COMPUTING THE FIRST EIGENELEMENTS OF SOME LINEAR OPERATORS USING A BRANCHING MONTE CARLO METHOD

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Abstract. In earlier works, we have developed a Monte Carlo method to compute the first eigenvalue of linear operators, which is based on the simulation of exit times. In this paper, we show how to use a branching method to handle in a better way the simulation of large exit times. We show furthermore that this new method provides naturally an estimation of the first eigenfunction of the adjoint operator. Numerical examples are given on the Laplace operator and on homogeneous neutron transport operators.

1. Introduction

The first eigenvalue of the neutron transport operator and of diffusion operator in a bounded domain gives often some relevant physical information regarding the large time behavior of the solutions of the associated Cauchy problems. In the case of diffusion operators (*e.g.* Laplace), this eigenvalue determines the speed of convergence toward the steady-state, which is the rate of absorption by the boundary in the probabilistic framework. In addition, the first eigenvalue also appears in some problems related to stochastic analysis: See [DV76] or [IW89, Chap. VI, § 8] for example. In the case of the neutron transport operator, the sign of this first eigenvalue determines if the system is sub-critical or super-critical [DL87b].

The numerical computation of the first eigenvalue and eigenfunction by a deterministic method requires to handle very large matrices obtained after a refined enough discretization of the operator. S. Maire and D. Talay [MT06] have shown how to estimate the first eigenvalue of the neutron transport operator by combining the Feynman-Kac representation of the solution of the relative Cauchy problem and the spectral expansion of its solution, following similar ideas in the field of

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particles methods (see [Kal81] for example). In the case of homogeneous neutron transport operators, this method reduces to the computation of the first time τ a particle exits from the domain. The idea is to estimate $F(t) = \mathbb{P}_x[\tau < t]$ when all the particles start from a single point x and to use the approximation $F(t) \sim C\exp(\lambda_1 t)$ for t large enough where $\lambda_1 < 0$ is the first eigenvalue sought. The eigenvalue λ_1 is then evaluated using a linear regression. This method was adapted to the Laplace operator in [LM07] and could be suitable for more general diffusion operators. In opposite to the neutron transport problem for which exact simulation schemes exist, the choice of a simulation scheme is crucial in this case. In the paper [LM07], we have also promoted the *random walk on squares* [MT99, CL02] and the *random walk on rectangles* [DL06] methods as the best ones for a polygonal domain D.

We consider the Cauchy problem

$$\frac{\partial u(t,x)}{\partial t} = Au(t,x) + c(x)u(t,x) \text{ with } u(0,\cdot) = u_0 \tag{1}$$

in a bounded domain D, where A is a linear operator with absorption on ∂D and c appears to be a gain or loss factor. In both cases, the solution u admits a Feynman-Kac representation

$$u(t,x) = \mathbb{E}_x\left[u_0(X_t)\exp\left(\int_0^t c(X_s)\,\mathrm{d}s\right)\mathbf{1}_{\tau>t}\right] \tag{2}$$

where $(X, \mathbb{P}_x)$ is the Markov process associated to the operator A and $\tau = \inf\{t \geq 0 \,|\, X_t \notin D\}$ is the first exit time from D. For instance, if A is the Laplace operator, *i.e.* $A = \frac{1}{2}\triangle$, the process X is just the Brownian motion. The processes related to transport operators are described in Section 4. We consider only homogeneous neutron transport problems, that is c is constant, and we choose $u_0 = 1$. The solution u writes

$$u(t,x) = \exp(ct)\mathbb{P}_x[t < \tau], \tag{3}$$

so that the value of $u(t,x)$ can be deduced from the distribution function of the first exit time τ. In the case of the Laplace operator, we also let $u_0 = 1$ and we set $c = 0$, so that the solution is just $u(t,x) = \mathbb{P}_x[t < \tau]$.

From an analytical point of view, the operator A generates a semigroup which has a density $p(t,x,y)$ with respect to the Lebesgue measure, and the solution u to (1) with a constant factor c may be written

$$u(t,x) = \exp(ct)\int_D p(t,x,y)u_0(y)\,\mathrm{d}y.$$

In both cases, an indirect application of the Kreĭn-Rutman theorem ([DL87a, Appendix of Chap. VIII], [Pin96a]) implies that there exists an eigenvalue λ_1 such that any element λ of its spectrum has a real part

smaller than λ_1. In addition, this eigenvalue has multiplicity one and its associated eigenfunction does not vanish on the open domain D.

Throughout this paper, we assume that when c is constant, the solution $u(t,x)$ may be expanded as

$$u(t,x) = \langle \varphi_1^*, u_0 \rangle \varphi_1(x) \exp((c+\lambda_1)t) + R(t,x) \tag{4}$$

with $R(t,x) = \mathrm{o}(\exp(\lambda_1 t))$, $\langle f, g \rangle = \int_D f(x)g(x)\,\mathrm{d}x$, φ_1^* is the first eigenfunction of the adjoint A^* of A such that $\varphi_1^* > 0$ and $\langle \varphi_1^*, \varphi_1 \rangle = 1$, and the initial condition u_0 is in a reasonable space of functions that contains the constant functions over the domain D. The expansion (4) holds for most of neutron transport operators used in practice, for self-adjoint operators with a compact resolvent such as the Laplace operator on a bounded domain, and more generally, for a large class of diffusion operators.

Using (3) and (4), the distribution function $F(t) = \mathbb{P}_x[\tau < t]$ of the first exit time τ of D is then expanded as

$$F(t) = 1 - \mathbb{P}_x[t < \tau] = 1 - \exp(-ct)(\langle 1, \varphi_1^* \rangle \exp(\lambda_1 t)\varphi_1(x) + R(t,x)).$$

The idea now is to approximate $F(t)$ by an empirical distribution function obtained by simulating the first exit time τ. Thus, we have developed some statistical methods to get λ_1 from this empirical distribution function.

The problems we get for estimating λ_1 are the following: we need to estimate $F(t)$ for $t > T$ with T large enough such that the approximation $1 - F(t) \simeq C\exp((\lambda_1 - c)t)$ is fair enough. On the other hand, as we use an empirical distribution function $F_N(t)$ with N samples to estimate $F(t)$, the variance of $\log(1 - F_N(t))$ explodes as $t \to \infty$. A first idea is to estimate $F_N(t)$ at two times t_0 and t_1 [Mai01, MT06]. Another possible approach, developed in [LM07], is to find a window $[t_0, t_1]$ on which $F_N(t)$ is a good approximation of $F(t)$ in $[t_0, t_1]$. A last possibility is to note that for $t > t_0$ and $c = 0$, the exit time τ from D is distributed like an exponential random variable of parameter $-\lambda_1$. Standard estimators like the maximum likelihood can then be used.

The aim of this article is to improve the results of [MT06] and [LM07]. We propose a variance reduction scheme on the empirical approximation of $F(t)$ which is very easy to implement. As a byproduct of this method, we can also estimate the first eigenfunction φ_1^* of the adjoint A^* of A. As the Laplace operator is self-adjoint, this first eigenfunction is also the first eigenfunction of $\frac{1}{2}\triangle$. For the neutron transport operator, the adjoint is also a neutron transport operator, so that the first eigenvalue of A may be computed using our method on A^*.

This new method is based on a branching mechanism which has been used in many fields (see for example [DM04, DMG05, CDMLL06, La06a, La06a], ...). As we are interested in the estimation of the asymptotic behavior of $F(t)$ when t is large, we may restrict ourselves to

estimate

$$\frac{F(t)-F(T)}{1-F(T)} = \mathbb{P}_x[\tau < t \,|\, \tau \geq T]$$

for a fixed $T > 0$ and $t \geq T$. We assume that we know the distribution π_T of the stochastic process X_T starting at x. By the Markov property, for $t > T$,

$$\mathbb{P}_x[\tau < t | \tau \geq T] = \mathbb{P}_{\pi_T}[\tau < t] = \int_D \mathbb{P}_y[\tau < t] \, \mathrm{d}\pi_T(y).$$

The algorithm is the following: we fix $T > 0$ and we get an estimator $\widehat{\pi}_T$ of π_T using a Monte Carlo method. Then we simulate the first exit time τ from D for the process X with $\widehat{\pi}_T$ as initial distribution, and we compute λ_1 using the methods previously discussed in [MT06, LM07].

The number of particles we use to estimate the empirical distribution function of τ given $\{t > T\}$ is the same as the number of particles we use to estimate $\widehat{\pi}_T$. This approach compensates the absorption of particles by the boundary. We may need to estimate $\widehat{\pi}_{T_1}$, ..., $\widehat{\pi}_{T_k}$ at some times $T_1 < \ldots < T_N$ using a branching mechanism at each of these times in order to get a good approximation of $\widehat{\pi}_T$. Not only this provides a much better approximation of $F(t)$ — up to multiplication and additive constants — when t is large, but $\widehat{\pi}_T$ approximates the first eigenfunction of A^* when T is large enough.

2. Estimating the first eigenvalue and its associated eigenfunction

The idea of the algorithm is to launch N particles starting at a given point x up to a fixed time T_1 and to record the positions of the particles that are still alive at this time. Then, we start again simulating N particles using the empirical distribution of X_{T_1} given $\{\tau > T_1\}$ as initial distribution. From the Markov property, the particles have a distribution close to $\mathbb{P}_x[\cdot|\tau > T_1]$. We can then use several slices $T_2, \ldots, T_k$ and then get a good approximation of the behavior of the particle given $\{\tau > T_k\}$.

2.1. The algorithm.

Our algorithm is the following

- Fix some times $T_0 = 0 < T_1 < T_2 < \ldots < T_k$, a number N of samples and a point $x \in D$. Set $\widehat{\pi}_{T_0} = \delta_x$.
- For i from 0 to $k-1$ do
  - Using $\widehat{\pi}_{T_i}$ as the initial distribution, simulate N independent realizations $\{\mathsf{X}^{(j)}\}_{j=1,\ldots,N}$ of $X_{(T_{i+1}-T_i)\wedge\tau}$, where τ is the first exit time from D.
  - Let $N(i)$ be the subset of $\{1,\ldots,N\}$ of random variables such that $\mathsf{X}^{(j)}$ belongs to D. Set $\widehat{\pi}_{T_{i+1}} = \frac{1}{|N(i)|}\sum_{j\in N(i)} \delta_{\mathsf{X}^{(j)}}$.
- Using $\widehat{\pi}_{T_k}$ as the initial distribution, simulate N realizations $\{\mathsf{t}^{(j)}\}_{j=1,\ldots,N}$ of the first exit time τ from D.

- Estimate λ_1 from $\{\mathsf{t}^{(j)}\}_{j=1,\dots,N}$ and estimate φ_1^* from the the realizations $\{\mathsf{X}^{(j)}\}_{j=1,\dots,N(i)}$ of the position of $X_{T_{i+1}}$.

Of course, the quality of the result is sensitive to the choices of $T_1,\dots,T_k$, N, and in a smaller way, to the starting point x. Yet, as we have shown in [LM07], the quality of the method used to simulate τ and X_t is one of the main concern for the precision of the estimators.

2.2. **How to choose the final time slice?** To get a good estimate of the first eigenvalue, we should choose the times $T_1,\dots,T_k$ in an appropriate way, and T_k should be large enough. As it was already noted, the distribution of $(X_{t+T})_{t\geq 0}$ for T large enough is essentially given by the first eigenvalue and the first eigenfunction. In particular, the density of X_{T_i} given $\{T_i<\tau\}$ and $X_{T_{i+1}}$ given $\{T_{i+1}<\tau\}$ tends to converge to the first eigenfunction φ_1^* (normalized to be a density of probability). One can then test the L^2-difference between two successive densities. A simpler criterion is obtained by setting

$$p_i=\mathbb{P}[\tau>T_{i+1}|\tau\geq T_i]\simeq\varphi_1(x)\langle 1,\varphi_1^*\rangle\exp(\lambda_1(T_{i+1}-T_i))$$

when T_i is large and choosing the first i such that p_i is close to p_{i+1}.

2.3. **Estimating the first eigenvalue from the empirical distribution function.** We present now few possible estimators of λ_1 from the simulated values of the first exit time τ.

(a) Interpolation method. This method is very simple. It was originally introduced by one of the author in his thesis [Mai01, MT06] (see also [LM07]). Given two times t_0 and $t_1>t_0$, we estimate $F(t_0)$ and $F(t_1)$ from the Monte Carlo simulation, which gives $\widehat{F}(t_0)$ and $\widehat{F}(t_1)$. If t_0 and t_1 are large enough, then

$$\lambda_{LI}(t_0,t_1)=\frac{1}{t_1-t_0}\log\left(\frac{\widehat{F}(t_1)}{\widehat{F}(t_0)}\right)$$

is an estimator for λ_1. In addition, one can give a confidence interval for λ_1 [LM07].

(b) Least square estimators. We construct the empirical distribution function $\widehat{F}(t)$ of $F(t)$ for t large enough and then estimate $\log(1-\widehat{F}(t))\simeq K+\lambda_1 t$ using a least square method.

The error between $\log(1-\widehat{F}(t))$ and $\log(1-F(t))$ is approximatively given by

$$\log(1-\widehat{F}(t))\simeq\log(1-F(t))+\frac{\eta\circ F^{-1}(t)}{\sqrt{N}(1-F(t))},$$

where $(\eta(t))_{t\in[0,1]}$ is a Brownian bridge. A consequence of this computation is that we shall consider t in some interval $[t_0,t_1]$ with t_0 large enough so that the first eigenvalue dominates in the approximation of

$F(t)$, and $t_1 > t_0$ not too large to keep the variance of the last term small.

Hence, we pick m points $\{\theta_i\}_{i=1,\dots,m}$ in $[t_0, t_1]$ and then we use the $(\theta_i, \log(1-\widehat{F}(\theta_i)))$'s as the points to perform the linear regression. Of course, this estimator depends on the choice of the θ_i. We have discussed in [LM07] how to choose the best estimator when relatively few points are used (with respect to the number of bins of the histogram used to construct $\widehat{F}$). Another possibility consists in using a linear interpolation of the discretely known function $\widehat{F}$ and then to use many points $\{\theta_i\}_{i=1,\dots,m}$. If we pick m random points $\{\theta_i\}_{i=1,\dots,m}$ on $[t_0, t_1]$, then the least square estimator is very stable with respect to the choice of the points when m is large (in our numerical example, we construct our histograms with 1,000 bins and $m = 10{,}000$). Note that the variability of the estimator as a function of the choice of $[t_0, t_1]$ is greater than the variability given by the confidence interval for the slope of the curve in the linear regression. The quality of the estimator may be deduced from the quantity $1 - R^2$, where R^2 is the coefficient of determination.

(c) Maximum likelihood. For T large enough, $\mathbb{P}_x[\tau > t | \tau > T] \simeq C\exp(\lambda_1 t)$. Then τ is an exponential random variable of parameter $-\lambda_1$ (see [BB96]). The density of τ given $\{\tau > T\}$ is $p(t,\lambda) = -\lambda\exp(-\lambda(t-T))$ with $\lambda = \lambda_1$. Hence, it is possible to use the standard estimators of the parameter of an exponential distribution. A natural estimator of λ_1 is the maximum likelihood estimator, *i.e.,* the value λ_{ML} which maximizes $\lambda \mapsto \prod_{i=1}^{M} p(\tau^{(i)}, \lambda)$, where $\{\tau^{(i)}\}_{i=1,\dots,M}$ are the values of τ greater than T, that is

$$\lambda_{ML} = -\frac{M}{\sum_{i=1}^{M}(\tau^{(i)} - T)}.$$

It is also a classical result that such an estimator is asymptotically normal. In addition, the variance of this estimator is known to be related to the Fisher information $I(\lambda_1)$ of the exponential distribution. This means that $\sqrt{M}(\lambda_{ML} - \lambda_1)$ converges to a normal distribution of mean 0 and variance $1/I(\lambda_1)$ with

$$I(\lambda) = \int_T^{+\infty} \frac{(\partial_\lambda p(t,\lambda))^2}{p(t,\lambda)}\,\mathrm{d}t = \frac{1}{\lambda^2}.$$

On this topic, see for example [Wil01].

(d) Other possible estimators. Other estimators have been proposed to estimate the parameter of an exponential distribution : see for example [RC93, GS99]. In the previously cited articles, the proposed estimators are robust ones and then less sensitive to the presence of outliers than the maximum likelihood.

2.4. **Estimating the first eigenfunction.** When $c = 0$, comparing (2) and (4) respectively with a general bounded, measurable function u_0 and with the function $u_0 = 1$ leads to

$$\mathbb{E}_x[u_0(X_t) \,|\, t < \tau] = \frac{\mathbb{E}_x[u_0(X_t); t < \tau]}{\mathbb{E}_x[1; t < \tau]} = \frac{\langle u_0, \varphi_1^* \rangle \varphi_1(x) \exp(\lambda_1 t) + \mathrm{o}(\exp(\lambda_1 t))}{\langle 1, \varphi_1^* \rangle \varphi_1(x) \exp(\lambda_1 t) + \mathrm{o}(\exp(\lambda_1 t))} \simeq \frac{\langle u_0, \varphi_1^* \rangle}{\langle 1, \varphi_1^* \rangle}$$

when the time t is large enough. Thus, the density of the position X_t given $\{t < \tau\}$ is $\varphi_1^*/\langle 1, \varphi_1^* \rangle$ for large t, assuming that $\varphi_1^* > 0$ in D (one knows that φ_1^* keep a constant sign over D).

The simplest way to estimate the first eigenvalue φ_1^* of the adjoint A^* of A consists in constructing an histogram of the positions X_t at a given time t for t large enough, for a sample of the surviving particles at this time. A less trivial way is to construct φ_1^* as a superposition of a distribution density — a kernel — around each simulated point (see [Sil86] for example). This gives a more regular density. In the numerical examples of Sections 3 and 4, we show that we can obtain good approximations of this eigenfunction using each of the two methods.

With λ_1, φ_1 and φ_1^*, we have a complete description of the solution of the Cauchy problem in large times for every initial functions and any point, as shown in the expansion (4). If the function φ_1 is not completely known, we know at least the value of φ_1 at the point where the simulation starts. Then we can estimate the solution to the Cauchy problem (4) at this point for any initial condition, when the time is large. Our algorithm allows us to estimate φ_1^*. In some cases, if A is self-adjoint or if the domain and the operator presents some symmetries, one can deduces φ_1 from φ_1^*. More generally, for a wide class of operators, it is still possible to apply our algorithm to the adjoint of A to estimate φ_1.

2.4.1. *On the adjoint of homogeneous neutron transport operator.* The neutron transport operator is a particular class of transport operators that particles submitted to collisions. The kind of operators we consider here are of type

$$Au(x,v) = \sum_{i=1}^{d} v_i \frac{\partial u}{\partial x_i}(x,v) + \nu \int_{\mathbf{V}} \pi(x,v,v')(u(x,v') - u(x,v)) \,\mathrm{d}v',$$

where $(x,v) \in D = \mathbf{S} \times \mathbf{V} \subset \mathbb{R}^d \times \mathbb{R}^d$, $\nu \in \mathbb{R}_+^*$ and $\pi(x,v,\cdot)$ is a distribution function on $\mathbf{V}$ for any $(s,v) \in D$. Thus, we simulate a particle with position X_t and velocity V_t. When a collision occurs at time t, the new velocity V_{t+} of the particle is chosen randomly using the density $\pi(X_t, V_t, \cdot)$. The particle then moves with constant velocity until the next collision that happens after an independent exponential time of parameter ν.

Formally, the adjoint A^* of A is

$$A^*u(x,v) = -\sum_{i=1}^{d} v_i \frac{\partial u}{\partial x_i}(x,v) + \nu \int_{\mathbf{V}} \pi(x,v',v)(u(x,v') - u(x,v))\,\mathrm{d}v',$$

If $\pi(x,\cdot,v)$ is also the density of a probability distribution, then one easily obtain that the solution to

$$\frac{\partial u(t,x,v)}{\partial t} = A^*u(t,x,v) \text{ on } D \text{ with } u(0,x,v) = u_0(x,v)$$

is equal to $\widehat{u}(t,x,-v) = u(t,x,v)$, where $\widehat{u}$ is solution to

$$\frac{\partial \widehat{u}(t,x,v)}{\partial t} = \widehat{A}\widehat{u}(t,x,v) \text{ on } \widehat{D} \text{ with } \widehat{u}(0,x,v) = u(x,-v)$$

with $\widehat{D} = \mathbf{S} \times (-\mathbf{V})$ and

$$\widehat{A}u(x,v) = \sum_{i=1}^{d} v_i \frac{\partial u}{\partial x_i}(x,v) + \nu \int_{-\mathbf{V}} \widehat{\pi}(x,v,v')(u(x,v') - u(x,v))\,\mathrm{d}v',$$
$$\widehat{\pi}(x,v,v') = \pi(x,-v',-v),\ (v,v') \in (-\mathbf{V})^2.$$

Hence, the first eigenfunction φ_1 of A is also the first eigenfunction of the adjoint of A^*, which may then be deduced from the first eigenfunction $\widehat{\varphi}_1$ of $\widehat{A}$ by $\varphi_1(x,v) = \widehat{\varphi}_1(x,-v)$.

Thus, under the assumption that $\pi(x,v,\cdot)$ and $\pi(x,\cdot,v)$ are probability densities — this hypothesis is really practical —, one can use our algorithm on $\widehat{A}$ to get the first eigenfunction φ_1 of A, as well as its first eigenvalue. As we will see it in the examples, there are realistic cases where one can deduce the first eigenfunction of A from the one of A^* using symmetry arguments.

The first eigenvalue of $\widehat{A}$ is equal to the first eigenvalue of A, so that taking the average of the two estimators for the first eigenvalue of A and $\widehat{A}$ gives a slightly better approximation of this quantity.

2.4.2. *On diffusion processes.* Of course, if A is the Laplace operator $\frac{1}{2}\triangle$, then $\varphi_1^* = \varphi_1$ since A est self-adjoint. Thus, our algorithm gives us directly the first eigenfunction of A.

We have also asserted in [LM07] that our approach can be used for a more general diffusion process whose infinitesimal generator is

$$A = \frac{1}{2}\sum_{i,j=1}^{d} a_{i,j}\frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{d} b_i \frac{\partial}{\partial x_i}.$$

Although A is not self-adjoint in general, under mild regularity assumptions on the coefficients and the domain, it has a discrete spectrum and there exists a real eigenvalue λ_1 such that any other (possibly complex) eigenvalue has a smaller real part: See [Pin96a] for example. In order to compute the first eigenvalue of A, an appropriate simulation scheme shall be used. The problem of obtaining a good approximation of the

first exit time from a domain has given rise to a large literature: see [MT99, Go00, JL05, BP06] for example.

The adjoint A^* of A is given by

$$A^* = \frac{1}{2}\sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j}(a_{i,j}\cdot) - \sum_{i=1}^{d} \frac{\partial}{\partial x_i}(b_i \cdot)$$

and our algorithm gives us directly the first eigenfunction φ_1^* of A^*. The first eigenvalue of A^* is also λ_1. If one wishes to compute the first eigenfunction φ_1 of A, one can use that A^{**} is equal to A and then, the first eigenfunction of the adjoint of A^* is φ_1. If the coefficients a and b are smooth enough, this operator A^* may be written

$$A^* = \frac{1}{2}\sum_{i,j=1}^{d} a_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{d} \beta_i \frac{\partial}{\partial x_i} + \gamma$$

with

$$\beta_i = \frac{1}{2}\sum_{j=1}^{d} \frac{\partial a_{i,j}}{\partial x_i} - b_i \text{ and } \gamma = \frac{1}{2}\sum_{i,j=1}^{d} \frac{\partial^2 a_{i,j}}{\partial x_i \partial x_j} - \sum_{i=1}^{d} \frac{\partial b_i}{\partial x_i}.$$

Note that if the coefficients are constant, then $\gamma = 0$, so that φ_1 may be computed by simulating the process associated to A^*.

We now deal with the case of a non-constant γ. The approach presented here can also be used to deal with a non-homogeneous creation/destruction rate c. Let L be the differential operator

$$L = \frac{1}{2}\sum_{i,j=1}^{d} a_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{d} \beta_i \frac{\partial}{\partial x_i}$$

so that $A^* = L + \gamma$. Let us assume that γ is bounded by a constant α, and let v be the solution to

$$\frac{\partial v}{\partial t} = Lv + \gamma v - \alpha v \text{ with } v(0,\cdot) = v_0$$

with a Dirichlet boundary condition on the boundary of the cylinder $\mathbb{R}_+ \times \partial D$. The solution v may be represented by the Feynman-Kac formula

$$v(t,x) = \mathbb{E}_x\left[v_0(Y_t)\exp\left(\int_0^t \gamma(Y_s)\,\mathrm{d}s - \alpha t\right); t < \tau\right]$$

where Y is the process generated by L. Let ζ be an exponential random variable of parameter 1. Then $v(t,x)$ may be written also

$$v(t,x) = \mathbb{E}_x\left[v_0(Y_t); \int_0^t \gamma(Y_s)\,\mathrm{d}s - \alpha t > \zeta \text{ and } t < \tau\right]. \tag{5}$$

On the other hand

$$v(t,x) \simeq \exp(\lambda_1^* t)\langle v_0, \psi_1^*\rangle \psi_1(x) \text{ when } t \text{ is large,} \tag{6}$$

where λ_1^* is the first eigenvalue of $A^* - \gamma = L^* - \gamma$ and ψ_1 is its first eigenfunction with $\langle \psi_1, \psi_1^* \rangle = 1$. Let us note that $\psi_1 = \varphi_1^*$, $\psi_1^* = \varphi_1$ and $\lambda_1^* = \lambda_1 - \alpha$. As above, we obtain from (5) and (6) that

$$\frac{\langle v_0, \varphi_1 \rangle}{\langle 1, \varphi_1 \rangle} \simeq \mathbb{P}_x \left[v_0(Y_t) \middle| \int_0^t \gamma(Y_s)\,\mathrm{d}s - \alpha t > \zeta \text{ and } t < \tau \right]$$

when t is large. Hence, a branching Monte Carlo may still be used. But here, unless $\gamma = 0$, one needs also to compute the integral $\int_0^{t\wedge\tau} \gamma(Y_s)\,\mathrm{d}s$ along the simulated paths of Y.

Computing numerically the first eigenvalue λ_1^* while estimating φ_1 also helps us to improve slightly the estimation of λ_1.

2.5. **Estimating the second eigenvalue of the Laplace operator?** As the Laplace operator with a Dirichlet boundary condition is self-adjoint, the spectrum $\{\lambda_k\}_{k\geq 1}$ of $\frac{1}{2}\triangle$ is countable, real and negative. In addition,

$$p(t,x,y) = \sum_{k\geq 1} \exp(\lambda_k t)\varphi_k(x)\varphi_k(y),\ t > 0,\ x, y \in D, \tag{7}$$

where we use the convention $\cdots \leq \lambda_3 \leq \lambda_2 < \lambda_1 < 0$ and the φ_k are the normalized eigenfunctions associated to λ_k. The distribution function $F(t) = \mathbb{P}_x[\tau < t]$ is given by the relation

$$1 - F(t) = \mathbb{E}_x[1; t < \tau] = \int_D p(t,x,y)\,\mathrm{d}y = \sum_{k\geq 1} e^{-\lambda_k t}\varphi_k(x) \int_D \varphi_k(y)\,\mathrm{d}y.$$

One may wonder whether or not it is possible to estimate — at least roughly — the second eigenvalue with this algorithm, as the density may be written

$$p(t,x,y) = e^{\lambda_1 t}\varphi_1(x)\varphi_1(y) + e^{\lambda_2 t}\varphi_2(x)\varphi_2(y) + r(t,x,y),$$

where $e^{-\lambda_2 t} r(t,x,y)$ decreases to 0 and both λ_1 and φ_1 are estimated using the previous algorithm. Two methods appear to be natural.

(a) Substract to $F_N(t)$ the estimation of the quantity $1 - \exp(\lambda_1 t)\varphi_1(x)\langle \varphi_1, 1 \rangle$ and estimate $\varphi_2 \langle \varphi_2, 1 \rangle \exp(\lambda_2 t)$ the same way λ_1 was estimated.

Instead of starting from the point x, one may also look for a probability measure μ on D such that $\int_D \varphi_1(x)\,\mathrm{d}\mu(x)$ is as small as possible. This is justified by

$$\begin{aligned}\mathbb{P}_\mu[T < \tau] &= \int_D \int_D p(t,x,y)\,\mathrm{d}y\,\mathrm{d}\mu(x) \\ &\simeq \left(\int_D \varphi_1\,\mathrm{d}\mu \right) \langle \varphi_1, 1 \rangle \exp(\lambda_1 t) + \left(\int_D \varphi_2\,\mathrm{d}\mu \right) \langle \varphi_2, 1 \rangle \exp(\lambda_2 t).\end{aligned}$$

The effect is then to increase the relative importance of the second eigenvalue while approximating $\mathbb{P}_\mu[T < \tau]$.

(b) Create a function $\varphi_1^\perp$ orthogonal with respect to the $\mathrm{L}^2(D)$ scalar product. If $\|\varphi_1\|_{\mathrm{L}^2(D)} = 1$, then $\varphi_1^\perp = 1 - \left(\int_D \varphi_1(y)\,\mathrm{d}y\right)\varphi_1$ is such a function. Then evaluate the quantities

$$v_i = \mathbb{E}_x[\varphi_1^\perp(X_{T_i}); T_i < \tau] \simeq \exp(\lambda_2 T_i)\varphi_2(x)\langle\varphi_2, \varphi_1^\perp\rangle$$

for $i = 1, 2$, where T_1 and T_2 are two times not too large. Then set $\lambda_2 = (T_1 - T_2)^{-1}\log(v_1/v_2)$.

On the test cases of Section 3, we have performed numerical experiments for both methods. Unfortunately, none of these methods has provided a stable enough estimator of λ_2.

3. Numerical examples on the Laplace operator

In this Section, we give two numerical examples related to the Laplace operators. The first test case is just a rectangle, where the eigenvalues and the eigenfunctions are explicitly known. This case gives us the inherent limit of the implementation of the Monte Carlo method: One cannot expect to get a better precision for a general case than for this case with the same number of samples. The second one has a slightly more complicated geometry and has been already studied in [LM07].

In the sequel, we denote by λ_{ML} the maximum likelihood estimator. The width of the 90 % confidence interval is $2\lambda_1\sqrt{1.64}/\sqrt{M}$, where M is the number of samples used to compute the maximum likelihood. We denote by $\lambda_{LS}(t_0, t_1)$ the least square estimator on the time interval $[t_0, t_1]$ and a large set of points ($m = 10{,}000$).

3.1. Case of a rectangle.

The eigenvalues and eigenfunctions of $\frac{1}{2}\triangle$ are explicitly known when D is the rectangle $[-L, L]\times[-\ell, \ell]$. We have for any integers $n, m \geq 1$,

$$\lambda_{n,m} = \frac{1}{2}\left(\left(\frac{n\pi}{2L}\right)^2 + \left(\frac{m\pi}{2\ell}\right)^2\right)$$
$$\text{and } \varphi_{n,m}(x, y) = \sin\left(\frac{n\pi}{2L}(x + L)\right)\sin\left(\frac{n\pi}{2\ell}(y + \ell)\right).$$

We consider the rectangle $D = [-2, 2] \times [-3/2, 3/2]$ for which the first eigenvalue $\lambda_{1,1}$ is -0.856735. In order to optimize the estimation of $\lambda_{1,1}$.

We perform five scenarios with N particles each. The results are summarized in Table 1. Except in Case (b), the particles start from the center of the rectangle in order to get a high number of living particles at time T_1.

We use several slices at times T_i, and we compute the empirical distribution function ψ_i of X_{T_i} obtained from the samples. To construct these functions, we use an histogram of cells of size 0.01×0.01. The functions ψ_i are normalized to have a L^2-norm equal to 1. In all cases, the L^2-norm of the difference between ψ_i and the adequately normalized eigenfunction $\varphi_{1,1}$ is around 0.5.

Simulation (a). We do not use the branching algorithm, so that we keep only the first exit times that are larger than 2.

Simulation (b). In order to get a comparison between the use of the empirical distribution function of X_T for T large enough instead of the density $\varphi_{1,1}/\int_D \varphi_{1,1}$, we draw randomly the starting point according to the probability law μ with density $\widehat{\varphi} = \varphi_{1,1}/\int_D \varphi_{1,1}$. With this initial distribution μ, since the eigenfunctions are orthogonal, let us note that $\mathbb{P}_\mu[\tau > t] = \exp(\lambda_1 t)$, so that τ is exactly an exponential random variable of parameter $-\lambda_1$.

Simulation (c). We use only one time slice at $T_1 = 2$. The probability that the particle is alive at time T_1 is $p_1 = 19.2\%$.

Simulation (d). We use the time slices $T_1 = 2$ and $T_2 = 4$. The probabilities of survival p_i at time T_i are $p_1 = 19.2\%$, $p_2 = 5.2\%$.

Simulation (e). We use the time slices $T_1 = 2$, $T_2 = 4$ and $T_3 = 6$. The probabilities of survival p_i at time T_i are $p_1 = 19.2\%$, $p_2 = 5.2\%$, $p_3 = 0.9\%$.

3.2. **A 2-dimensional test case.** Our estimation algorithm was presented in [LM07] on a 2-dimensional test case, which is the domain presented in Figure 1. The results are then compared with the ones obtained with the `pdetool` package from `Matlab`. Using a very fine mesh, this deterministic solver gives the value $\lambda_1 = 0.73952$. Our numerical results are given in Table 2.

Simulation (a). Here, there is no branching. For the Maximum likelihood estimator, we keep only the values of τ that are greater than 2, which means that we use only 36 % of the particles.

Simulation (b). We use only a time slice at $T = 2$. Regarding the first eigenvalue, we compute φ_1 at time T with an histogram with square cell 0.05×0.05, which we compare with the eigenfunction given by Matlab. The L^2-norm of the difference between these two functions is 0.1.

Simulation (c). We use two time slices at $T_1 = 2$ and $T_2 = 4$. The proportion of particles remaining at the first slice is $p_1 = 36\%$ and at the second slice is $p_2 = 8\%$. The L^2-norm of the difference between the eigenfunction given by the Monte Carlo Method at time $T = 4$ and the one given by the finite element method is 0.1.

Estimator	value	$1-R^2$
Exact value	-0.856735	
Simulation (a) $N=10^6$, $\theta=1$ unit		
λ_{ML} $(\tau \geq 2)$	$-0.8525 \pm 2.5 \cdot 10^{-3}$	
$\lambda_{LS}(2,4)$	-0.8527	$2 \cdot 10^{-6}$
$\lambda_{LS}(2,6)$	-0.8518	$3 \cdot 10^{-6}$
$\lambda_{LS}(2,8)$	-0.8521	$2 \cdot 10^{-5}$
Simulation (a) $N=10^7$, $\theta=10$ unit		
λ_{ML} $(\tau \geq 2)$	$-0.8554 \pm 8 \cdot 10^{-4}$	
$\lambda_{LS}(2,4)$	-0.8553	$5 \cdot 10^{-7}$
$\lambda_{LS}(2,6)$	-0.8569	$8 \cdot 10^{-6}$
$\lambda_{LS}(2,8)$	-0.8580	$6 \cdot 10^{-6}$
Simulation (b) $N=10^6$, $\theta=3.5$ unit		
λ_{ML} $(\tau \geq 0)$	$-0.8570 \pm 1.1 \cdot 10^{-3}$	
$\lambda_{LS}(0,2)$	-0.8571	$2 \cdot 10^{-6}$
$\lambda_{LS}(0,4)$	-0.8588	$4 \cdot 10^{-6}$
$\lambda_{LS}(0,6)$	-0.8564	$7 \cdot 10^{-6}$
$\lambda_{LS}(0,8)$	-0.8556	$15 \cdot 10^{-6}$
Simulation (c) $N=10^6$, $\theta=3$ unit		
λ_{ML} $(\tau \geq 2)$	-0.8564 ± 10^{-3}	
$\lambda_{LS}(2,4)$	-0.8568	$6 \cdot 10^{-6}$
$\lambda_{LS}(2,6)$	-0.8571	$7 \cdot 10^{-7}$
$\lambda_{LS}(2,8)$	-0.8615	$6 \cdot 10^{-5}$
Simulation (d) $N=10^6$, $\theta=4.5$ unit		
λ_{ML} $(\tau \geq 4)$	-0.8577 ± 10^{-3}	
$\lambda_{LS}(4,6)$	-0.8567	$1.2 \cdot 10^{-6}$
$\lambda_{LS}(4,8)$	-0.8577	$1.4 \cdot 10^{-6}$
$\lambda_{LS}(4,10)$	-0.8549	$7.0 \cdot 10^{-6}$
Simulation (e) $N=10^6$, $\theta=6$ unit		
λ_{ML} $(\tau \geq 6)$	-0.8564 ± 10^{-3}	
$\lambda_{LS}(6,8)$	-0.8573	$4 \cdot 10^{-7}$
$\lambda_{LS}(6,10)$	-0.8565	$9 \cdot 10^{-7}$
$\lambda_{LS}(6,12)$	-0.8569	$2.6 \cdot 10^{-6}$

TABLE 1. Estimation of the first eigenvalue of the rectangle using a sample size N. The quantity θ gives the relative execution time.

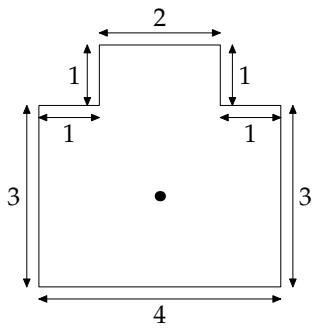

FIGURE 1. A 2-dimensional domain. The dot represents the starting point.

Reference value	-0.73952	
Estimator	value	$1-R^2$
Simulation (a) $N=10^6$, $\theta=1$ unit		
λ_{ML} $(\tau\geq 2)$	$-0.7373 \pm 1.5\cdot 10^{-3}$	
$\lambda_{LS}(2,4)$	-0.7403	$2.0\cdot 10^{-5}$
$\lambda_{LS}(2,6)$	-0.7381	$1.1\cdot 10^{-5}$
$\lambda_{LS}(2,8)$	-0.7378	$1.5\cdot 10^{-5}$
Simulation (a) $N=10^7$, $\theta=10$ unit		
λ_{ML} $(\tau\geq 2)$	$-0.7374 \pm 0.5\cdot 10^{-3}$	
$\lambda_{LS}(2,4)$	-0.7397	$2.7\cdot 10^{-6}$
$\lambda_{LS}(2,6)$	-0.7387	$0.8\cdot 10^{-6}$
$\lambda_{LS}(2,8)$	-0.7367	$5.5\cdot 10^{-6}$
Simulation (b) $N=10^6$, $\theta=2.5$ unit		
λ_{ML} $(\tau\geq 2)$	$-0.7378 \pm 0.9\cdot 10^{-3}$	
λ_{ML} $(\tau\geq 3)$	$-0.7373 \pm 1.3\cdot 10^{-3}$	
$\lambda_{LS}(2,4)$	-0.7366	$1.0\cdot 10^{-6}$
$\lambda_{LS}(2,6)$	-0.7378	$7\cdot 10^{-7}$
$\lambda_{LS}(3.5,5.5)$	-0.7390	$8\cdot 10^{-7}$
$\lambda_{LS}(2,8)$	-0.7392	$1.2\cdot 10^{-6}$
Simulation (c) $N=10^6$, $\theta=4.2$ unit		
λ_{ML} $(\tau\geq 4)$	$-0.7389 \pm 0.9\cdot 10^{-3}$	
λ_{ML} $(\tau\geq 5)$	$-0.7389 \pm 1.3\cdot 10^{-3}$	
$\lambda_{LS}(4,6)$	-0.7396	$1.9\cdot 10^{-6}$
$\lambda_{LS}(4,8)$	-0.7391	$1.5\cdot 10^{-6}$
$\lambda_{LS}(4,10)$	-0.7375	$3.5\cdot 10^{-6}$

TABLE 2. Estimation of the first eigenvalue of the $2d$-test case using a sample size N. The quantity θ gives the relative execution time.

Remark 1. Let us note that with (7), if one knows λ_1 and ψ_1, then one can approximate the density $p(t,x,y)$ of the Laplace operator as $p(t,x,y)=\exp(\lambda_1 t)\varphi_1(x)\varphi_1(y)$ for t large enough. This gives a large time approximation of the solution of the Cauchy problems

$$\frac{\partial u(t,x)}{\partial t}=\frac{1}{2}\triangle u(t,x) \text{ with } u(0,x)=u_0(x)$$

for any function u_0, since $u(t,x)=\int_D p(t,x,y)u_0(y)\,\mathrm{d}y$.

4. Numerical examples on Neutron transport operators

4.1. **The Lehner-Wing model.**

4.1.1. *Description and stochastic representation.* We study the Cauchy problem

$$\frac{\partial u}{\partial t}=-v\frac{\partial u}{\partial x}-u(t,x,v)+\frac{c}{2}\int_V u(t,x,v')\,\mathrm{d}v'$$

with initial conditions $u(x,v,0)=1$ and absorption boundary conditions. The spatial domain is $\mathbf{S}=]0,d[$, the velocity domain is $\mathbf{V}=]-1,1[$ and c is a positive constant. This model is homogeneous and isotropic and we rewrite it as

$$\frac{\partial u}{\partial t} = Au(t,x,v) + (c-1)\,u(t,x,v) \tag{8}$$

with

$$Au = -v\frac{\partial u}{\partial x} + c\left\{\frac{1}{2}\int_V u(t,x,v')\,\mathrm{d}v' - u(t,x,v)\right\}$$

to give the stochastic representation of its solution. Let us consider the velocity $(V_t)_{t\geq 0}$ of a particle with collisions at random times. After a collision, the velocity has a uniform distribution on $\mathbf{V}$. The cumulative distribution of the time between two collisions is

$$1-\exp\left[-\int_0^t c\,\mathrm{d}s\right] = 1-\exp\left(-ct\right).$$

The process we consider now is solution $(X_t,V_t)_{t\geq 0}$ of the differential equation $\frac{\mathrm{d}X_t}{\mathrm{d}t}=-V_t$ with initial conditions $X_0=x$ and $V_0=v$. The infinitesimal generator of this process $(X_t,V_t)_{t\geq 0}$ is A. The solution of (8) may then be written

$$u(t,x,v)=\exp((c-1)t)\mathbb{P}_{x,v}[\tau>t]$$

where τ is the exit time from $D=\mathbf{S}\times\mathbf{V}$ for the process $(X_t,V_t)_{t\geq 0}$ with $X_0=x$ and $V_0=v$ under $\mathbb{P}_{x,v}$.

This model is known as the *Lehner-Wing model* [DL87b, Chap. 21, p. 1164] and is also called *multiplying slabs* [DS].

There are two kinds of eigenvalues problems in neutron transport. The first one is the criticality computation. In our problem, it consists in finding the value of the parameter c such that the first eigenvalue of the operator $Bu=Au+(c-1)u$ is equal to 0. This means that the first eigenvalue λ_1 of A is equal to $1-c$, since the first eigenvalue of B is λ_1+c-1. The second kind of problem is the computation of this eigenvalue for a given value of c.

Here, we first consider that we know a very good approximation of the parameter c corresponding to the critical value. In this situation, we have to check that the first eigenvalue is fairly close to 0 using our estimator. Second, we take two values of c below and above the critical value and we compute the corresponding first eigenvalues and we compute the critical parameter using the secant method.

4.1.2. *In the critical case.* We consider in our numerical examples to simulate $(X_t,V_t)_{t\geq 0}$ when the spatial domain $\mathbf{S}$ is $]0,8[$. The value of the critical parameter c is equal to 1.03639014 (See [DS]).

In our branching algorithms, we use slices at times $T_1=40$, $T_2=80$ and $T_3=120$. In order to estimate the first eigenvalue of A, we use the interpolation estimator $\lambda_{LI}(t_0,t_1)$ with or without branching using

	With branching		Without branching	
N	10^6	10^7	10^6	10^7
$\alpha_{LI}(T_1,T_2)$	$2.2\cdot10^{-5}$	$1.0\cdot10^{-5}$	$6.5\cdot10^{-5}$	$0.2\cdot10^{-5}$
$\alpha_{LI}(T_2,T_3)$	$-3.3\cdot10^{-5}$	$1.4\cdot10^{-5}$	$1.6\cdot10^{-4}$	$9.0\cdot10^{-5}$
$\alpha_{LI}(T_1,T_3)$	$-5.4\cdot10^{-6}$	$1.2\cdot10^{-5}$	$1.1\cdot10^{-4}$	$5.1\cdot10^{-5}$
Error max	$3.3\cdot10^{-5}$	$1.1\cdot10^{-5}$	$1.6\cdot10^{-4}$	$9\cdot10^{-5}$
Relative Time	2	20	1	10

TABLE 3. Estimation of the first eigenvalue α of B for the critical value of c with N particles. The starting point is $(x,v)=(4,-0.2)$.

	$c=c_{\min}=1.036$		$c=c_{\max}=1.037$	
N	10^6	10^7	10^6	10^7
$\alpha_{LI}(T_1,T_2)$	-0.000435	-0.000415	0.000633	0.000610
$\alpha_{LI}(T_2,T_3)$	-0.00423	-0.000430	0.000564	0.00062
$\alpha_{LI}(T_1,T_3)$	-0.000429	-0.00042	0.000598	0.000615

TABLE 4. Estimation of the first eigenvalue α of B for c close to the critical value with N particles. The starting point is $(x,v)=(4,-0.2)$.

the values of $F(t_0)=\mathbb{P}_{x,v}[\tau<t_0]$ and $F(t_1)=\mathbb{P}_{x,v}[\tau<t_1]$ (See Section 2.3). The probabilities $p_i=1-F(T_i)$ the particle is still alive at time T_i are $p_1=30.7\,\%$, $p_2=7.2\,\%$ and $p_3=1.7\%$. The ratio $p_2/p_1=0.2333$ and $p_3/p_2=0.2334$ are pretty close. This confirms that the system has reach the steady-state regime after time T_1. When the successive ratios p_{i+1}/p_i takes a stationary value, the behavior of the system is dominated by the first eigenvalue and eigenfunction. In Table 3, we do not report the first eigenvalue λ_1 of A but the first eigenvalue $\alpha=c-1+\lambda_1$ of B which shall be close to 0.

4.1.3. *Computation of the criticality factor.* We are going to use the secant method to compute the criticality factor. In Table 4, we compute the values of $\alpha=c-1+\lambda_1$ for $c=c_{\min}=1.036$ and $c=c_{\max}=1.037$ using the previous method assuming for the sake of simplicity that we are already near criticality. The estimator we use for λ_1 is still the one given by linear interpolation, and we set $\alpha_{LI}(t_0,t_1)=c-1+\lambda_{LI}(t_0,t_1)$.

The approximation of the criticality factor is then

$$\widehat{c}=c_{\min}-\alpha_{\min}\frac{c_{\max}-c_{\min}}{\alpha_{\max}-\alpha_{\min}}=1.036406$$

with $\alpha_{\min}=-0.000421$ and $\alpha_{\max}=0.00615$ are obtained by averaging the 3 estimators of Tables 4 with $N=10^7$ particles. The value of $\widehat{c}$ is close to $1.5\cdot10^{-5}$ to the true one. In the previous paper [MT06], such an accuracy had required $N=10^9$ simulations.

4.1.4. *Estimation of the solution of the Cauchy problem in large time.* We show how the estimation of the first eigenfunction provides a complete description of the solution to (8) when the time is large.

Using the spectral expansion, the solution $u(t,x,v)$ to (8) with the initial condition $u(0,x,v)=1$ may be written

$$u(t,x,v) = \exp((c-1)t)(\beta(x,v)\exp(\lambda_1 t) + \mathrm{o}(\exp(\lambda_1 t))) \tag{9}$$

where λ_1 is the first eigenvalue of the neutron transport operator A and $\beta(x,v) = \langle 1, \varphi_1^*\rangle \varphi_1(x,v)$. As $u(t,x,v) = \exp((c-1)t)\mathbb{P}_{x,v}[t<\tau]$, the quantity λ_1 is related to the rate of absorption of the particles by the boundary. The function $\beta(x,v)$ is equal to $\langle 1, \varphi_1^*\rangle \varphi_1(x,v)$, where φ_1 and φ_1^* denote the first eigenfunctions of A and A^* with $\langle \varphi_1^*, \varphi_1\rangle = 1$ (see for example Chap. XXI, § 3 in [DL87b]).

The interpolation method or the least square method also give the value of $\beta_0 = \beta(x_0,v_0)$ at the starting point (x_0,v_0) of the particles, which can also be deduced from $\beta_0 \exp(\lambda_1 t) = \mathbb{P}_{x_0,v_0}[t<\tau]$. With the branching method, we can approximate

$$\psi_1^*(x,v) = \frac{\varphi_1^*(x,v)}{\langle 1, \varphi_1^*\rangle}$$

with the density of (X_T, V_T) for T large enough. We set $\psi_1(x,v) = \varphi_1(x,v)\langle 1, \varphi_1^*\rangle$. Using this expression for $\beta(x,v)$, the solution to (9) with $u(0,\cdot,\cdot) = u_0$ becomes

$$u(t,x,v) = \langle u_0, \psi_1^*\rangle \exp((c-1-\lambda_1)t)\psi_1(v,x) + \mathrm{o}(\exp((c-1-\lambda_1)t)).$$

where $\psi_1^*(x,v)$ can be estimated from the simulations. From the estimation of $\psi_1^*(x,v)$ and β_0, one can estimate $\psi_1(x_0,v_0)$ at the starting point (x_0,v_0).

Using the symmetries properties of the coefficients of the neutron transport operator and the symmetries of the domain, we get that $\psi_1(x,v) = \psi_1^*(d-x,-v)$.

We give a numerical illustration of this in the critical case above with 10^7 particles. For $\beta_0 = \beta(x_0,v_0)$ with $(x_0,v_0) = (4,-0.2)$, using the times T_2 and T_3, we obtain $\beta_0 \simeq 1.316$.

We now estimate ψ_1 — the density of (X_T, V_T) at time $T = 80$ — from the positions $(X_T^{(i)}, V_T^{(i)})$ of the J_0 particles remaining at this time. We then use a convolution kernel so that

$$\psi_1(x,v) = \frac{1}{2\pi J_0 h^2} \sum_{i=1}^{J_0} \exp\left(-\frac{(x-X^{(i)})^2}{2h^2}\right) \exp\left(-\frac{(v-V^{(i)})^2}{2h^2}\right).$$

With $h = 0.1$, we compute $\psi_1(4,-0.2)$ and we obtain 0.0883 which leads to an approximation of $K = \langle 1, \psi_1^*\rangle = 14.9$. Thus, in the critical case,

$$u(t,x,v) = K\psi_1(x,v) + \mathrm{o}(\exp((c-1+\lambda_1)t)).$$

We have also computed $\psi_1(4, 0.2) = 0.0892$ thanks to the same kernel approximation, which should be equal by a symmetry argument to $\psi_1(4, -0.2)$. The difference between $\psi_1(x_0, v)$ and $\psi_1(x_0, -v)$ with $x_0 = 4$ in the middle of $\mathbf{S}$ provides us with a test for checking a possible error in the algorithm. This also indicates the best precision one can expect on ψ_1.

Thus, with simulations starting from a single point, we obtain a complete description of $u(t, x, v)$ for any $(x, v) \in D$ and t large enough.

We can use this description for some rare events estimations. For example, if one needs to compute $\mathbb{P}_{x,v}[\tau > T]$ for a larger value of T than one used in this simulation, one can use the approximation

$$\mathbb{P}_{x,v}[\tau > T] \simeq \exp(\lambda_1 T) K\psi_1(x, v).$$

This can also simplify the simulation of rare some events. Thanks to the Markov property, we have for any measurable event Γ that depends only on what happens after a time T large enough,

$$\mathbb{P}_{x,v}[(X_t, V_t)_{t\geq T} \in \Gamma] \simeq K\psi_1(x, v) \exp(\lambda_1 T)\mathbb{P}_{\psi_1^*}[(X_t, V_t)_{t\geq 0} \in \theta_T^{-1}\Gamma],$$

where $(\theta_t)_{t\geq 0}$ is the shift operator of the Markov process. Thus, one has only to perform a Monte Carlo estimation of $\mathbb{P}_{\psi_1^*}[(X_t, V_t)_{t\geq 0} \in \theta_T^{-1}\Gamma]$ to get an estimation of $\mathbb{P}_{x,v}[(X_t, V_t)_{t\geq T} \in \Gamma]$.

4.2. **Multiplying spheres.** We now consider a similar problem where the positions of the particles take their values in a ball and the velocities take their values in the unit sphere. The numerical resolution of such a problem requires the discretization of 5 variables by means of deterministic methods.

4.2.1. *The physical model.* We now consider the Cauchy problem

$$\frac{\partial u(t, x, v)}{\partial t} = -v\nabla_x u(t, x, v) + (c - 1)u(t, x, v) + c\left(\frac{1}{4\pi}\int_{\mathbb{S}_2} u(t, x, v')\,\mathrm{d}v' - u(t, x, v)\right)$$

with an initial condition $u(x, v, 0) = 1$ and absorption boundary conditions. The velocity domain is the unit sphere $\mathbb{S}_2$, the spatial domain is the unit ball of radius d and c plays the same role than in the previous model. The solution of this equation is

$$u(t, x, v) = \exp((c - 1)t)\mathbb{P}_{x,v}[\tau > t],$$

where the transport process $(X_t, V_t)_{t\geq 0}$ is solution of the differential equation $\frac{\mathrm{d}X_t}{\mathrm{d}t} = -V_t$ with initial conditions $X_0 = x$ and $V_0 = v$. The velocity after a collision has a uniform law on $\mathbb{S}_2$. The cumulative distribution of the time between two collisions is

$$1 - \exp\left(-\int_0^t c\,\mathrm{d}s\right) = 1 - \exp(-ct).$$

c	1.138	0.1384602	1.139
$\alpha_{LI}(T_1, T_2)$	-0.000419	$7.1 \cdot 10^{-5}$	0.00067
$\alpha_{LI}(T_2, T_3)$	-0.000540	$1.8 \cdot 10^{-5}$	0.00056
$\alpha_{LI}(T_1, T_3)$	-0.000480	$4.7 \cdot 10^{-5}$	0.00061
Mean	-0.00052	$4.5 \cdot 10^{-5}$	0.000613

TABLE 5. Estimation of the first eigenvalue α of B for the multiplying spheres models with $N = 10^7$ particles.

The simulation of $(X_t, V_t)_{t \geq 0}$ is explained in [Mai01, MT06, LM07].

4.2.2. *Numerical results.* We compute an approximation of the criticality factor when $d = 4$ using the least square method in the approximation of the principal eigenvalues. We perform the simulation using the time slices at times $T_1 = 20$, $T_2 = 40$ and $T_3 = 60$ using $N = 10^7$ particles for values of c close to the critical one. The criticality factor is about 1.1384602 [DS]. The principal eigenvalues of B relative to $c = 1.138$ and $c = 1.139$ are respectively about $-5 \cdot 10^{-4}$ and $6 \cdot 10^{-4}$. The approximation of the criticality factor, given by the secant method, is $c \simeq 1.138459$ which corresponds to an error of about 10^{-6}. In the previous paper [MT06], such an accuracy had required $N = 2 \cdot 10^9$ simulations.

5. Conclusion

In the estimation of the first eigenvalue with a Monte Carlo method, the branching algorithm is a very satisfactory way to improve the quality of the simulation proposed in [LM07]. On all the numerical tests, the branching algorithm has provided a better accuracy than our previous method for comparable simulation times. Indeed, with the previous method, the Monte Carlo error was roughly of order $1/\sqrt{pN}$, where p was the proportion of particles we keep to estimate the first eigenvalue. As long time estimates are needed, the value of p was rather small. With the branching algorithm, the Monte Carlo error is roughly of order $1/\sqrt{N}$. Using empirical distribution of the positions of the particles at given time instead of the exact distribution has a low impact on the quality of the estimation.

In addition, this method gives us a way to estimate the first eigenfunction of the adjoint operator using the density of the empirical distribution of the remaining particles. This could be important for some applications, especially in the neutron transport criticality problem. In addition, it may help to improve and quicken the estimation of the probability of some events occurring after a large time. Similar Monte Carlo techniques can also be used to simulate the first eigenfunction of the operator when the latter is not self-adjoint, nor the eigenfunctions of the operator and its adjoint are related by symmetry relations.

From this approximation of the eigenfunctions, we can also express an approximation of the solution to the Cauchy problem for large times and for any point, while the simulation only requires a single starting point.

The only drawback of this method is that it requires to store large amount of data. Note that however, that amount of data increases only linearly with the dimension. On the other hand, the computational cost does not really depend on the dimension. In addition, the branching algorithm is easy to implement, and hence may be used for high-dimensional problems.

References

[BB96] N. Balakrishnan and A. P. Basu. *The Exponential Distribution: Theory, Methods, and Applications*. Gordon and Breach, 1996.

[BP06] F.M. Buchmann and W.P. Petersen. An exit probability approach to solving high dimensional Dirichlet problems. *SIAM J. Sci. Comput.*, 28(3):1153–1166, 2006.

[CDMLL06] F. Cérou, P. Del Moral, F. LeGland and P. Lezaud. Genetic genealogical model in rare event analysis. *ALEA*, 1:181–203, 2006.

[CL02] F. Campillo and A. Lejay. A Monte Carlo method without grid for a fractured porous domain model. *Monte Carlo Methods Appl.*, 8(2):129–148, 2002.

[DS] E.B. Dahl and N.G. Sjostrand. Eigenvalue spectrum of multiplying slabs and spheres for monoenergetic neutrons with anisotropic scattering. *Nulc. Sci. Eng.*, 69:114–125, 1979.

[DL87a] R. Dautray and J.-L. Lions. *Spectre des opérateurs*. Vol. 5 of *Analyse Mathématique et Calcul Numérique pour les Sciences et Techniques*, Masson, 1987.

[DL87b] R. Dautray and J.-L. Lions. *Évolution : numérique, transport*. Vol. 9 of *Analyse Mathématique et Calcul Numérique pour les Sciences et Techniques*, Masson, 1987.

[DL06] M. Deaconu and A. Lejay. A random walk on rectangles algorithm. *Methodol. Comput. Appl. Probab.*, 8(1):135–151, 2006.

[DM04] P. Del Moral. *Feynman-Kac formulae*. Probability and its Applications. Springer-Verlag, New York, 2004. Genealogical and interacting particle systems with applications.

[DMG05] P. Del Moral and J. Garnier. Genealogical particle analysis of rare events. *Ann. Appl. Probab.*, 15(4):2496–2534, 2005.

[DV76] M.D. Donsker and S.R.S. Varadhan. On the principal eigenvalue of second-order elliptic differential operators. *Comm. Pure Appl. Math.*, 29(6):595–621, 1976.

[GS99] U. Gather and V. Schultze. Robust estimation of scale of an exponential distribution. *Statist. Neerlandica*, 53(3):327–341, 1999.

[Go00] E. Gobet. Weak approximation of killed diffusion using Euler schemes. *Stochastic Process. Appl.* 87(2):167–197, 2000.

[IW89] N. Ikeda and S. Watanabe. *Stochastic differential equations and diffusion processes*. 2nd ed., North-Holland Mathematical Library, 24. North-Holland Publishing Co., Amsterdam; Kodansha, Ltd., Tokyo, 1989.

[JL05] K.M. Jansons and G.D. Lythe. Multidimensional exponential timestepping with boundary test. *SIAM J. Sci. Comput.* 27(3):793–808, 2005.

[Kal81] M.H. Kalos. *Équation du transport*. École CEA-EDF-INRIA sur les méthodes de Monte-Carlo, INRIA reports, 1981.

[La06a] A. Lagnoux. Rare event simulation. *Probab. Engrg. Inform. Sci.* 20(1):45–66, 2006.

[LM07] A. Lejay and S. Maire. Computing the principal eigenvalue of the laplace operator by a stochastic method. *Math. Comput. Simulation*, 73(3):351–363, 2007.

[LR06] A. Lagnoux Renaudie. *Analyse des modèles de branchement avec duplication des trajectoires pour l'étude des événements rares*. PhD thesis, Université Toulouse 3, 2006.

[Mai01] S. Maire. *Réduction de variance pour l'intégration numérique et pour le calcul critique en transport neutronique*. PhD thesis, Université de Toulon et de Var, 2001.

[MT99] G.N. Milstein and M.V. Tretyakov. Simulation of a space-time bounded diffusion. *Ann. Appl. Probab.*, 9(3):732–779, 1999.

[MT06] S. Maire and D. Talay. On a Monte Carlo method for neutron transport criticality computations. *IMA J. Numer. Anal.*, 26(4):657–685, 2006.

[Pin96a] R.G. Pinsky. *Positive Harmonic Functions and Diffusion*, Cambridge University Press, 1996.

[RC93] P. J. Rousseeuw and C. Croux. Alternatives to the median absolute deviation. *J. Amer. Statist. Assoc.*, 88(424):1273–1283, 1993.

[Sil86] B.W. Silverman. *Density estimation for statistics and data analysis*, Monographs on Statistics and Applied Probability. Chapman & Hall, London, 1986.

[Wil01] D. Williams. *Weighing the odds*. Cambridge University Press, Cambridge, 2001.

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