_+ \times \Omega_x^n \times \mathbb{R}_v^n \times \mathbb{R}_w^n)$.

Then the problem

$$\begin{cases} \frac{\partial f}{\partial t} + v \cdot \nabla_x f + af = \mathcal{K}f + Q & (t, x, v) \in]0, T[\times \Omega \times \mathbb{R}^n \\ \upharpoonright f t = 0 = f^{in} \\ \upharpoonright f \Gamma^- = f_b^- \end{cases}$$

has a unique generalized solution $f \in \mathbf{C}_b([0, T] \times \Omega \times \mathbb{R}^n)$.

4 The use of Monte Carlo methods to solve the linear Boltzmann equation

The transport equation in an infinite medium with its corresponding deterministic collisional component can be expressed as:

$$\partial_t u(x, t, \mathbf{v}) + \mathbf{v} \cdot \nabla u(x, t, \mathbf{v}) + v \sigma_t(x, t, \mathbf{v}) u(x, t, \mathbf{v}) = v \sigma_s(x, t, \mathbf{v}) \int P(x, t, \mathbf{v}, \mathbf{v}') u(x, t, \mathbf{v}') d\mathbf{v}' \quad (3)$$

Where

$$\sigma_s(x, t, \mathbf{v}) = \int \sigma_s(x, t, \mathbf{v}, \mathbf{v}') d\mathbf{v}', \quad P(x, t, \mathbf{v}, \mathbf{v}') = \frac{\sigma_s(x, t, \mathbf{v}, \mathbf{v}')}{\sigma_s(x, t, \mathbf{v})}$$

The approach involves a series of variable changes. The initial step involves re-expressing the transport equation 3 with respect to a characteristic $x + vt$. As a result, it transforms into:

$$\partial_s u(x + \mathbf{v}s, s, \mathbf{v}) = -v \sigma_t(x + \mathbf{v}s, s, \mathbf{v}) u(x + \mathbf{v}s, s, \mathbf{v}) + v \sigma_s(x + \mathbf{v}s, s, \mathbf{v}) \int P(x + \mathbf{v}s, s, \mathbf{v}, \mathbf{v}') u(x + \mathbf{v}s, s, \mathbf{v}') d\mathbf{v}' \quad (4)$$

Let's multiply both sides of the equation by:

$$e^{\int_0^s v \sigma_t(x + \mathbf{v}\alpha, \alpha, \mathbf{v}) d\alpha}$$

Following that, we obtain

$$\partial_s [u(x + \mathbf{v}s, s, \mathbf{v}) e^{\int_0^s v \sigma_t(x + \mathbf{v}\alpha, \alpha, \mathbf{v}) d\alpha}] = e^{\int_0^s v \sigma_t(x + \mathbf{v}\alpha, \alpha, \mathbf{v}) d\alpha} v \sigma_s(x + \mathbf{v}s, s, \mathbf{v}) \int P(x + \mathbf{v}s, s, \mathbf{v}, \mathbf{v}') u(x + \mathbf{v}s, s, \mathbf{v}') d\mathbf{v}'$$

We get after integrating the equation 4 between $[0, t]$:

$$\begin{aligned} u(x + \mathbf{v}t, t, \mathbf{v}) &= u_0(x, \mathbf{v}) \exp \left(- \int_0^t v \sigma_t(x + \mathbf{v}\alpha, \alpha, \mathbf{v}) d\alpha \right) \\ &+ \int_0^t \int v \sigma_s(x + \mathbf{v}s, s, \mathbf{v}) u(x + \mathbf{v}s, s, \mathbf{v}') e^{-\int_s^t v \sigma_t(x + \mathbf{v}\alpha, \mathbf{v}) d\alpha} P(x + \mathbf{v}s, s, \mathbf{v}, \mathbf{v}') d\mathbf{v}' ds \end{aligned} \quad (5)$$

We obtain:

$$\begin{aligned}
u(x, t, \mathbf{v}) &= u_0(x - \mathbf{v}t, \mathbf{v}) \exp \left(- \int_0^t v \sigma_t(x - \mathbf{v}(t - \alpha), \alpha, \mathbf{v}) d\alpha \right) \\
&+ \int_0^t \int v \sigma_s(x - \mathbf{v}(t - s), s, \mathbf{v}) u(x - \mathbf{v}(t - s), s, \mathbf{v}') e^{-\int_s^t v \sigma_t(x - \mathbf{v}(t - \alpha), \mathbf{v}) d\alpha} P(x - \mathbf{v}(t - s), s, \mathbf{v}, \mathbf{v}') d\mathbf{v}' ds
\end{aligned} \tag{6}$$

We also have:

$$\begin{aligned}
\exp \left(- \int_0^t v \sigma_t(x - \mathbf{v}(t - \alpha), \alpha, \mathbf{v}) d\alpha \right) &= \exp \left(- \int_0^t v \sigma_t(x - \mathbf{v}\alpha, t - \alpha, \mathbf{v}) d\alpha \right) \\
&= \int_t^\infty v \sigma_t(x - \mathbf{v}s, t - s, \mathbf{v}) \exp \left(- \int_0^s v \sigma_t(x - \mathbf{v}\alpha, t - \alpha, \mathbf{v}) d\alpha \right) ds
\end{aligned} \tag{7}$$

Then the integral representation of 3 is provided by:

$$\begin{aligned}
u(x, t, \mathbf{v}) &= \int_t^\infty u_0(x - \mathbf{v}t, \mathbf{v}) v \sigma_t(x - \mathbf{v}s, t - s, \mathbf{v}) \exp \left(- \int_0^s v \sigma_t(x - \mathbf{v}\alpha, t - \alpha, \mathbf{v}) d\alpha \right) ds \\
&+ \int_0^t \int v \sigma_s(x - \mathbf{v}(t - s), s, \mathbf{v}) u(x - \mathbf{v}(t - s), s, \mathbf{v}') e^{-\int_s^t v \sigma_t(x - \mathbf{v}(t - \alpha), \mathbf{v}) d\alpha} P(x - \mathbf{v}(t - s), s, \mathbf{v}, \mathbf{v}') d\mathbf{v}' ds
\end{aligned} \tag{8}$$

5 Semi analog MC scheme

Developing a Monte Carlo scheme involves introducing a group of random variables along with their associated probability measure to express 8 as an expectation. The selection of this set of random variables is not unique, resulting in various Monte Carlo schemes with distinct properties.

6 Numerical tests/results

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7 Conclusion