

Resolution of the linear Boltzmann equation by Monte Carlo method

Antoine Boucher
Gabriel Rodiere
Clément Aumonier
Guillaume Doyen
Khaoula El Maddah
Supervisor : Gael Poette

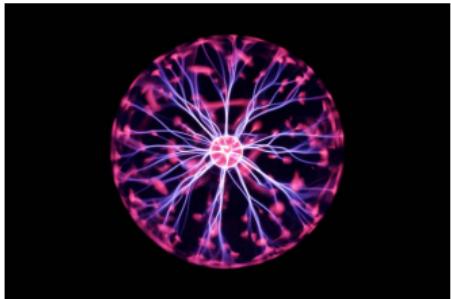
Wednesday, 31st January 2024



Table of contents

- 1 Introduction
- 2 Monte Carlo method
- 3 The existence and uniqueness of the solution
- 4 Resolution of the equation
- 5 The semi-analog MC scheme
- 6 Numerical results
- 7 Tests
- 8 Conclusion

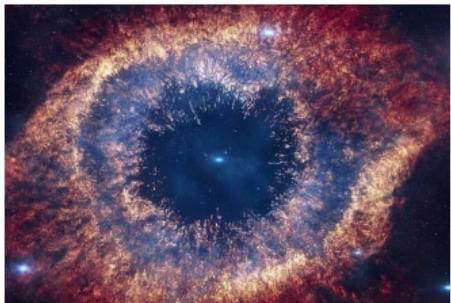
Fields of Application for the Boltzmann Equation



Plasma physics



Fluid dynamic



Astrophysics



Rarefied Gas Dynamics

What is Monte Carlo?

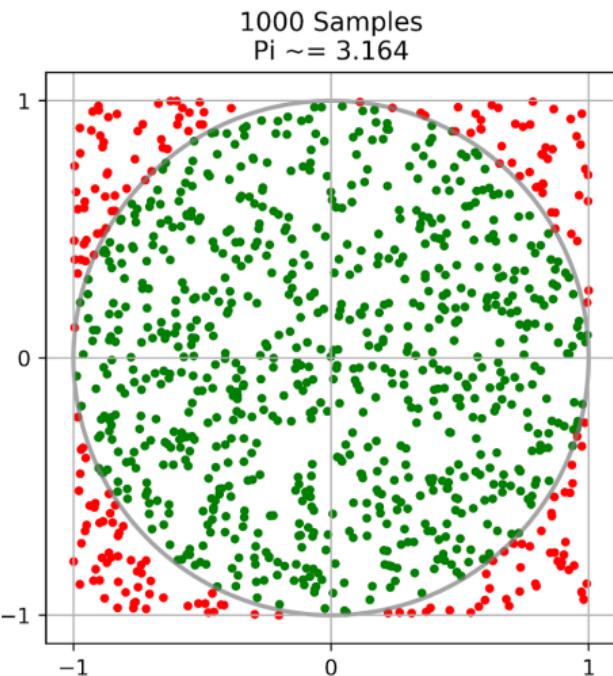


Stanislaw Ulam and Nicholas Metropolis



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 :

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

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

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

Boltzmann equation

The transport equation can be expressed as:

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

Where

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

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 $\mathbf{x} + \mathbf{v}s$. It transforms into:

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

After multiplying both sides of the equation by:

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

Following that, we obtain:

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

Integration of the equation

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

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

After a variable change, we obtain:

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

The integral form of the Boltzmann equation

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

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

Problem : the solution depends on its own integral !

↳ Let's introduce a numerical recursive MC scheme !

Semi-analog scheme

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

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

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

We introduce the specified random variables :

$$\begin{cases} \tau \text{ with probability measure } f_\tau(\mathbf{x}, t, \mathbf{v}) ds, \\ \mathbf{v}' \text{ with probability measure } P_{\mathbf{v}'}^s(\mathbf{x}, t, s, \mathbf{v}, \mathbf{v}') dv' \end{cases}$$

Expression of the solution

We found the following **expectation** value:

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

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:

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

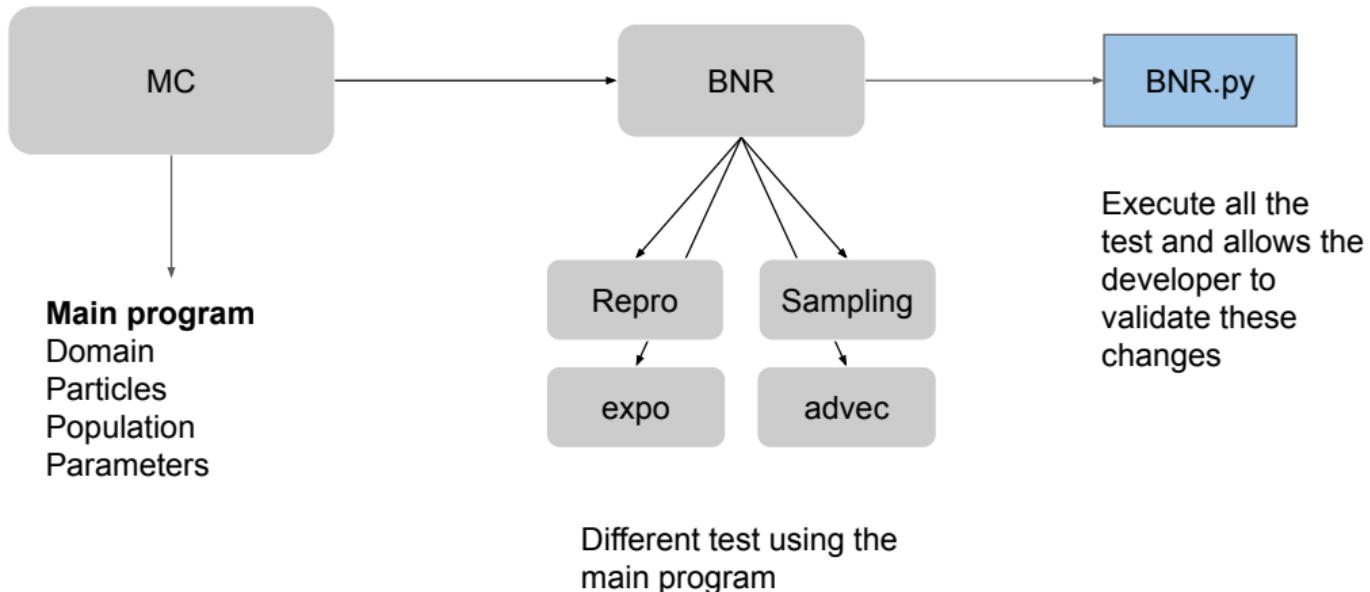
Monte Carlo Particle Transport Algorithm

```

1: Let  $u(\mathbf{x}, t, \mathbf{v}) \leftarrow 0$ ;
2: for  $p \in [1; N_{MC}]$  do
3:   set  $s_p = t$ 
4:   set  $\mathbf{x}_p = \mathbf{x}$ 
5:   set  $\mathbf{v}_p = \mathbf{v}$ 
6:   set  $w_p(t) = N_{MC}$ 
7:   while  $s_p > 0$  and  $w_p > 0$  do
8:     if  $\mathbf{x}_p \notin D$  then
9:       apply_BCs( $\mathbf{x}_p, s_p, \mathbf{v}_p$ )
10:      end if
11:      Sample  $\tau \sim f_\tau(\mathbf{x}_p, s_p, \mathbf{v}_p, s)$  ds
12:      if  $\tau > s_p$  then           ← Census/Contribution
13:         $\mathbf{x}_p \leftarrow \mathbf{x}_p + s_p \mathbf{v}_p$ 
14:         $s_p \leftarrow 0$ 
15:         $u(\mathbf{x}, t, \mathbf{v})^+ = w_p u_0(\mathbf{x}_p, \mathbf{v}_p)$ 
16:      else                      ← Scattering/Collision
17:         $w_p \leftarrow \frac{\sigma_s(\mathbf{x}_p, s_p - \tau, \mathbf{v}_p)}{\sigma_t(\mathbf{x}_p, s_p - \tau, \mathbf{v}_p)} w_p$ 
18:        Sample  $\mathbf{v}' \sim P_{\mathbf{v}'}^s(\mathbf{x}_p, s_p, \tau, \mathbf{v}_p, \mathbf{v}')$  d $\mathbf{v}'$ 
19:         $\mathbf{x}_p \leftarrow \mathbf{x}_p + \mathbf{v}_p \tau$ 
20:         $s_p \leftarrow s_p - \tau > 0$ 
21:      end if
22:    end while
23:  end for

```

Architecture of the code



Samplings of τ and \mathbf{v}_p

The variables are sampled as follows :

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

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

1D results

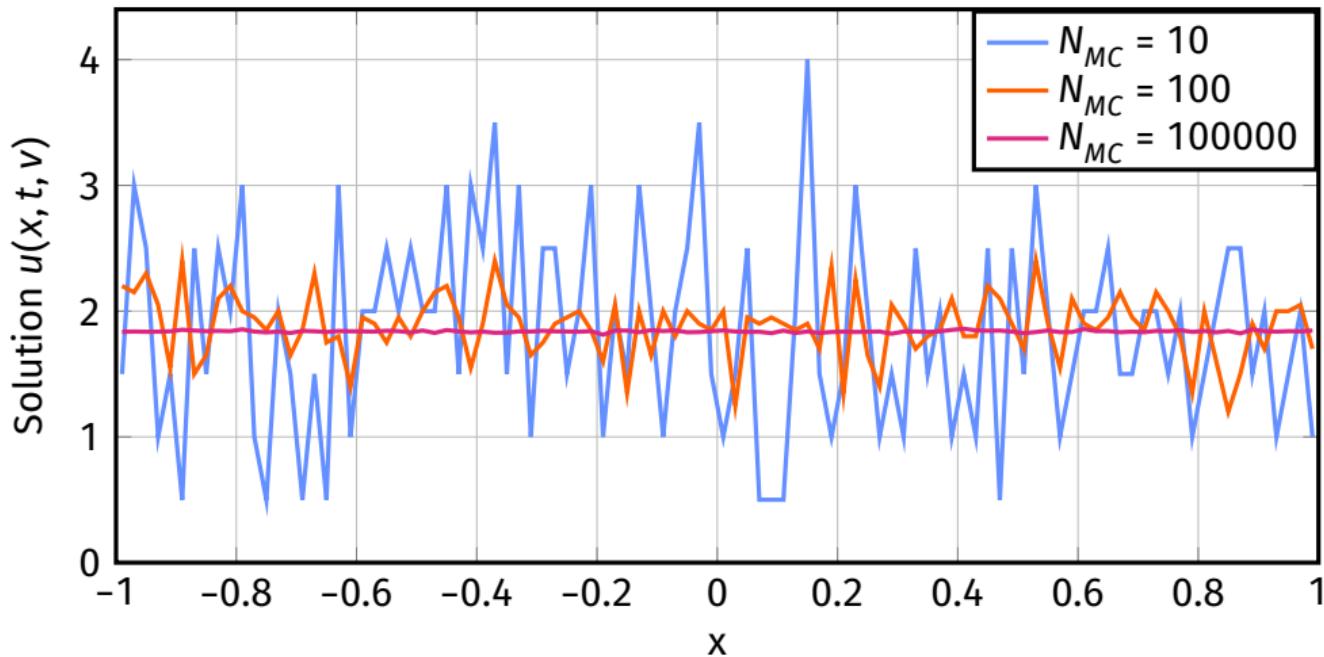
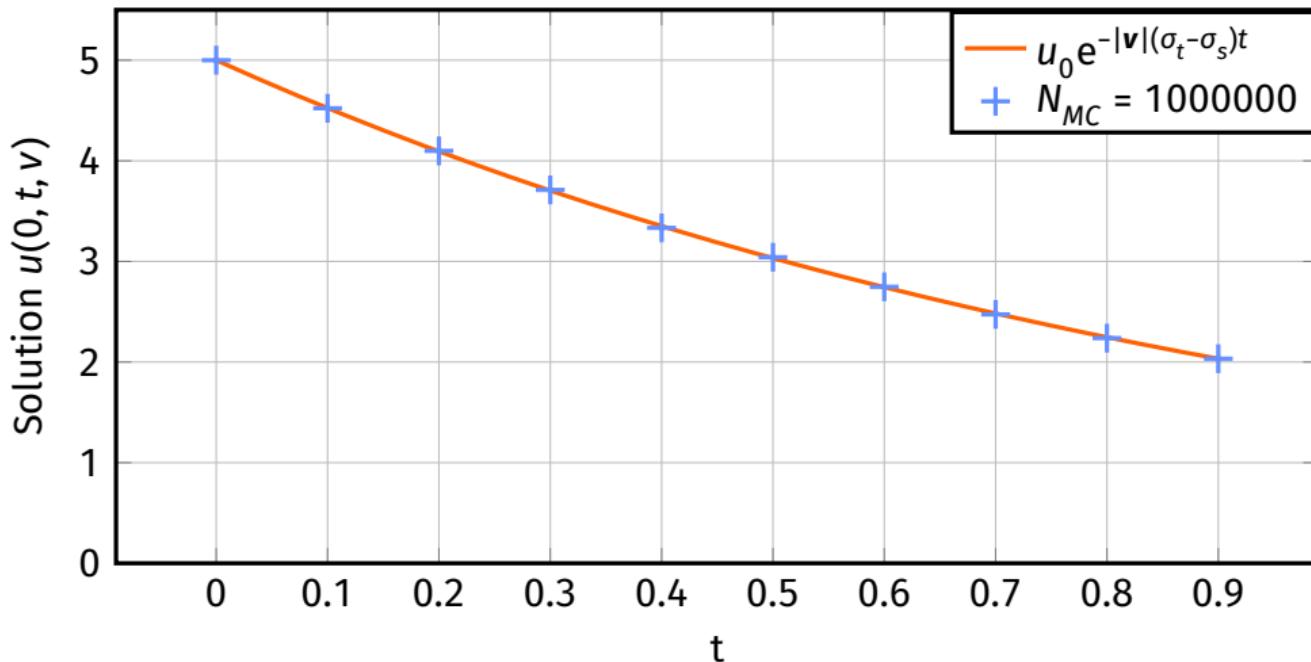


Figure 1: Solution refinement with N_{MC} in 1D.

1D results

Figure 2: Solution in 1D with $\sigma_s = 0$.

1D results

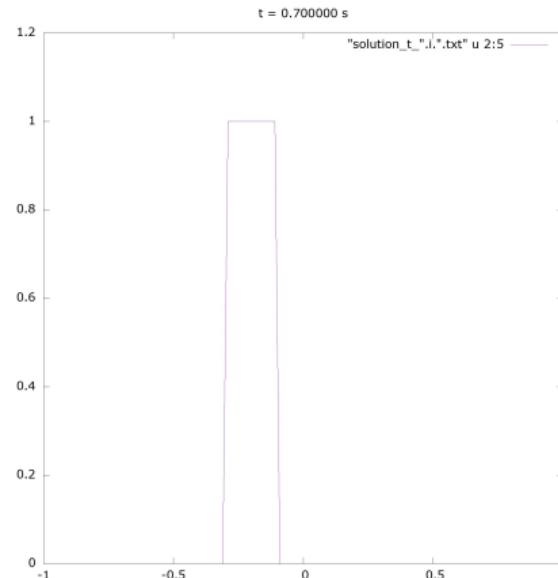
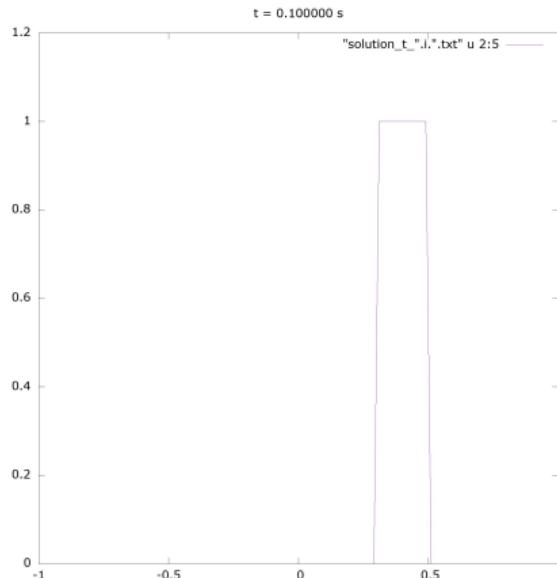


Figure 3: Solution in 1D with $\sigma_s = \sigma_t = 0$.

Advection

When the $\sigma_S = \sigma_T = 0$, the explicit solution is given by:

$$u(x, t, w) = u_0(x - vwt, w)$$

Absorption

The exponential test used a computation of the main program with σ_t and σ_s constant. With this configuration we can calculate the integrale of the exact solution as :

$$\int_{\Omega} U(t) d_x = \int_{\Omega} U_0 d_x e^{-v(\sigma_t - \sigma_s)t}$$

When the $\sigma_s = 0$ and $\sigma_T = 1$.

Transparency scattering

When the $\sigma_S = 0.5$ and $\sigma_T = 1$

Conclusion

- extension to 2d/3d easy
- use of recursivity
- Possibility to change scheme (backward/forward, analog/semi-analog/non-analog) to compare them
- Parallelization ;
- elaborate more tests ;
- Boundary conditions
- Site ;

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>.