Resolution of the linear Boltzmann equation by Monte Carlo method

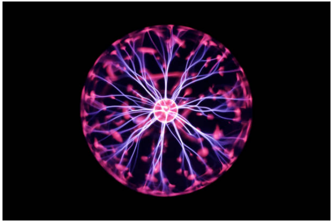
Antoine Boucher
Gabriel Rodiere
Clément Aumonier
Guillaume Doyen
Khaoula El Maddah

Wednesday, 31st January 2024

BORDEAUX INP Enseirb-Matmeca

Table of contents

Fields of Application for the Boltzmann Equation



Plasma physics

Fluid dynamic

Astrophysics

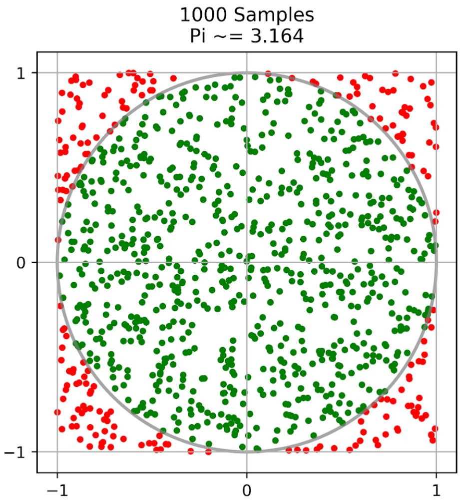
Rarefied Gas Dynamics

What is Monte Carlo?

Stanislaw Ulam and Nicholas Metropolis

Monaco

Example of the calculation of π



An estimate of π is given by:

$$\pi_N = \frac{\text{Number of stones within the circle}}{4N}$$

Cauchy problem

Cauchy problem with damping a and a source term S:

$$\begin{cases} \partial_t u(\boldsymbol{x}, t, \boldsymbol{v}) + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} u(\boldsymbol{x}, t, \boldsymbol{v}) + a(\boldsymbol{x}, t, \boldsymbol{v}) u(\boldsymbol{x}, t, \boldsymbol{v}) = S(\boldsymbol{x}, t, \boldsymbol{v}), \quad \boldsymbol{x} \in \mathbb{R}^n, \quad t > 0. \\ u(0, \boldsymbol{x}, \boldsymbol{v}) = u_0(\boldsymbol{x}, \boldsymbol{v}) \end{cases}$$

Then using the method of characteristics, we get the unique solution:

$$u(\boldsymbol{x}, t, \boldsymbol{v}) = \left(u_0(\boldsymbol{x} - t\boldsymbol{v}, \boldsymbol{v}) + \int_0^t S(\boldsymbol{x} + (s - t)\boldsymbol{v}, s, \boldsymbol{v}) \, \mathrm{d}s \right) \mathrm{e}^{-\int_0^t a(\boldsymbol{x} + (t - \tau)\boldsymbol{v}, \tau, \boldsymbol{v}) \, \mathrm{d}\tau}$$

Boltzmann equation

The transport equation can be expressed as:

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

Where

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

σ_t: the total cross-section
σ_s: the scattering cross-section
$v\sigma_t$: a damping term

Després, Golse, and Allaire 2018, Poëtte 2019 & Lapeyre, Pardoux, and Sentis 1998

Method of characteristics

The initial step is re-expressing the transport equation with respect to a characteristic $\boldsymbol{x} + \boldsymbol{v}s$. It transforms into:

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

After multiplying both sides of the equation by:

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

Following that, we obtain:

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

Integration of the equation

We get after integrating the equation between $(0, t)$:

$$u(\boldsymbol{x} + \boldsymbol{v}t, t, \boldsymbol{v}) = u_0(\boldsymbol{x}, \boldsymbol{v}) \exp\left(- \int_0^t v\sigma_t\left(\boldsymbol{x} + \boldsymbol{v}\alpha, \alpha, \boldsymbol{v}\right) \, \mathrm{d}\alpha\right)$$
$$+ \int_0^t \int v\sigma_s\left(\boldsymbol{x} + \boldsymbol{v}s, s, \boldsymbol{v}\right) u\left(\boldsymbol{x} + \boldsymbol{v}s, s, \boldsymbol{v}'\right) e^{-\int_s^t v\sigma_t(\boldsymbol{x}+\boldsymbol{v}\alpha, \boldsymbol{v}) \, \mathrm{d}\alpha} P\left(\boldsymbol{x} + \boldsymbol{v}s, s, \boldsymbol{v}, \boldsymbol{v}'\right) \, \mathrm{d}\boldsymbol{v}' \, \mathrm{d}s$$

After a variable change, we obtain:

$$u(\boldsymbol{x}, t, \boldsymbol{v}) = u_0(\boldsymbol{x} - \boldsymbol{v}t, \boldsymbol{v}) \exp\left(- \int_0^t v\sigma_t\left(\boldsymbol{x} - \boldsymbol{v}(t - \alpha), \alpha, \boldsymbol{v}\right)\right)$$
$$+ \int_0^t \int v\sigma_s\left(\boldsymbol{x} - \boldsymbol{v}(t - s), s, \boldsymbol{v}\right) u\left(\boldsymbol{x} - \boldsymbol{v}(t - s), s, \boldsymbol{v}'\right)$$
$$e^{-\int_s^t v\sigma_t(x - \boldsymbol{v}(t-\alpha), \boldsymbol{v}) \, \mathrm{d}\alpha} P\left(\boldsymbol{x} - \boldsymbol{v}(t - s), s, \boldsymbol{v}, \boldsymbol{v}'\right) \, \mathrm{d}\boldsymbol{v}' \, \mathrm{d}s$$

The integral form of the Boltzmann equation

The integral representation of the transport equation is then provided by:

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

Problem: the solution depends on its own integral!
↳ Let’s introduce a recursive numerical MC scheme!

Semi-analog scheme

For the semi-analog scheme, we introduce the probability measure of the interaction time:

$$f_\tau(\boldsymbol{x}, t, \boldsymbol{v}, s)\, \mathrm{d}s = 1_{[0,\infty[}(s)\, v\sigma_t(\boldsymbol{x} - \boldsymbol{v}s, t - s, v) e^{-\int_0^s v\sigma_t(\boldsymbol{x} - \boldsymbol{v}\alpha, t-\alpha, v)\, \mathrm{d}\alpha}\, \mathrm{d}s$$

for all $(\boldsymbol{x}, t, \boldsymbol{v}) \in D \times (0, T) \times \mathbb{R}^3$

We introduce the specified random variables:

$$\begin{cases} \tau \text{ with probability measure } f_\tau(\boldsymbol{x}, t, \boldsymbol{v})\ \mathrm{d}s, \\ \boldsymbol{V}' \text{ with probability measure } P^s_{\boldsymbol{V}'}(\boldsymbol{x}, t, s, \boldsymbol{v}, \boldsymbol{v}')\ \mathrm{d}v' \end{cases}$$

Expression of the solution

We found the following **expectation** value:

$$u(\mathbf{x}, t, \mathbf{v}) = \mathbb{E}\left[1_{[t,\infty[}(\tau)\, u_0(\mathbf{x} - \mathbf{v}t, \mathbf{v}) + 1_{[0,t[}(\tau)\, \frac{\sigma_s(\mathbf{x} - \mathbf{v}\tau, t - \tau, \mathbf{v})}{\sigma_t(\mathbf{x} - \mathbf{v}\tau, t - \tau, \mathbf{v})} u(\mathbf{x} - \mathbf{v}\tau, t - \tau, \mathbf{V}')\right]$$

We seek solutions that possess this specific structure:

$$u_p(\mathbf{x}, t, \mathbf{v}) = w_p(t)\, \delta_x(\mathbf{x}_p(t))\, \delta_{\mathbf{v}}(\mathbf{v}_p(t))$$

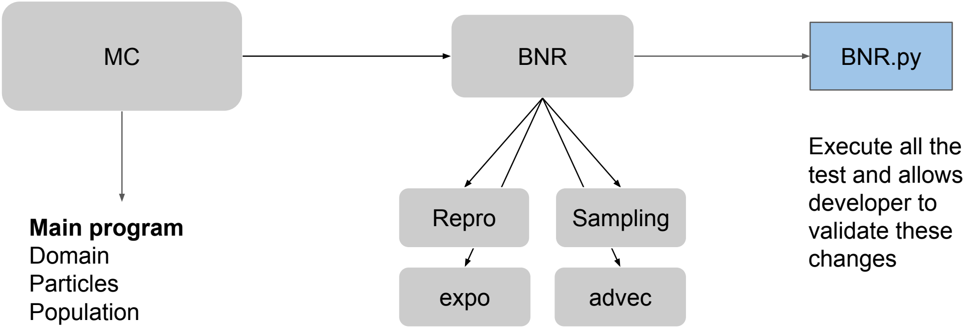
Replacing u_p in the equation yields:

$$\begin{cases} w_p(t) = 1_{[0,\infty[}(\tau) w_p(0) + 1_{[0,t[}(\tau) \dfrac{\sigma_s}{\sigma_t}\Big(x\mathbf{x}_p(t - \tau), t - \tau, \mathbf{v}_p(t - \tau)\Big)\, w_p(t - \tau), \\ \mathbf{x}_p(t) = 1_{[0,\infty[}(\tau)(\mathbf{x}_0 - \mathbf{v}t) + 1_{[0,t[}(\tau)(\mathbf{x}_{t-\tau} - \mathbf{v}\tau), \\ \mathbf{v}_p(t) = 1_{[0,\infty[}(\tau)\mathbf{v} + 1_{[0,t[}(\tau)\mathbf{V}'. \end{cases}$$

Monte Carlo Particle Transport Algorithm

Let $u(\boldsymbol{x}, t, \boldsymbol{v}) \leftarrow 0$;
for $p \in [\![1; N_{MC}]\!]$ **do**
  set $s_p = t$
  set $\boldsymbol{x}_p = \boldsymbol{x}$
  set $\boldsymbol{v}_p = \boldsymbol{v}$
  set $w_p(t) = N_{MC}$
  while $s_p > 0$ and $w_p > 0$ **do**
    if $\boldsymbol{x}_p \notin D$ **then**
      apply_BCs$(\boldsymbol{x}_p, s_p, \boldsymbol{v}_p)$
    end if
    Sample $\tau \rightsquigarrow f_\tau(\boldsymbol{x}_p, s_p, \boldsymbol{v}_p, s)\,ds$
    if $\tau > s_p$ **then** ←Census/Contribution
      $\boldsymbol{x}_p \leftarrow \boldsymbol{x}_p + s_p \boldsymbol{v}_p$
      $s_p \leftarrow 0$
      $u(\boldsymbol{x}, t, \boldsymbol{v}) += w_p u_0(\boldsymbol{x}_p, \boldsymbol{v}_p)$
    else ←Scattering/Collision
      $w_p \leftarrow \frac{\sigma_s(\boldsymbol{x}_p, s_p - \tau, \boldsymbol{v}_p)}{\sigma_t(\boldsymbol{x}_p, s_p - \tau, \boldsymbol{v}_p)} w_p$
      Sample $\boldsymbol{v}_p \rightsquigarrow P^s_{\boldsymbol{v}'}(\boldsymbol{x}_p, s_p, \tau, \boldsymbol{v}_p, \boldsymbol{v}')\,d\boldsymbol{v}'$
      $\boldsymbol{x}_p \leftarrow \boldsymbol{x}_p + \boldsymbol{v}_p \tau$
      $s_p \leftarrow s_p - \tau > 0$
    end if
  end while
end for

Architecture of the code



Main program
Domain
Particles
Population
Parameters

Different test using the main program

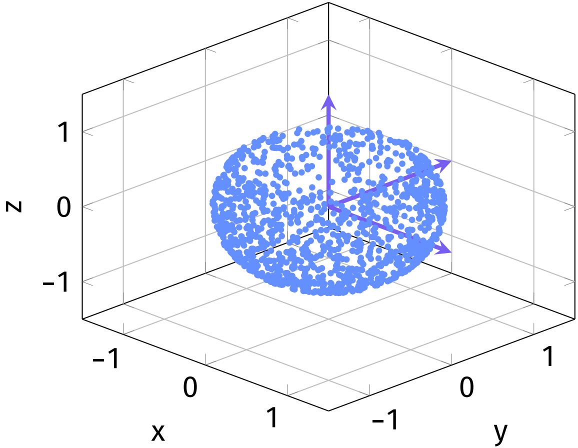
Execute all the test and allows the developer to validate these changes

Samplings of τ and $\boldsymbol{v}_p$

The variables are sampled as follows:

$$\tau = -\frac{\log U}{\sigma_t(\boldsymbol{x}_p, s_p, \boldsymbol{v}_p)|\boldsymbol{v}_p|} \text{ where } U \rightsquigarrow U[0;1].$$

$\boldsymbol{v}_p$ is sampled uniformly on the 3D unit sphere.



1D results

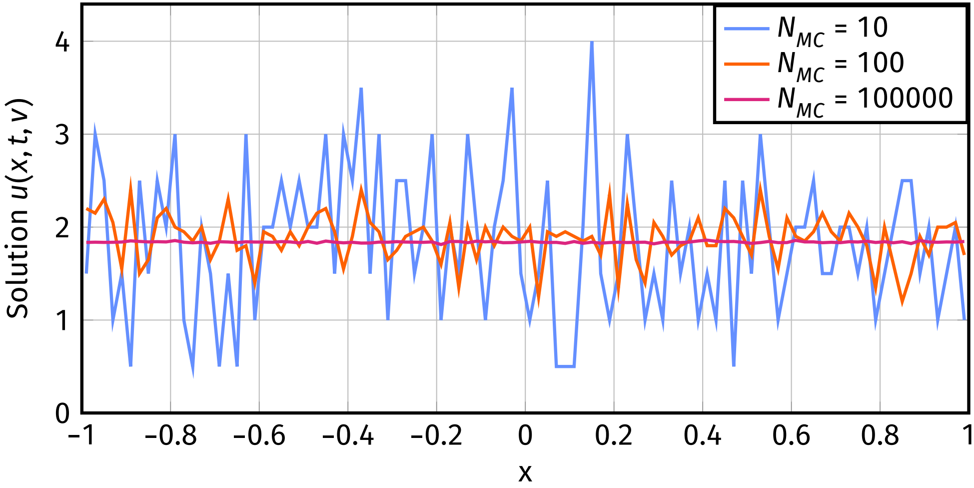


Figure 1: Solution refinement with N_{MC} in 1D.

1D results

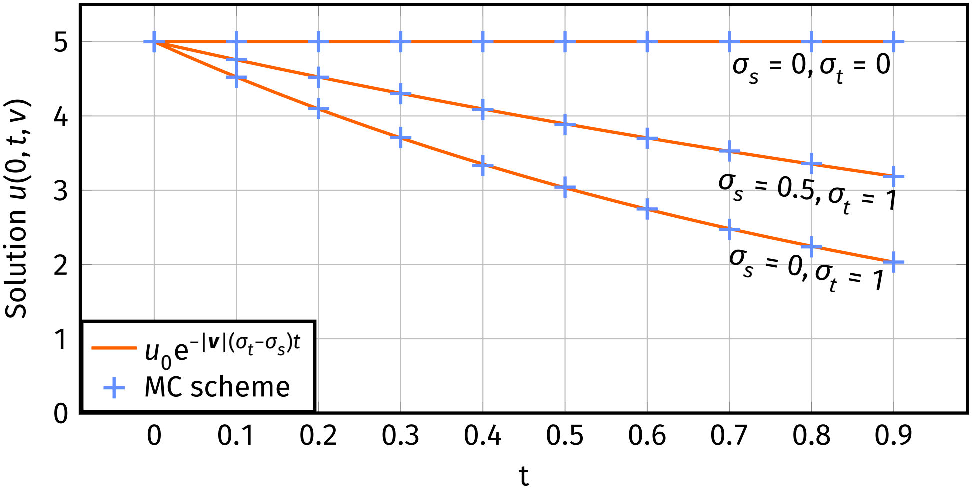


Figure 2: Solution in 1D over time with an intermediate regime.

1D results

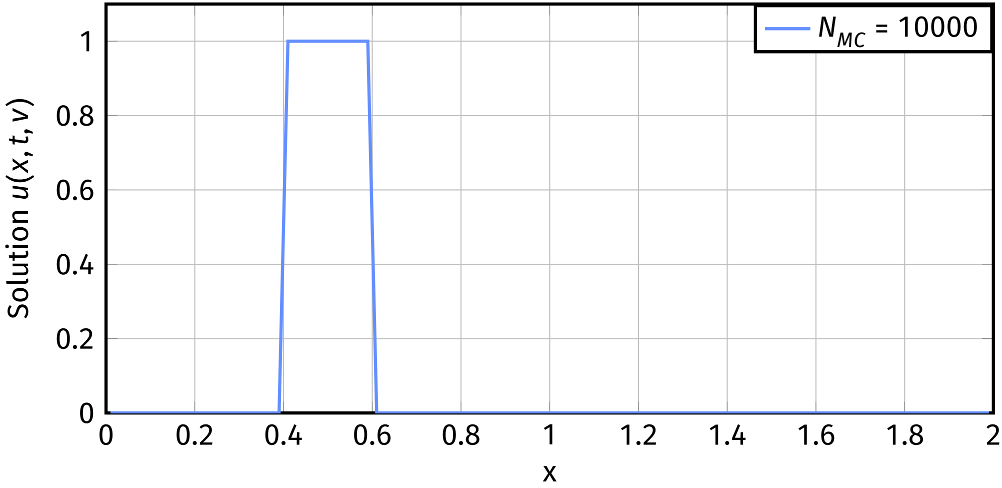
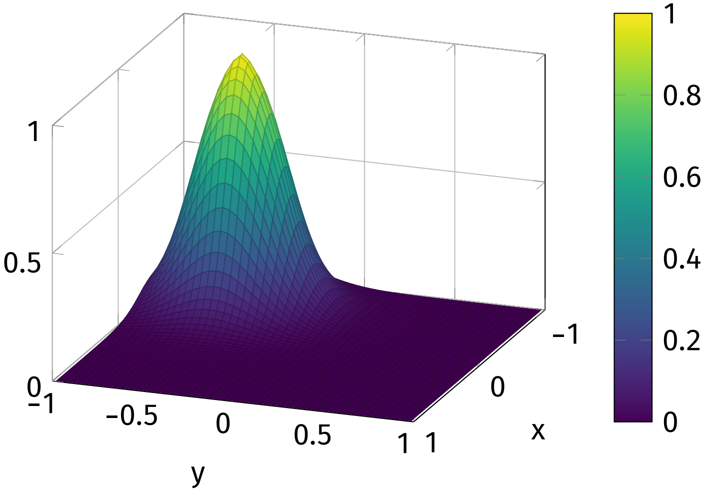


Figure 3: Solution in 1D with $\sigma_s = \sigma_t = 0$.

2D Transparent medium

When $\sigma_t = \sigma_s = 0$, the explicit solution is given by:

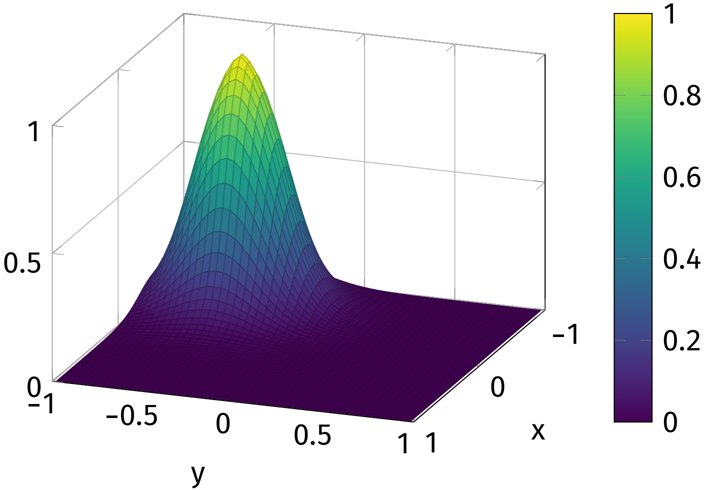
$$u(\boldsymbol{x}, t, \boldsymbol{v}) = u_0(\boldsymbol{x} - \boldsymbol{v}t, \boldsymbol{v})$$



2D Absorbing medium

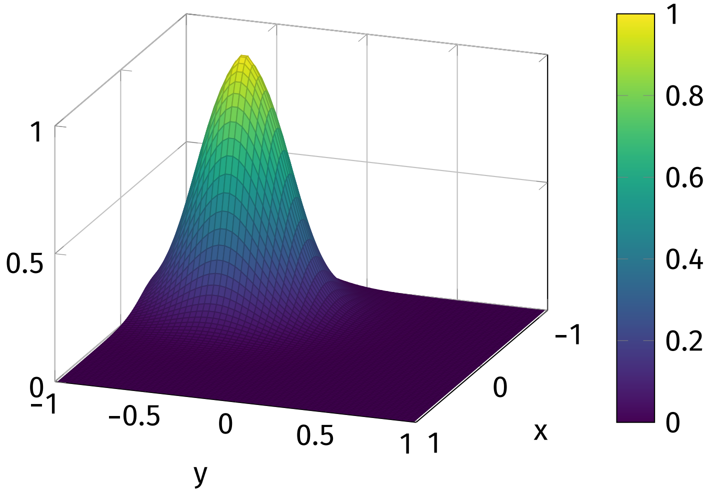
When $\sigma_s = 0$ and $\sigma_t = 1$, an exact solution is known:

$$u(\mathbf{x}, t, \mathbf{v}) = \left(u_0(\mathbf{x} - t\mathbf{v}, \mathbf{v})\right) \mathrm{e}^{-\int_0^t v\sigma_t(\mathbf{x}+(t-\tau)\mathbf{v},\tau,\mathbf{v})\,\mathrm{d}\tau}$$



2D Absorption-scattering medium

With $\sigma_s = 0.5$ and $\sigma_t = 1$: no exact solution is known.



Conclusion

Main interests of MC schemes:

- uses recursive formulation,
- 2D/3D w/o extra cost,
- multiple schemes (backward here for radiation/forward, analog/semi-analog/non-analog) depending on the application,
- immediate parallelization.

Possible improvements:

- elaborate more tests,
- implement more boundary conditions,

Website

Homepage Bibliography Numerical Results Download

Solving the linear Boltzmann equation using Monte-Carlo methods

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

Summary

The study of particle transport in various physical systems plays a pivotal role in understanding complex phenomena across diverse scientific domains. One fundamental equation that governs the behavior of particles is the linear Boltzmann equation, which describes the evolution of particle distribution in phase space. This equation has broad applications, ranging from nuclear reactor physics and radiation shielding design to medical imaging and astrophysics.

In this project, we delve into the numerical solution of the linear Boltzmann equation, leveraging the powerful Monte Carlo method. Monte Carlo methods have proven to be versatile and efficient tools for tackling complex problems in physics, finance, and engineering. By applying these methods to the linear Boltzmann equation, we aim to develop a computational framework that provides accurate and reliable solutions to intricate particle transport problems.

Furthermore, we introduce a semi-analog Monte Carlo scheme as a method to solve our problem. Ultimately, this project aims to contribute to the understanding and application of the linear Boltzmann equation, offering a valuable computational tool for solving real-world problems in particle transport.

Contents

On this page, readers can find the resources derived from the conducted research and the corresponding numerical outcomes. Additionally, the report and the presentation for this project is available on this page, ready for download.

For further resources, only one adress:

Resolution of the linear Boltzmann equation by Monte Carlo method

References

Després, Bruno, François Golse, and Grégoire Allaire (2018). *Transport et diffusion*. OCLC: 1107840142. Palaiseau: École polytechnique. ISBN: 978-2-7302-1675-3.

Lapeyre, Bernard, Étienne Pardoux, and Rémi Sentis (1998). *Méthodes de Monte-Carlo pour les équations de transport et de diffusion*. Mathématiques et applications 29. Berlin: Springer. ISBN: 978-3-540-63393-8.

Poëtte, Gaël (Sept. 2019). "CONTRIBUTION TO THE MATHEMATICAL AND NUMERICAL ANALYSIS OF UNCERTAIN SYSTEMS OF CONSERVATION LAWS AND OF THE LINEAR AND NONLINEAR BOLTZMANN EQUATION". Habilitation à diriger des recherches. Université de Bordeaux 1. URL: `https://hal.science/tel-02288678`.