Resolution of the linear Boltzmann equation by Monte Carlo method

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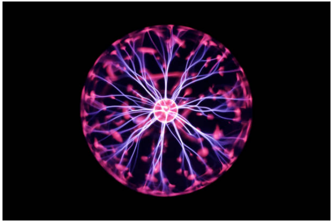
Fields of Application for the Boltzmann Equation



Plasma physics

Fluid dynamic

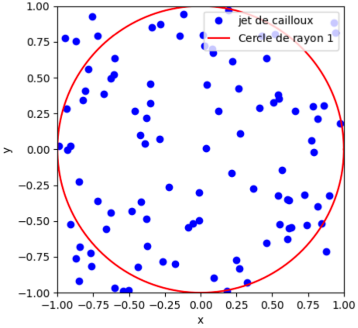
Astrophysics

Rarefied Gas Dynamics

Example of the calculation of π

We draw a circle with a radius of $r = 1$ inscribed in a square of side length 2. We throw stones in the air and count the number of stones within the circle. An estimate of π is given by

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



Special cas with Absorption and Source Term

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:

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

In this case, if $u_0 \in \mathcal{C}^1(\mathbb{R}^n)$, then using the method of characteristics, we can still demonstrate that the Cauchy problem has a unique solution $u \in \mathcal{C}^1(\mathbb{R}_+ \times \mathbb{R}^n)$. This solution is given as follows:

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

Boltzmann equation

This work is based on **noauthor_transport_2018**, **poette:tel-02288678** & **lapeyre_methodes_1998**.
The transport equation in an infinite medium with its corresponding deterministic collisional component can be expressed as:

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

Where

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

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

Variable change

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

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

Equation Transformation with Multiplication and Integration

After multiplying both sides of the equation by:

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

Following that, we obtain

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

Integration of the equation

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

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

After a variable change, we obtain:

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

Re-expression of the exponential

We also have:

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

The integral form of the Boltzmann equation

Then the integral representation of the transport equation is provided by:

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

Problem : the solution depends on its own integral ! $\longrightarrow$ Let's introduce a numerical MC scheme !

Semi-analog scheme

Developing a Monte Carlo scheme involves introducing random variables and their associated probability measure to express the equation as an expectation. The choice of this set of random variables is not unique, leading to different Monte Carlo schemes with distinct properties.

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

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

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

We introduce the specified random variables corresponding to the previously identified probability measures.

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

Expression of the solution

We found the following expectation value:

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

Essentially, the process of constructing a Monte Carlo scheme is based on searching for solutions of expectation that possess this specific structures:

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

Replacing u_p in the equation yields:

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

Monte Carlo Particle Transport Algorithm

Let $u(\boldsymbol{x}, t, \boldsymbol{v}) \leftarrow 0$;
for $p \in [\![1; \mathrm{N}_{\mathrm{MC}}]\!]$ **do**
  set $s_p = t$
  set $\boldsymbol{x}_p = \boldsymbol{x}$
  set $\boldsymbol{v}_p = \boldsymbol{v}$
  set $w_p(t) = \mathrm{N}_{\mathrm{MC}}$
  while $s_p > 0$ and $w_p > 0$ **do**
    if $\boldsymbol{x}_p \notin \mathcal{D}$ **then**
      apply_BCs$(\boldsymbol{x}_p, s_p, \boldsymbol{v}_p)$
    end if
    $\tau \leftarrow \mathrm{P} \rightsquigarrow f_\tau(\boldsymbol{x}_p, s_p, s, \boldsymbol{v}_p)\,\mathrm{d}s$
    if $\tau > s_p$ **then**
      $\boldsymbol{x}_p \leftarrow \boldsymbol{x}_p + s_p \boldsymbol{v}_p$
      $s_p \leftarrow 0$
      $u(\boldsymbol{x}, t, \boldsymbol{v}) += w_p u_0(\boldsymbol{x}_p, \boldsymbol{v}_p)$
    else
      $w_p \leftarrow \frac{\sigma_s(\boldsymbol{x}_p, s_p - \tau, \boldsymbol{v}_p)}{\sigma_t(\boldsymbol{x}_p, s_p - \tau, \boldsymbol{v}_p)} w_p$
      $\boldsymbol{v}_p \leftarrow \mathbf{V}' \rightsquigarrow \mathrm{P}_{\mathbf{V}'} s(\boldsymbol{x}_p, s_p, \tau, \boldsymbol{v}_p, \boldsymbol{v}')\,\mathrm{d}\boldsymbol{v}'$
      $\boldsymbol{x}_p \leftarrow \boldsymbol{x}_p + \boldsymbol{v}_p \tau$
      $s_p \leftarrow s_p - \tau > 0$
    end if
  end while
end for

Sampling of τ and v_p

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

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

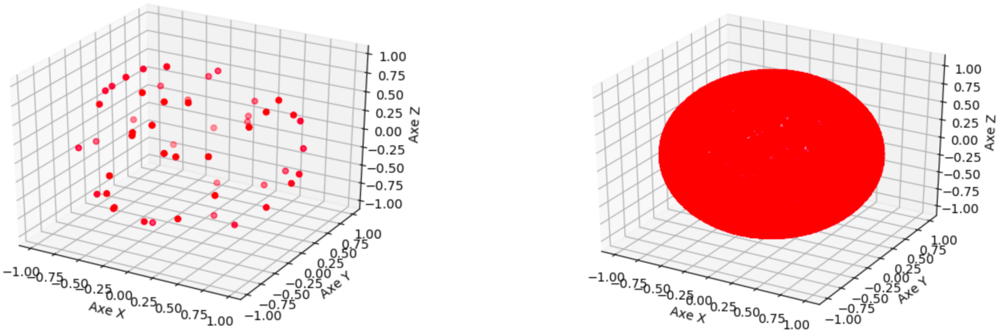


Figure 1: Plot of the sampling of $\boldsymbol{v}_p$ for nMC $= 50$ and 10000 points.

1D results

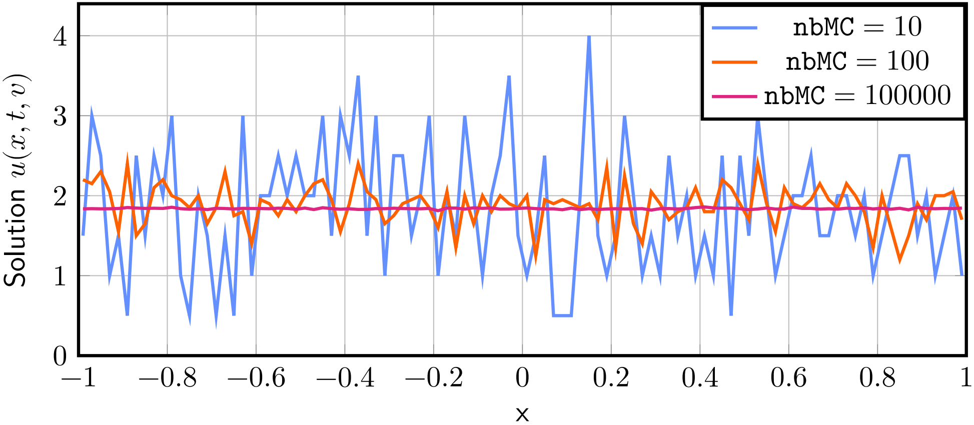


Figure 2: Solution refinement with nbMC in 1D.

1D results

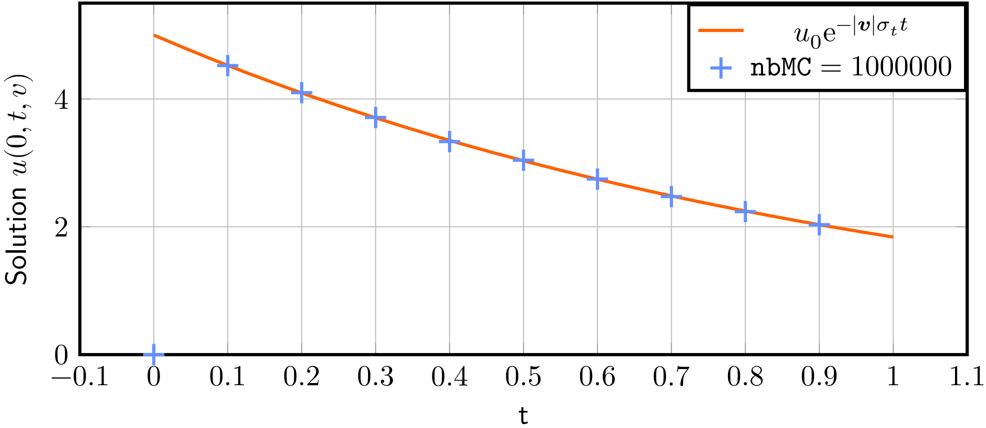


Figure 3: Solution in 1D with $\sigma_s = 0$.

1D results

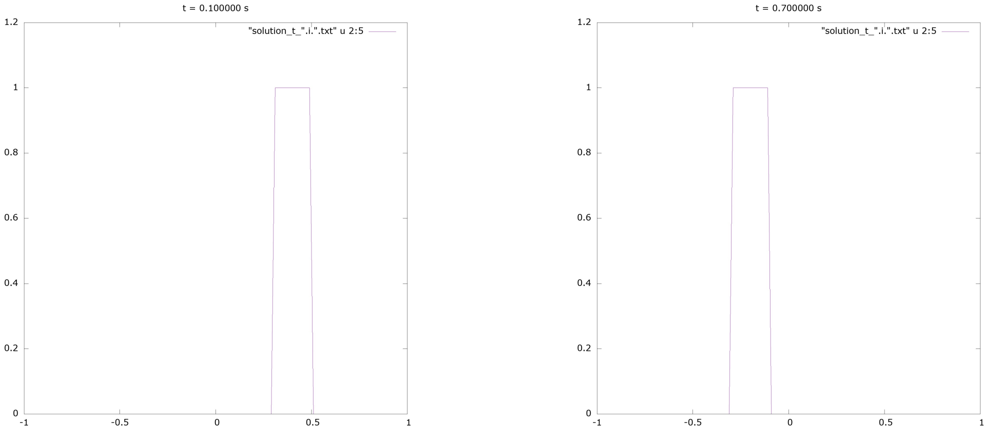


Figure 4: Solution in 1D with $\sigma_s = \sigma_t = 0$.

2D result

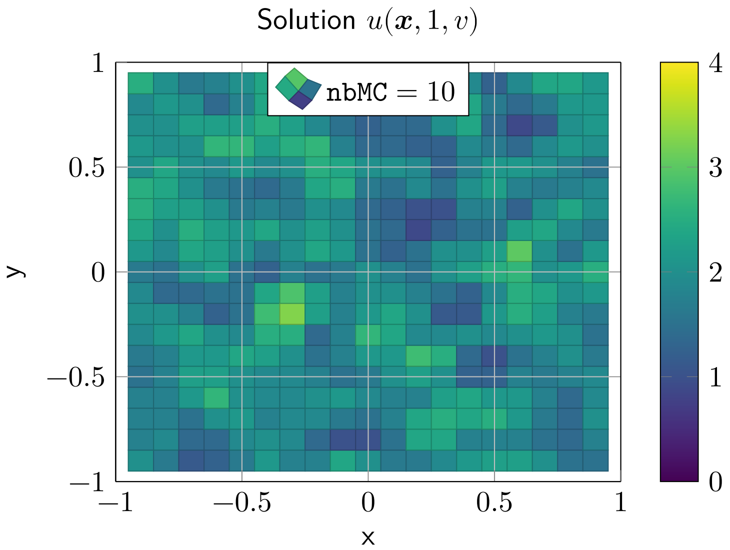


Figure 5: Solution in 2D with 20×20 points.

References