

ON A MONTE CARLO METHOD FOR NEUTRON TRANSPORT CRITICALITY COMPUTATIONS

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ABSTRACT. We give a stochastic representation of the principal eigenvalue of some homogeneous neutron transport operators. Our construction is based upon the Feynman–Kac formula for integral transport equations, and uses probabilistic techniques only. We develop a Monte Carlo method for criticality computations. We numerically test this method on various homogeneous and inhomogeneous problems, and compare our results with those obtained by standard methods.

1. INTRODUCTION

The aim of this paper is three-fold. We first study a stochastic representation of the principal eigenvalue of a simple homogeneous neutron transport operator. We then propose a Monte Carlo method for the criticality analysis of homogeneous neutron transport problems, and we test this method in a case where it can be mathematically justified. Finally, we consider more realistic inhomogeneous test-cases which suggest that the method can be applied in rather general situations.

The evolution of a population of neutrons is modelled by a density function $u(t, x, v)$ which depends on the position x in a domain D , the velocity v in a domain V , and the time t . This function is a solution of the Cauchy problem in the domain $\mathbb{R}_+ \times D \times V$,

$$(1.1) \quad \frac{\partial u}{\partial t}(t, x, v) = \mathcal{T}u(t, x, v),$$

where the neutron transport operator \mathcal{T} is defined as

$$(1.2) \quad \mathcal{T}u(t, x, v) = -v\nabla_x u(t, x, v) - \Sigma_{\text{tcs}}(x, v)u(t, x, v) + \int_V \Sigma_{\text{sf}}(x, z, v)u(t, x, z)dz + S(t, x, v).$$

Here, $S(t, x, v)$ represents a source term and $\Sigma_{\text{tcs}}(x, v)$ represents the total cross section. The definition of the function $\Sigma_{\text{sf}}(x, z, v)$ involves the scattering cross section Σ_s and the fission cross section Σ_f which characterize the physical properties of the nuclear reactor which is usually highly heterogeneous [4]. The boundary conditions depend on the behaviour of the neutrons at the boundary. In this paper we focus on the specific criticality transport equation

$$(1.3) \quad \frac{\partial u}{\partial t}(t, x, v) = \mathcal{T}^\lambda u(t, x, v),$$

where

$$\begin{aligned} \mathcal{T}^\lambda u(t, x, v) &= -v\nabla_x u(t, x, v) - \Sigma_{\text{tcs}}(x, v)u(t, x, v) + \int_V \Sigma_s(x, z, v)u(t, x, z)dz \\ &\quad + \frac{1}{\lambda} \int_V \Sigma_f(x, z, v)u(t, x, z)dz. \end{aligned}$$

In this model the production of neutrons comes from fission only. The parameter $\lambda > 0$ is related to the number of neutrons created by a fission. We will say that the model is spatially homogeneous when the coefficients Σ_{tcs} , $\Sigma_s(x, z, v)$ and Σ_f depend on the velocity variable only.

Under weak assumptions on the physical model, using analysis tools and especially the Krein-Rutman theorem, one can show that the principal eigenvalue of \mathcal{T}^λ is real and simple, and that its eigenfunction is positive: see, e.g., Mika [17]. Let α_0^λ be the principal eigenvalue of the operator \mathcal{T}^λ . If $\alpha_0^\lambda = 0$, there is a perfect balance between the production and the absorption of the neutrons. The corresponding λ is often

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called the *keff* coefficient. If $\alpha_0^\lambda < 0$, the reactor is subcritical and if $\alpha_0^\lambda > 0$, the reactor is supercritical. The number of neutrons decays or grows exponentially fast according to the sign of α_0^λ . Furthermore, under weak hypotheses, α_0^λ is a decreasing function of λ which tends to $+\infty$ when λ tends to 0 and is negative for λ large enough (see, e.g., Dautray–Lions [7]).

In criticality studies one desires to compute the value of λ for which the principal eigenvalue α_0^λ of the operator \mathcal{T}^λ is as close to zero as possible. Therefore one must find the largest value λ such that there exists a solution Ψ to the following equation in the domain $D \times V$ with appropriate boundary conditions:

$$v\nabla_x \Psi(x, v) + \Sigma_{\text{tcs}}(x, v)\Psi(x, v) - \int_V \Sigma_s(x, z, v)\Psi(x, z)dz = \frac{1}{\lambda} \int_V \Sigma_f(x, z, v)\Psi(x, z)dz.$$

For theoretical considerations see, e.g., Vidav [21]. For other criticality analyses see, e.g., Bardos et al. [3].

The numerical calculation of the *keff* coefficient and its eigenfunction by deterministic methods is achieved by using the power method on the fission part of the transport operator. Setting

$$L\Psi := v\nabla_x \Psi(x, v) + \Sigma_{\text{tcs}}(x, v)\Psi_t(x, v) - \int_V \Sigma_s(x, z, v)\Psi(x, z)dz$$

and

$$F\Psi := \int_V \Sigma_f(x, z, v)\Psi(x, z)dz,$$

the n th-step of the algorithm consists in solving the equation

$$\bar{L}\Psi_n = \frac{1}{\lambda_{n-1}}\bar{F}\Psi_{n-1},$$

where

$$\lambda_n := \lambda_{n-1} \frac{\int_D \int_V \Psi_n(x, v)dx dv}{\int_D \int_V \Psi_{n-1}(x, v)dx dv},$$

and \bar{L} and \bar{F} are discretizations of the operators L and F .

The most commonly used discretization methods are the nodal methods, finite differences and finite elements for the spatial discretization, and the so called discrete ordinates SN and spherical harmonics PN methods for the velocity variables: see, e.g., Lewis [16], Planchard [19], Karp [12], Warin [22]. With these methods a good approximation may be difficult to achieve, especially for three-dimensional problems, because of their complexity. Therefore it is worth considering Monte Carlo methods since these methods are less sensitive than deterministic methods to the dimensional effect and to the heterogeneity of the nuclear reactor: see, e.g., Lapeyre et al. [15] and Kalos [11]. Monte Carlo methods are used to approximate α_0^λ , λ being fixed: one simulates particles, computes the numbers $N(t_1)$ and $N(t_2)$ of particles which are inside the domain D at times t_1 and t_2 , and then uses the estimator

$$\alpha_0^\lambda \simeq \frac{1}{t_2 - t_1} \ln\left(\frac{N(t_2)}{N(t_1)}\right).$$

This estimator relies on the approximation

$$N(t) \simeq N(0) \exp(\alpha_0^\lambda t)$$

(see [11]). Monte Carlo methods are also used to approximate the *keff* coefficient; this consists of solving the sequence of equations

$$(1.4) \quad L\Psi_{n+1} = \frac{1}{\lambda_{n-1}}F\Psi_n$$

by means of a stochastic particle method: see, e.g., Brockway et al. [2]. Here we propose a new Monte Carlo method which avoids the numerical resolution of PDEs in the whole domain.

The organization of the paper is as follows. In Section 2 we describe the stochastic representation of the solution of the general transport equation (1.1) and of the principal eigenvalue α_0^λ of the transport operator by means of the Feynman–Kac formula. We then explain how to combine the Monte Carlo approximation of this solution and its formal eigenfunction expansion to give a numerical approximation of α_0^λ . In Section 3, we consider a particular homogeneous model; using probabilistic tools only, we obtain another stochastic representation of the principal eigenvalue. Sections 4 and 5 are devoted to the numerical computation of the

principal eigenvalue and of the criticality factor for homogeneous models. The last two sections are devoted to more realistic inhomogeneous models. Different variance reduction techniques are developed and tested.

2. REFINED MONTE CARLO SIMULATIONS FOR CRITICALITY STUDIES OF SPATIALLY HOMOGENEOUS AND INHOMOGENEOUS MODELS

Consider the neutron transport operator \mathcal{T} defined in (1.2). As explained in our introduction, we aim to approximate by a Monte Carlo method the principal eigenvalue of the operator \mathcal{T} in order to determine the k_{eff} coefficient. Of course, the principal eigenvalue may not be isolated and simple. Several sets of sufficient conditions are available in the literature: see, e.g., Dautray–Lions [7] and Mokhtar–Kharroubi [18].

2.1. A deterministic representation of the principal eigenvalue. We recall some properties of \mathcal{T} (see Chapters 1 and 21 in Dautray–Lions [7]). Suppose that \mathcal{T} admits eigenvalues with finite multiplicity and no accumulation point in a strip $\{z \in \mathcal{C}; A_1 < \operatorname{Re} z \leq A_2\}$, the remaining part of the spectrum being located in the half-space $\{z \in \mathcal{C}; \operatorname{Re} z \leq A_1\}$. Then the operator \mathcal{T} is the infinitesimal generator of a semi-group $G(t)$ of the class \mathcal{C}^0 in $L^2(D \times V)$; the spectrum of $G(t)$ admits a principal eigenvalue α_0 which is real and simple. Moreover, there exists $\beta < \alpha_0$ such that

$$(2.1) \quad G(t) = e^{\alpha_0 t} P_0 + \mathcal{O}(e^{\beta t}),$$

where P_0 is the projector in $L^2(D \times V)$ on the eigenspace associated to α_0 (see [7, Chap. 21, Sec. 3, proof of Prop. 6]). Therefore, if D is a bounded domain and $u(t, x, v)$ is the solution to the Cauchy problem (1.3) with absorption boundary conditions (no incoming neutrons, see below) and initial condition $u(0, x, v) = u_0(x, v)$, one has

$$(2.2) \quad u(t, x, v) = e t \mathcal{T} u_0(x, v) = G(t) u_0(x, v) = e \alpha_0 t P_0 u_0(x, v) + \mathcal{O}(e \beta t) \text{ in } L^2(D \times V).$$

Remark. For example, the following assumptions ensure the above property for the spectrum of $G(t)$: the domain D is bounded and convex; V is a closed ball which includes 0; the kernels Σ_s and Σ_f do not depend on x (see [7, Chap. 21, Sec. 3]).

Let E be a subdomain of $D \times V$. Set

$$(2.3) \quad g_E(t) = \frac{1}{\operatorname{vol}(E)} \int \int_E u(t, x, v) \, dx dy.$$

It results from (2.2) that

$$(2.4) \quad \lim_{t \rightarrow \infty} \frac{1}{t} \log g_E(t) = \alpha_0.$$

We now aim to deduce a Monte Carlo method from that formula.

2.2. Transport processes and Feynman–Kac formulae.

2.2.1. Transport processes for transport equations in $\mathbb{R}_+ \times \mathbb{R}^k \times V$. Consider general transport equations in $\mathbb{R}_+ \times D \times V := \mathbb{R}_+ \times \mathbb{R}^k \times V$, that we write in the form

$$\mathcal{T}u(t, x, v) := b(x, v) \nabla_x u(t, x, v) + \Theta(x, v) \left[\int_V u(t, x, z) \Pi^{x, v}(z) dz - u(t, x, v) \right] + c(x, v) u(t, x, v)$$

which appears to be convenient for probabilistic interpretations.

Such equations describe particles which move and collide at random times with particles of another type. The motion of each moving particle can be described by a stochastic process X_t which solves the differential equation

$$(2.5) \quad \frac{dX_t}{dt} = b(X_t, V_t),$$

where V_t is a jump process which models the velocity of the particle; the jump times of (V_t) are the times at which the particle collides.

Suppose that the function b is measurable and

$$\exists K > 0, \quad |b(x_1, v) - b(x_2, v)| \leq K |x_1 - x_2| \text{ for all } x_1, x_2, v.$$

The law of the velocity V_t after a collision, knowing that $(X_t, V_t) = (x, v)$ just before the collision, has a bounded density denoted by $\Pi^{x, v}(z)$ which is measurable w.r.t. (x, v, z) . We now describe the law of the

collision times. Let T_n be the elapsed time between the n -th and $(n+1)$ -st collisions. The conditional law of T_n , knowing that $(X_t, V_t) = (x, v)$ when the n -th collision occurs, has the following distribution function:

$$F^{x,v}(t) = 1 - \exp \left[- \int_0^t \Theta(\xi_s(x, v), v) ds \right],$$

where $\xi_s(x, v)$ is the solution of

$$\frac{d\xi_s}{ds} = b(\xi_s, v)$$

with $\xi_0 = x$, and the function Θ is measurable, positive and bounded. Under these assumptions, it is well known that the stochastic transport process (X_t, V_t) is well defined and is a strong Markov process (see, e.g., [6]).

2.2.2. Feynman–Kac formulae. Suppose first that $D = \mathbb{R}^k$ and that the functions u_0 and c are measurable and bounded. Then the solution $u(t, x, v)$ satisfies the Feynman–Kac formula

$$(2.6) \quad u(t, x, v) = \mathbb{E}_{x,v} \left[u_0(X_t, V_t) \exp \left(\int_0^t c(X_s, V_s) ds \right) \right],$$

where $\mathbb{E}_{x,v}$ is the law of the Markov process (X_t, V_t) starting at point x with velocity v at time 0.

Suppose now that D is a bounded domain. We suppose that there are no incoming neutrons, that is,

$$(2.7) \quad \begin{cases} u(t, x, v) = 0 \text{ for all } x \text{ on the boundary of } D \text{ such that } b(x, v) \cdot n(x) > 0, \\ \text{where } n(x) \text{ denotes the inward normal vector to the boundary.} \end{cases}$$

This boundary condition is the so called ‘‘absorption Dirichlet boundary condition’’. The Feynman–Kac formula then writes

$$(2.8) \quad u(t, x, v) = \mathbb{E}_{x,v} \left[\mathbb{I}_{\tau^D > t} u_0(X_t, V_t) \exp \left(\int_0^t c(X_s, V_s) ds \right) \right],$$

where τ^D is the first exit time of (X_t) from D . See, e.g., [6] and [1].

We can rewrite (2.8) in terms of a killed transport process: let (X_t^D, V_t^D) denote the killed Markov process defined by

$$\mathbb{P}((X_t^D, V_t^D) \in B) = \mathbb{P}((X_t, V_t) \in B, \tau^D > t)$$

for all Borel subset B of $D \times V$. Then

$$(2.9) \quad u(t, x, v) = \mathbb{E}_{x,v} \left[u_0(X_t^D, V_t^D) \exp \left(\int_0^t c(X_s^D, V_s^D) ds \right) \right].$$

2.3. Monte Carlo methods.

2.3.1. Standard Monte Carlo simulations. The approximation of $u(t, x, v)$ can be obtained using a standard Monte Carlo method. Let the processes $Z_t^{(i)}(x, v)$, $1 \leq i \leq N$, be independent copies of the process

$$Z_t(x, v) = \mathbb{I}_{\tau^D > t} u_0(X_t, V_t) \exp \left(\int_0^t c(X_s, V_s) ds \right)$$

where (X_t, V_t) is issued from (x, v) . Then

$$u(t, x, v) \simeq \frac{1}{N} \sum_{i=1}^N Z_t^{(i)}(x, v).$$

To compute the mean value $g_E(t)$, we simulate the processes $Z_t^{(i)}(x^i, v^i)$, $1 \leq i \leq N$, where the N starting points (x^i, v^i) are independent and uniformly distributed in E , and we compute

$$(2.10) \quad \overline{g_E}(t) := \frac{1}{N} \sum_{i=1}^N Z_t^{(i)}(x^i, v^i).$$

In view of (2.4) and (2.10) one may thus compute α_0 by using a Monte Carlo method. In Section 4 we will see that the accuracy is poor because the variance of the simulation quickly increases with t . We therefore

recommend the following two variants. Of course, their efficiency will decrease when β is very close to α_0 . However this difficulty occurs with any other numerical method.

2.3.2. *Interpolation method.* We deduce from (2.2) that

$$(2.11) \quad \frac{1}{t} \log(g_E(t)) \simeq \alpha_0 + \frac{\log(K_0)}{t} + o(e^{(\beta-\alpha_0)t})$$

for all t large enough and all subdomains E of the domain D . Choose t_1, t_2 large enough and define the new estimator

$$\alpha_0(t_1, t_2) = \frac{\log(\bar{g}_2) - \log(\bar{g}_1)}{t_2 - t_1}$$

of α_0 , where we have set: \bar{g}_E is the Monte Carlo approximation of g_E defined as in (2.3) and $\bar{g}_i := g_E(t_i)$ ($i = 1, 2$). Using the confidence interval

$$\bar{g}_1 - 1.96 \frac{\sigma_1}{\sqrt{N}} \leq g_1 \leq \bar{g}_1 + 1.96 \frac{\sigma_1}{\sqrt{N}}$$

and assuming that $\frac{\sigma_1}{\bar{g}_1 \sqrt{N}} \ll 1$ we obtain

$$\log(\bar{g}_1) - 1.96 \frac{\sigma_1}{\bar{g}_1 \sqrt{N}} \leq \log(g_1) \leq \log(\bar{g}_1) + 1.96 \frac{\sigma_1}{\bar{g}_1 \sqrt{N}}.$$

We thus have

$$\frac{\log\left(\frac{g_2}{g_1}\right)}{t_2 - t_1} - \frac{1.96N^{-\frac{1}{2}}}{t_2 - t_1} \left(\frac{\sigma_1}{\bar{g}_1} + \frac{\sigma_2}{\bar{g}_2}\right) \leq \alpha_0(t_1, t_2) \leq \frac{\log\left(\frac{g_2}{g_1}\right)}{t_2 - t_1} + \frac{1.96}{\sqrt{N}(t_2 - t_1)} \left(\frac{\sigma_1}{\bar{g}_1} + \frac{\sigma_2}{\bar{g}_2}\right)$$

with probability 0.9 at least.

2.3.3. *Least-squares approximation.* In order to make a global use of the information given by the computation of the solution at the different times, one may use least-squares approximations of α_0 and $\log(K_0)$ by choosing times t_1, \dots, t_m and minimizing

$$\sum_{i=1}^m \left(\alpha_0 + \frac{\beta}{t_i} - \frac{1}{t_i} \log(g_E(t_i)) \right)^2.$$

Here we continue to assume that the remainder term of (2.2) is negligible. This procedure provides an estimator of α_0 which, according to our numerical experiments, seems more accurate than the previous ones.

Before analyzing numerically the above refinements of the direct Monte Carlo simulations (see Sections 4-7 below), we consider a homogeneous one-dimensional model which allows us to express α_0 in terms of the tail of the distribution of the first exit time of (X_t) from the domain D .

3. A PROBABILISTIC REPRESENTATION OF THE PRINCIPAL EIGENVALUE

In this section we show that, for particular models, (2.4) can be replaced by an equality of the type

$$\alpha_0 = \lim_{t \rightarrow \infty} \frac{1}{t} \log(u(t, x, v))$$

for all (x, v) , which will allow us to also prove that α_0 can be approximated by simulating exit times of (X_t) only. Our technique is fully probabilistic. Our assumptions essentially concern the sub-Markovian transition operator of a killed stochastic transport process. Notice that the expansion (2.2) holds almost everywhere only, whereas the probabilistic representation holds everywhere, and that it may allow one to study the sensitivity of the principal eigenvalue with respect to various parameters of the model, as it has been done for elliptic operators and small viscosity parameters (see, e.g., Kifer [14]).

3.1. The principal eigenvalue of an elliptic operator. The stochastic representation of the principal eigenvalue of a general elliptic operator \mathcal{L} is usually achieved by combining the Feynman–Kac formula for the Cauchy problem

$$\begin{cases} \frac{\partial u}{\partial t}(t, x) = \mathcal{L}u(t, x), \\ u(x, 0) = 1, \end{cases}$$

and, when it exists, the eigenfunction expansion of the function,

$$u(t, x) = \sum_{j=0}^{\infty} c_j \exp(\alpha_j t) \Psi_j(x),$$

where the α_j 's are the eigenvalues of \mathcal{L} arranged in decreasing order and the Ψ_j 's are the corresponding eigenfunctions. Using this method, Kac [10] gives the following stochastic representation for the principal eigenvalue of the operator

$$\mathcal{L}u = \frac{1}{2} \Delta u - ku,$$

where k is a continuous function from \mathbb{R} in $[0, \infty)$ such that $\lim_{x \rightarrow \pm\infty} k(x) = \infty$:

$$\alpha_0 = \lim_{t \rightarrow \infty} \frac{1}{t} \log \mathbb{E}_x \exp \left(- \int_0^t k(B_s) ds \right)$$

for all $x \in \mathbb{R}$, where B_t is a Brownian motion. Freidlin [8] considers a general elliptic operator \mathcal{L} with Dirichlet boundary conditions in a bounded domain D in \mathbb{R}^k . Let τ^D be the first exit time from D of the stochastic process X_t^x whose generator is \mathcal{L} . The principal eigenvalue α_0 satisfies

$$\alpha_0 = \lim_{t \rightarrow +\infty} \frac{1}{t} \log \mathbb{P}(\tau^D > t).$$

Probabilistic proofs of this result are given in Freidlin [8] and in Friedman [9]. These proofs deeply use the fact that \mathcal{L} is the generator of a diffusion process. As we are concerned by generators of transport processes we follow another method developed by Kifer [14]. This method relies on the hypothesis that the transition probability of the killed diffusion process has a density which is bounded from above and below by strictly positive constants. For transport processes, this hypothesis may be too stringent: for example, consider the model studied in Subsection 3.3 below; for small times, the transition density may not exist and for large times, this density tends to 0 when the space coordinate tends to 0 and the velocity coordinate is positive. We thus have to add arguments to Kifer's ones.

3.2. The principal eigenvalue of a transport operator. Let ρ be a real number. Consider bounded domains D and V , and the Cauchy problem in $\mathbb{R}_+ \times D \times V$:

$$(3.1) \quad \frac{\partial u}{\partial t}(t, x, v) = b(x, v) \nabla_x u(t, x, v) + \Theta(x, v) \left[\int_V u(t, x, z) \Pi^{x, v}(z) dz - u(t, x, v) \right] + \rho u(t, x, v),$$

with a bounded initial condition $u(0, x, v) = u_0(x, v)$ and the absorption boundary condition (2.7). We suppose that the assumptions made in the subsection 2.2.2 on b , Θ and $\Pi^{x, v}$ hold in force. In view of (2.8) one has

$$(3.2) \quad u(t, x, v) = \mathbb{E}_{x, v} [u_0(X_t, V_t) \exp(\rho t) \mathbb{1}_{t < \tau^D}],$$

where τ^D is the first exit time of (X_t) from D .

We state a classical result for Markov processes which is a straightforward consequence of the fact that the function

$$t \rightarrow \log \sup_{(x, v) \in D \times V} \mathbb{P}_{x, v}(\tau^D > t)$$

is subadditive.

Lemma 3.1. *Suppose that b , Θ and $\Pi^{x, v}$ satisfy the hypotheses listed in the Subsection 2.2. The quantity*

$$\frac{1}{t} \log \sup_{(x, v) \in D \times V} \mathbb{P}_{x, v}(\tau^D > t)$$

has a finite limit β_ρ when t goes to $+\infty$.

We now prove that we can remove the supremum in the previous formula. The hypotheses of the following result seem rather abstract. However we will see in Subsection 3.3 below an example where these hypotheses can be verified without too much difficulty, and that the guidelines of our verification can obviously be adapted to other models.

Recall that (X_t^D, V_t^D) denotes the killed Markov process defined by

$$\mathbb{P}((X_t^D, V_t^D) \in B) = \mathbb{P}((X_t, V_t) \in B, \tau^D > t)$$

for all Borel subset B of D .

Theorem 3.2. *In addition to the hypotheses of Lemma 3.1, assume that there exists $T^* > 0$ such that, for all $T > T^*$, there exists a positive and measurable function $p^D(T, (x, v), (x_1, v_1))$ satisfying*

$$\mathbb{E}_{x,v}[f(X_t, V_t)\mathbb{1}_{\tau^D > t}] = \mathbb{E}_{x,v}[f(X_t^D, V_t^D)] = \int_V \int_D p^D(t, (x, v), (x_1, v_1))f(x_1, v_1)dx_1dv_1$$

for all bounded Borel measurable functions f . In addition, suppose that there exists a Borel subset A of $D \times V$ such that

$$(3.3) \quad \operatorname{ess\,inf}_{(x_1, v_1) \in A} p^D(T, (x, v), (x_1, v_1)) > 0,$$

and

$$(3.4) \quad \operatorname{ess\,sup}_{(x_1, v_1) \in D \times V} p^D(T, (x, v), (x_1, v_1)) < \infty.$$

Finally, suppose that

$$(3.5) \quad \exists \kappa > 0, \int \int_A \mathbb{P}_{x,v}(\tau^D > t)dx dv \geq \kappa \int \int_{A^c} \mathbb{P}_{x,v}(\tau^D > t)dx dv \text{ for all } t > 0.$$

i) Let β_ρ be defined as in the preceding lemma. Then, for all $(x, v) \in D \times V$ we have

$$(3.6) \quad \lim_{t \rightarrow +\infty} \frac{1}{t} \log(\mathbb{P}_{x,v}(\tau^D > t)) = \beta_\rho.$$

ii) Assume that $0 < c_1 \leq u_0(x, v) \leq c_2 < \infty$ for some positive real numbers c_1 and c_2 . For all $(x, v) \in D \times V$ we have

$$\lim_{t \rightarrow \infty} \frac{1}{t} \log(u(t, x, v)) = \beta_\rho + \rho.$$

Remark. Under the assumptions made in Subsection 2.1, in view of the expansion (2.2) and using (3.6), we have

$$(3.7) \quad \alpha_0 = \lim_{t \rightarrow +\infty} \frac{1}{t} \log(\mathbb{P}_{x,v}(\tau^D > t)) + \rho.$$

A Monte Carlo approximation of α_0 can thus consist in approximating the distribution function of τ^D for an arbitrarily fixed initial condition: see Sections 4 and 5 below for numerical experiments.

Proof. The claim ii) is a straightforward consequence of i) since, in view of (2.8), we have

$$c_1 \exp(\rho t) \mathbb{P}_{x,v}(\tau_D > t) \leq u(t, x, v) \leq c_2 \exp(\rho t) \mathbb{P}_{x,v}(\tau^D > t).$$

We now prove i) by adapting a proof used in Kifer [14, chap.III]. Fix (x, v) in D and let $t > T$. We have

$$\mathbb{P}_{x,v}(\tau^D > t) = \int_V \int_D p^D(t, (x, v), (x_1, v_1))dx_1dv_1.$$

From the Markov property it follows that

$$\mathbb{P}_{x,v}(X_t^D \in D) = \int_V \int_D p^D(T, (x, v), (x_1, v_1)) \mathbb{P}_{x_1, v_1}(\tau^D > t - T)dx_1dv_1,$$

which implies the following two inequalities

$$(3.8) \quad \mathbb{P}_{x,v}(X_t^D \in D) \geq \operatorname{ess\,inf}_{(x_1, v_1) \in A} p^D(T, (x, v), (x_1, v_1)) \int \int_A \mathbb{P}_{x_2, v_2}(\tau^D > t - T)dx_2dv_2,$$

and

$$(3.9) \quad \begin{aligned} \mathbb{P}_{x,v}(X_t^D \in D) &\leq \operatorname{ess\,sup}_{(x_1,v_1) \in D \times V} p^D(T, (x,v), (x_1,v_1)) \times \int_V \int_D \mathbb{P}_{x_2,v_2}(\tau^D > t - T) dx_2 dv_2 \\ &\leq \left(1 + \frac{1}{\kappa}\right) \operatorname{ess\,sup}_{(x_1,v_1) \in D \times V} p^D(T, (x,v), (x_1,v_1)) \times \int_A \int_A \mathbb{P}_{x_2,v_2}(\tau^D > t - T) dx_2 dv_2, \end{aligned}$$

where κ is as in (3.5). From Lemma 3.1 and inequality (3.9) we have

$$(3.10) \quad \beta_\rho \leq \liminf_{t \rightarrow +\infty} \frac{1}{t} \log \int_A \int_A \mathbb{P}_{x_2,v_2}(\tau^D > t - T) dx_2 dv_2.$$

In addition, in view of (3.8), we have

$$(3.11) \quad \beta_\rho \geq \limsup_{t \rightarrow +\infty} \frac{1}{t} \log \mathbb{P}_{x,v}(\tau^D > t) \geq \limsup_{t \rightarrow +\infty} \frac{1}{t} \log \int_A \int_A \mathbb{P}_{x_2,v_2}(\tau^D > t - T) dx_2 dv_2.$$

We gather the inequalities (3.11) and (3.10): it turns out that all the inequalities are, in fact, equalities. In particular,

$$\lim_{t \rightarrow +\infty} \frac{1}{t} \log(\mathbb{P}_{x,v}(\tau^D > t)) = \beta_\rho.$$

□

3.3. The principal eigenvalue of a homogeneous one-dimensional model. The aim of this subsection is to show how the hypotheses of Theorem 3.2 can be verified in practice. We consider a rather simple model which, however, requires nontrivial arguments. For technical reasons and to simplify the presentation, we limit ourselves to a one-dimensional model. Nevertheless, our presentation involves the main ingredients to handle multi-dimensional homogeneous models as well.

3.3.1. Description of the model. Consider the Cauchy problem in $\mathbb{R}_+ \times \mathbb{R} \times V$:

$$(3.12) \quad \frac{\partial u}{\partial t}(t, x, v) = -v \frac{\partial u}{\partial x}(t, x, v) + c \left\{ \frac{1}{2(1-\delta)} \int_{V_\delta} u(t, x, v') dv' - u(t, x, v) \right\} + (c-1)u(t, x, v),$$

with a positive initial condition $(0, x, v) = u_0(x, v)$ and boundary absorption conditions (2.7). We suppose:

$$(3.13) \quad \begin{cases} \text{the space domain is } D := (0, d) \text{ and the velocity domain is} \\ V_\delta := (-1, -\delta) \cup (\delta, 1) \text{ with } 0 < \delta < 1; \\ \text{the constant } c \text{ is strictly positive;} \\ u(t, 0, v) = 0 \text{ for all } v > 0 \text{ and } t \geq 0; \\ u(t, d, v) = 0 \text{ for all } v < 0 \text{ and } t \geq 0. \end{cases}$$

According to Subsection 2.2.2, we construct the following stochastic transport process:

$$(3.14) \quad \begin{cases} \frac{dX_t}{dt} = -V_t; \\ \text{the law of the velocity } V_t \text{ after a collision is the uniform law on } V_\delta; \\ \text{the distribution function of the conditional law, knowing that } (X_t, V_t) = (x, v) \\ \text{when the } n\text{-th collision occurs, of the elapsed time} \\ \text{before the next collision is } F^{x,v}(t) = 1 - \exp(-ct). \end{cases}$$

Notice that the condition that the velocity is bounded away from 0 is also encountered in spectral studies of transport operators: cf., e.g., Dautray–Lions [7, Chap. 21]).

We now prove that the hypotheses of theorem 3.2 are satisfied, that is, inequalities (3.3), (3.4), and (3.5). We choose $A := (\frac{d}{4}, \frac{3d}{4}) \times V_\delta$.

3.3.2. *A bound from above for the density $p^D(t, (x, v), (x_1, v_1))$.* In order to prove that (3.4) holds, we start with an elementary result concerning the transport process related to equation (3.12) without boundary conditions, that is, when $D = \mathbb{R}$. We still assume that $c > 0$.

Lemma 3.3. *Let (X_t, V_t) be the transport process defined as in (3.14). If the law of (X_0, V_0) admits a density $p_0(\xi, \nu)$ in $L^\infty(\mathbb{R} \times V_\delta)$ with respect to the Lebesgue measure on $\mathbb{R} \times V_\delta$, then (X_t, V_t) admits a density $p(t, \xi, \nu)$ in $L^\infty(\mathbb{R} \times V_\delta)$ and*

$$(3.15) \quad \forall t > 0, \operatorname{ess\,sup}_{\xi \in \mathbb{R}} \int_{V_\delta} p(t, \xi, \nu) d\nu \leq \operatorname{ess\,sup}_{\xi \in \mathbb{R}} \int_{V_\delta} p(0, \xi, \nu) d\nu.$$

Proof. The existence of the density is a standard result on transport jump processes (see Dautray-Lions [7, chap.3]). In order to get the bound from above, we observe that the density $p(t, \xi, \nu)$ is a weak solution to the Fokker–Planck equation in $\mathbb{R}_+ \times \mathbb{R} \times V_\delta$

$$\frac{\partial p}{\partial t}(t, \xi, \nu) = \nu \frac{\partial p}{\partial \xi}(t, \xi, \nu) + c \left\{ \frac{1}{2(1-\delta)} \int_{V_\delta} p(t, \xi, \nu') d\nu' - p(t, \xi, \nu) \right\}$$

with initial condition

$$p(0, \xi, \nu) = p_0(\xi, \nu).$$

As p_0 is bounded and measurable, we can interpret the above Fokker–Planck equation as a transport equation of the type (1.1), and thus write $p(t, \xi, \nu)$ as the solution of the integral equation

$$p(t, \xi, \nu) = p_0(\xi + \nu t, \nu) \exp(-ct) + \frac{c}{2(1-\delta)} \int_0^t \int_{V_\delta} p(s, \xi + \nu(t-s), \nu') \exp(c(s-t)) d\nu' ds$$

(see [6, Chap.3, Sec. 3.2.1]). Gronwall's lemma implies that $p(t, \xi, \nu)$ is bounded and thus integrable w.r.t. ν . A second application of Gronwall's lemma then leads to (3.15). \square

We now consider problems satisfying (3.13).

Proposition 3.4. *For all $(x, v) \in D$ and $T > \frac{3d}{\delta}$, the transition probability of (X_T^D, V_T^D) starting at (x, v) admits a density $p^D(T, (x, v), (x_1, v_1))$ with respect to the Lebesgue measure on D . Moreover, there exists $M > 0$ such that*

$$\operatorname{ess\,sup}_{(x_1, v_1) \in D} p^D(T, (x, v), (x_1, v_1)) \leq M.$$

Remark. We emphasize that, in the above statement and in the proof below, the specific form of the velocity domain V_δ is used to ensure the existence of the density p^D . Indeed, suppose that $V_\delta = (-1, 1)$ (which corresponds to the Lehner–Wing model that we will consider in Section 4 for numerical illustrations). Then, for all $t > 0$, one has $\mathbb{P}_{x,0}(X_t^D = x, V_t^D = 0, S_1 > t) > 0$, and therefore the law of (X_t^D, V_t^D) has an atomic component.

Proof. We first prove the existence of the density p^D . Let B_0 be a Borel subset of D with zero Lebesgue measure. We aim to show that

$$\mathbb{P}_{x,v}((X_T^D, V_T^D) \in B_0) = 0$$

for all $T > \frac{3d}{\delta}$. Fix $T > \frac{3d}{\delta}$. We have

$$\mathbb{P}_{x,v}((X_T^D, V_T^D) \in B_0) = \mathbb{P}_{x,v}((X_T^D, V_T^D) \in B_0, S_2 \leq T),$$

where S_2 is the second collision time. Indeed, since $T > \frac{3d}{\delta}$, if two collisions do not occur before T , the process has been absorbed at the boundary, and hence

$$\mathbb{P}_{x,v}((X_T^D, V_T^D) \in B_0, S_2 > T) = 0.$$

We also have

$$\mathbb{P}_{x,v}((X_T^D, V_T^D) \in B_0, S_2 \leq T) \leq \mathbb{P}_{x,v}((X_T, V_T) \in B_0, S_2 \leq T),$$

where (X_t, V_t) is the Markov transport process associated to the transport equation in the whole space. We now observe

$$\mathbb{P}_{x,v}((X_T, V_T) \in B_0, S_2 \leq T) = \mathbb{E} \int \int_G \mathbb{P}_{x+\theta_1 v + \theta_2 V_1, V_2}((X_{T-\theta_1-\theta_2}, V_{T-\theta_1-\theta_2}) \in B_0) c^2 e^{-c\theta_1 - c\theta_2} d\theta_1 d\theta_2,$$

where $G := \{0 < \theta_1, 0 < \theta_2, \theta_1 + \theta_2 \leq T\}$, and V_1, V_2 are independent copies of the uniform law on V_δ . Let (θ_1, θ_2) be in G . The pair

$$(x + \theta_1 v + \theta_2 V_1, V_2)$$

admits a density with respect to the Lebesgue measure, and therefore Lemma 3.3 implies that

$$\mathbb{P}_{x+\theta_1 v+\theta_2 V_1, V_2}((X_{T-\theta_1-\theta_2}, V_{T-\theta_1-\theta_2}) \in B_0) = 0 \text{ a.s..}$$

We thus have proved the existence of the density $p^D(T, (x, v), (x_1, v_1))$.

We now exhibit a bound from above for $p^D(T, (x, v), (x_1, v_1))$. Without loss of generality we assume $v > 0$. For technical reasons we now need to consider the first three collision times. We observe that, since $T > \frac{3d}{\delta}$,

$$\mathbb{P}_{x,v}((X_T^D, V_T^D) \in B_0, S_3 > T) = 0.$$

Set $\tilde{G} := \{0 < \theta_i, (1 \leq i \leq 3), \theta_1 + \theta_2 + \theta_3 \leq T\}$. Now, for all Borel subset B of D we have

$$\begin{aligned} & \mathbb{P}_{x,v}((X_T^D, V_T^D) \in B) \\ & \leq \mathbb{E} \int \int_{\tilde{G}} \mathbb{P}_{x+\theta_1 v+\theta_2 V_1+\theta_3 V_2, V_3}((X_{T-\theta_1-\theta_2-\theta_3}, V_{T-\theta_1-\theta_2-\theta_3}) \in B) c^2 e^{-c(\theta_1 + \theta_2 + \theta_3)} d\theta_3 d\theta_2 d\theta_1. \end{aligned}$$

Fix θ_1, θ_2 and θ_3 in \tilde{G} . In view of Lemma 3.3, the law of (X_s, V_s) has a density $q_{x,v,\theta_1,\theta_2,\theta_3}(s, \xi, \nu)$ when the initial law is the law of $(x + \theta_1 v + \theta_2 V_1 + \theta_3 V_2, V_3)$. It is easy to check that the density of $x + \theta_1 v + \theta_2 V_1 + \theta_3 V_2$ is bounded from below by $C_\delta \inf(\frac{1}{\theta_2}, \frac{1}{\theta_3})$ for some C_δ which does not depend on the θ_i 's. Observe that this bound from below is a function of (θ_2, θ_3) which is locally integrable w.r.t. $d\theta_2 d\theta_3$ around the origin. We now use (3.15) and, for some new constant C_δ we get

$$\mathbb{P}_{x,v}((X_T^D, V_T^D) \in B) \leq C_\delta \int \int_{\tilde{G}} \inf(\frac{1}{\theta_2}, \frac{1}{\theta_3}) e^{-c(\theta_1 + \theta_2 + \theta_3)} d\theta_3 d\theta_2 d\theta_1 < \infty.$$

That completes the proof. \square

3.3.3. A bound from below for the transition density of (X_t^D, V_t^D) . Our aim is now to prove that (3.4) and (3.5) hold.

Proposition 3.5. *As above, let $T > \frac{3d}{\delta}$ and let A denote the set $(\frac{d}{4}, \frac{3d}{4}) \times V_\delta$. (Improperly!) set*

$$A^c := ((0, \frac{d}{4}) \cup (\frac{3d}{4}, d)) \times V_\delta.$$

i) We have

$$\text{ess inf}_{(y,u) \in A} p^D(T, (x, v), (y, u)) > 0.$$

ii) There is a constant $\kappa > 0$, such that

$$\int \int_A \mathbb{P}_{x,v}(\tau^D > t) dx dv \geq \kappa \int \int_{A^c} \mathbb{P}_{x,v}(\tau^D > t) dx dv \text{ for all } t > 0.$$

Proof. We first prove ii). Let $(x, v) \in A$ and let t_A (respectively, t_D) be the deterministic exit time from A (respectively, D) in free motion from x with velocity v . We have

$$\begin{aligned} \mathbb{P}_{x,v}(\tau^D > t) & \geq \mathbb{P}_{x,v}(X_t^D \in D, t_A \leq S_1 \leq t_D) \\ & = \mathbb{E} \int_{t_A}^{t_D} \mathbb{P}_{x+s_1 v, Y}(X_{t-s_1}^D \in D) \psi_{S_1}(s_1) ds_1, \end{aligned}$$

where Y is uniformly distributed on the velocity space and

$$\psi_{S_1}(s_1) = c \exp(-cs_1).$$

We obviously have

$$\mathbb{P}_{x+s_1 v, Y}(X_{t-s_1}^D \in D) \geq \mathbb{P}_{x+s_1 v, Y}(X_t^D \in D) \text{ a.s.,}$$

and therefore

$$\mathbb{P}_{x,v}(\tau^D > t) \geq \frac{1}{2(1-\delta)} \mathbb{E} \int_{V_\delta} \int_{t_A}^{t_D} \mathbb{P}_{x+s_1 v, v_1}(X_t^D \in D) \psi_{S_1}(s_1) ds_1 dv_1.$$

First assume that $v < 0$. We then have $x + vt_D = 0$ and $x + vt_A = \frac{d}{4}$. Using that $\psi_{S_1}(s_1) \geq c \exp(-cd)$ and the change of variable $x_1 = x + s_1 v$, and observing that $1/|v| > 1$, we get

$$\mathbb{P}_{x,v}(\tau^D > t) \geq \frac{c}{2(1-\delta)} \exp\left(-\frac{cd}{\delta}\right) \int_{V_\delta} \int_0^{\frac{d}{4}} \mathbb{P}_{x_1, v_1}(X_t^D \in D) dx_1 dv_1.$$

On the other hand, if $v > 0$, we have $x + vt_D = d$ and $x + vt_A = \frac{3d}{4}$. Proceeding as above we get

$$\mathbb{P}_{x,v}(\tau^D > t) \geq \frac{c}{2(1-\delta)} \exp\left(-\frac{cd}{\delta}\right) \int_{V_\delta} \int_{\frac{3d}{4}}^d \mathbb{P}_{x_1, v_1}(X_t^D \in D) dx_1 dv_1.$$

Hence

$$\mathbb{P}_{x,v}(\tau^D > t) + \mathbb{P}_{d-x,-v}(\tau^D > t) \geq \frac{c}{2(1-\delta)} \exp\left(-\frac{cd}{\delta}\right) \times \int \int_{A^c} \mathbb{P}_{x_1, v_1}(X_t^D \in D) dx_1 dv_1.$$

Using the symmetry of the domain, we have

$$\mathbb{P}_{x,v}(\tau^D > t) = \mathbb{P}_{d-x,-v}(\tau^D > t),$$

which implies that

$$\mathbb{P}_{x,v}(\tau^D > t) \geq \frac{c}{4(1-\delta)} \exp\left(-\frac{cd}{\delta}\right) \int \int_{A^c} \mathbb{P}_{x_1, v_1}(X_t^D \in D) dx_1 dv_1.$$

It remains to integrate w.r.t. x and v to obtain ii).

We now turn to i). It suffices to prove that

$$\exists \beta > 0, P_{x,v}(X_T^D \in (y - \varepsilon, y + \varepsilon), V_T^D \in (u - \frac{\varepsilon}{2T}, u + \frac{\varepsilon}{2T})) > \beta \varepsilon^2$$

for all $(x, v) \in D \times V$ and $(y, u) \in A$ and all ε small enough. We first build a deterministic path starting at (x, v) , reaching (y, u) at time T and staying sufficiently far from the boundary of D . We define γ_1 such that the location x_1 at the first collision time s_1 satisfies $\gamma_1 \geq \frac{\inf(x, 1-x)}{2}$. Then the motion goes toward y and stays at a distance at least $\frac{\gamma}{2}$ from the boundary by moving and colliding $N - 1$ times at distinct times s_j with velocities v_j . The last part of the path at the velocity u lasts $T - s_{N-1}$. The idea is now to build sufficiently many random paths from this deterministic path. We let S_j be the collisions times and V_j^D the corresponding velocities. We also let $\gamma_2 = \min(\gamma_1, \frac{\gamma}{2})$, choose $\varepsilon > 0$ small compared to γ_2 , and η such that the intervals $G_j = [s_j - \eta, s_j + \eta]$ and $H_j = [v_j - \eta, v_j + \eta]$ are included in the support of the S_j and the V_j^D . Thus all the paths that we can build from these values stay in D . We now define

$$\begin{aligned} D_1 &= [y - \varepsilon \leq x + S_1 v + \sum_{j=1}^{N-2} (S_{j+1} - S_j) V_j^D + (T - S_{N-1}) V_{N-1}^D \leq y + \varepsilon], \\ D_2 &= [S_j \in G_j \ \forall j \leq N - 1], \\ D_3 &= [V_j^D \in H_j \ \forall j \leq N - 2], \\ D_4 &= [u - \frac{\varepsilon}{2T} \leq V_{N-1}^D \leq u + \frac{\varepsilon}{2T}], \\ D_5 &= [S_N \geq T]. \end{aligned}$$

We thus have

$$\mathbb{P}_{x,v}((X_T^D, V_T^D) \in ([y - \varepsilon, y + \varepsilon] \times [u - \frac{\varepsilon}{2T}, u + \frac{\varepsilon}{2T}])) \geq \mathbb{P}_{x,v}(D_1 \cap D_2 \cap D_3 \cap D_4 \cap D_5).$$

Integrating with respect to the laws of V_{N-1}^D and S_N , using that $S_{N-1} \leq T \leq S_N$ and letting

$$\begin{aligned} D_6 &= [y - \varepsilon \leq x + S_1 v + \sum_{j=1}^{N-2} (S_{j+1} - S_j) V_j^D + (T - S_{N-1})(u - \frac{\varepsilon}{2T})], \\ D_7 &= [x + S_1 v + \sum_{j=1}^{N-2} (S_{j+1} - S_j) V_j^D + (T - S_{N-1})(u + \frac{\varepsilon}{2T}) \leq y + \varepsilon], \end{aligned}$$

we can bound the previous expression from below by

$$\frac{\varepsilon}{2T(1-\delta)} \exp(-cT) \mathbb{P}_{x,v}(D_2 \cap D_3 \cap D_6 \cap D_7).$$

Let

$$D_8 := [y - \frac{\varepsilon}{2} \leq x + S_1 v + \sum_{j=1}^{N-2} (S_{j+1} - S_j) V_j^D + (T - S_{N-1}) u \leq y + \frac{\varepsilon}{2}].$$

An integration provides

$$\begin{aligned} \mathbb{P}_{x,v}(D_2 \cap D_3 \cap D_8) &= \int_{G_1} \dots \int_{G_{N-1}} \int_{H_1} \dots \int_{H_{N-2}} \varphi_{S_1, \dots, S_{N-1}}(t_1, \dots, t_{N-1}) \\ &\quad \psi_{V_1^D, \dots, V_{N-2}^D}(y_1, \dots, y_{N-2}) \mathbb{I}_{D_9}(t_1, \dots, t_{N-1}) dt_1 \dots dt_{N-1} dy_1 \dots dy_{N-2}, \end{aligned}$$

where

$$D_9 = [y - \frac{\varepsilon}{2} \leq x + t_1 v + \sum_{j=1}^{N-2} (t_{j+1} - t_j) y_j + (T - t_{N-1}) u \leq y + \frac{\varepsilon}{2}],$$

The previous expression is bounded from below by

$$C_1 \int_{G_1} \dots \int_{G_{N-1}} \int_{H_1} \dots \int_{H_{N-2}} \mathbb{I}_{D_9}(t_1, \dots, t_{N-1}) dt_1 \dots dt_{N-1} dy_1 \dots dy_{N-2}$$

with

$$C_1 = \inf_{t_i \in G_i} \varphi_{S_1, \dots, S_{N-1}}(t_1, \dots, t_{N-1}) \inf_{y_i \in H_i} \psi_{V_1^D, \dots, V_{N-2}^D}(y_1, \dots, y_{N-2}).$$

We now let $\theta_1 = t_1, \theta_2 = t_2 - t_1, \dots, \theta_{N-1} = t_{N-1} - t_{N-2}$ to transform the above integral into an integral of the form

$$\int_{G_1} \dots \int_{G_{N-1}} \int_{Z_1} \dots \int_{Z_{N-2}} \mathbb{I}_{D_{10}}(\theta_1, \dots, \theta_{N-1}) d\theta_1 \dots d\theta_{N-1} dy_1 \dots dy_{N-2},$$

where

$$D_{10} = [y - \frac{\varepsilon}{2} \leq x + T u + \theta_1 (v - u) + \sum_{j=2}^{N-1} \theta_j (y_{j-1} - u) \leq y + \frac{\varepsilon}{2}].$$

A change of variables allows us to transform the domain into $[0, 1]^{2N-1}$, and therefore we now have to bound from below an integral of the form

$$\int_0^1 \dots \int_0^1 \mathbb{I}_{q - \frac{\varepsilon}{2} \leq x_1 + \sum_{j=2}^{N-1} x_j y_j \leq q + \frac{\varepsilon}{2}} dx_1 \dots dx_{N-1} dy_2 \dots dy_{N-1}.$$

We observe that

$$\int_0^1 \int_0^1 f(xy) dx dy = \int_0^1 -\ln(t) f(t) dt$$

for all bounded measurable functions f . Similarly, the change of variables $u_1 = x_1$ and $u_j = x_j y_j, j \geq 2$, leads us to

$$I := \int_0^1 \dots \int_0^1 \prod_{j=2}^{N-1} (-\ln(u_j)) \mathbb{I}_{q - \frac{\varepsilon}{2} \leq \sum_{j=2}^{N-1} u_j \leq q + \frac{\varepsilon}{2}} du_1 \dots du_{N-1}.$$

There exists $\zeta > 0$ such that

$$J := \int_0^1 \int_0^\zeta \dots \int_0^\zeta \prod_{j=2}^{N-1} (-\ln(u_j)) \mathbb{I}_{q - \frac{\varepsilon}{2} \leq \sum_{j=2}^{N-1} u_j \leq q + \frac{\varepsilon}{2}} du_1 \dots du_{N-1}$$

is strictly positive. For such a $\zeta >$ we have

$$I \geq (-\ln(\zeta))^{N-2} \int_0^1 \int_0^\zeta \dots \int_0^\zeta \mathbb{I}_{q - \frac{\varepsilon}{2} \leq \sum_{j=2}^{N-2} u_j \leq q + \frac{\varepsilon}{2}} du_1 \dots du_{N-1}.$$

A final normalization leads us to a bound from below of the type

$$\int_0^1 \dots \int_0^1 \mathbb{I}_{\tilde{q} - \tilde{\varepsilon} \leq \sum_{j=1}^{N-1} x_j \leq \tilde{q} + \tilde{\varepsilon}} dx_1 \dots dx_{N-1}$$

for some $\tilde{\varepsilon} > 0$ and $\tilde{c} > \tilde{\varepsilon}$, which is nothing else than

$$\mathbb{P}(\tilde{q} - \tilde{\varepsilon} \leq S \leq \tilde{q} + \tilde{\varepsilon}),$$

where S is the sum of $N - 1$ uniform and independent random variables. Its density Ψ_S satisfies $\Psi_S(\tilde{c}) > 0$ since, by construction, $\tilde{c} \in (0, N - 1)$. Thus

$$\mathbb{P}(\tilde{q} - \tilde{\varepsilon} \leq S \leq \tilde{q} + \tilde{\varepsilon}) \geq \theta \tilde{\varepsilon}$$

for some $\theta > 0$, from which the conclusion follows. \square

4. NUMERICAL EXPERIMENTS FOR THE LEHNER–WING MODEL

4.1. Description and stochastic representation. In this section we study the Cauchy problem

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

with the initial condition $u(0, x, v) = u_0(x, v)$ and the absorption boundary condition (2.7). The spatial domain is $(0, A)$, the velocity domain is $V = (-1, 1)$ and c is a positive constant. This homogeneous and isotropic model is known as the Lehner–Wing model [7, Chap. 18] and is also called multiplying slabs ([5]). We have to find the value of the constant c such that the system is critical. In spite of the fact that the velocity domain contains 0, one can prove that the principal eigenvalue is real and simple: see [7, Chap. 18].

From

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

we get the stochastic representation

$$u(t, x, v) = \exp((c - 1)t) \mathbb{E}_{x,v} [u_0(X_t, V_t) \mathbb{I}_{t < \tau^D}].$$

The velocity after a collision has a uniform law on V . The cumulative distribution of the time between two collisions is $F^{x,v}(t) = 1 - \exp(-ct)$. For any fixed c we compute the principal eigenvalue using the estimators described in Section 2. To compute the criticality factor, that is, the critical value of c , we then use the fact that the principal eigenvalue is an increasing function of c .

4.2. Numerical computation of $u(t, x, v)$. We compute

$$u(t, x, v) = \exp((c - 1)t) \mathbb{E}_{x,v} [u_0(X_t, V_t) \mathbb{I}_{t < \tau^D}]$$

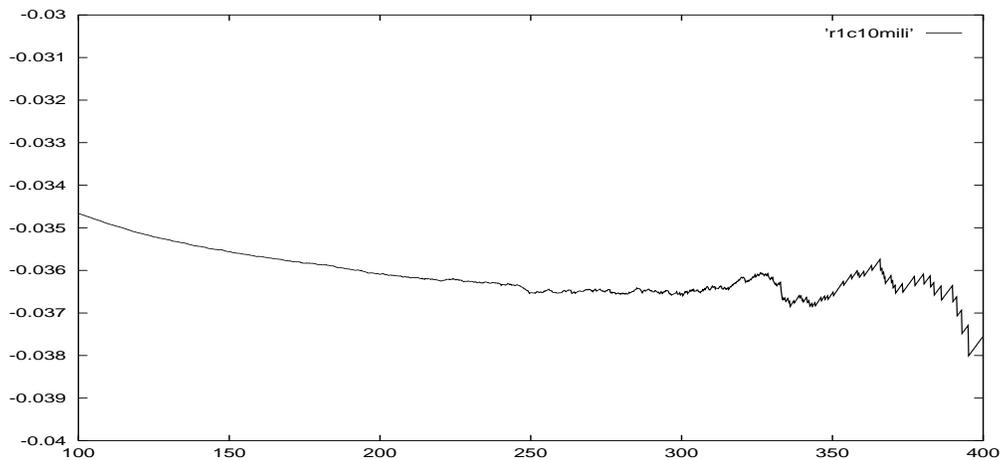
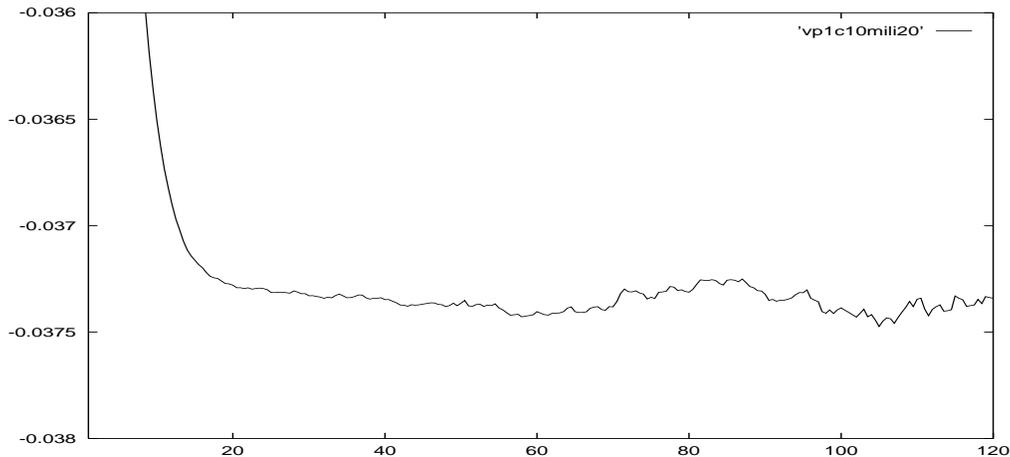
by using a Monte Carlo method. The initial condition u_0 can be arbitrarily chosen because we are only interested in computing the principal eigenvalue. Nevertheless we choose $u_0 \equiv 1$ for the following two reasons. First, the stationary solution tends to $u_0 \equiv 1$ and the criticality factor tends to 1 when the spatial domain increases to \mathbb{R} ; therefore, if the spatial domain is large enough, the initial solution $u_0 \equiv 1$ is close to the eigenfunction relative to the principal eigenvalue, which ensures that the leading term in the right-hand side of (2.2) dominates the remaining term even for small values of t . Second, the solution simplifies to

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

which reduces the cost of the simulation.

4.3. Approximation of the principal eigenvalue by the direct method. We study this model with $A = 8$, and the trajectories start from $E = [3.5, 4.5] \times [-0.5, 0.5]$. We make the trajectories start near the center of the spatial domain with small velocities because we desire that the trajectories reach the boundary as late as possible. We choose $c = 1$, which leads to a subcritical system. Fig. 4.1 shows the time evolution of the direct approximation $\bar{\alpha}_0(t) := \frac{1}{t} \log(g_E(t))$ obtained with 10^6 trajectories for $100 \leq t \leq 400$.

It is difficult to deduce an accurate estimate of the principal eigenvalue from this figure. The value seems to be around -0.037. We can easily explain why the direct method does not work well: we have to compute the probability of an event which becomes rarer and rarer when time increases (for only 5 of our 10^6 simulated trajectories is τ^D larger than 400) and, in addition, we have to compute the logarithm of this probability.

FIGURE 4.1. Direct method ; x -axis: t ; y -axis: $\bar{\alpha}_0(t)$ FIGURE 4.2. Interpolation method ; x -axis: t_1 ; y -axis: $\alpha_0(t_1, t_1 + 20)$

4.4. Approximation of the principal eigenvalue by the interpolation method. We now consider the interpolation method of Section 2.3.2. Figure 4.2 shows the time evolution of the estimators $\alpha_0(t_1, t_2)$ considered as a function of t_1 , after having fixed $t_2 - t_1 = 20$, which appears to be a good choice in terms of variance reduction (we have again used 10^6 trajectories). It shows that the interpolation method is more stable than the direct method, and that the principal eigenvalue is close to -0.0374 .

The following table summarizes the results obtained with 10^9 trajectories for three different values of t_1 (the very large number of trajectories ensures highly accurate approximations of $\alpha_0(t_1, t_2)$). The confidence intervals are (binf, bsup).

t_1	binf	$\alpha_0(t_1, t_2)$	bsup
50	-3.736110^{-2}	-3.734410^{-2}	-3.732610^{-2}
55	-3.736010^{-2}	-3.734110^{-2}	-3.732210^{-2}
60	-3.736410^{-2}	-3.734410^{-2}	-3.732110^{-2}

The three confidence intervals and the three values $\alpha_0(t_1, t_2)$ are almost identical, which indicates that the remaining term in (2.11) is negligible. We approximate α_0 by $\alpha_0(50, 70)$. We notice that the length of the confidence interval is around 4×10^{-5} , and that practitioners often desire a 10^{-5} accuracy for the criticality factor.

4.5. Approximation of the principal eigenvalue by least squares approximation. Figure 4.3 shows the time evolution of least squares estimators $\alpha_0(t_p, t_q, m)$ of the principal eigenvalue. We choose $m = 400$ and $20 \leq t_p \leq 100$. The other parameters are as in Subsection 4.3. Compared to the interpolation method, the least squares method appears to be much better. Actually it provides an approximation of the principal eigenvalue within $[-0.0374, -0.0373]$, which means that the accuracy is of order 10^{-4} .

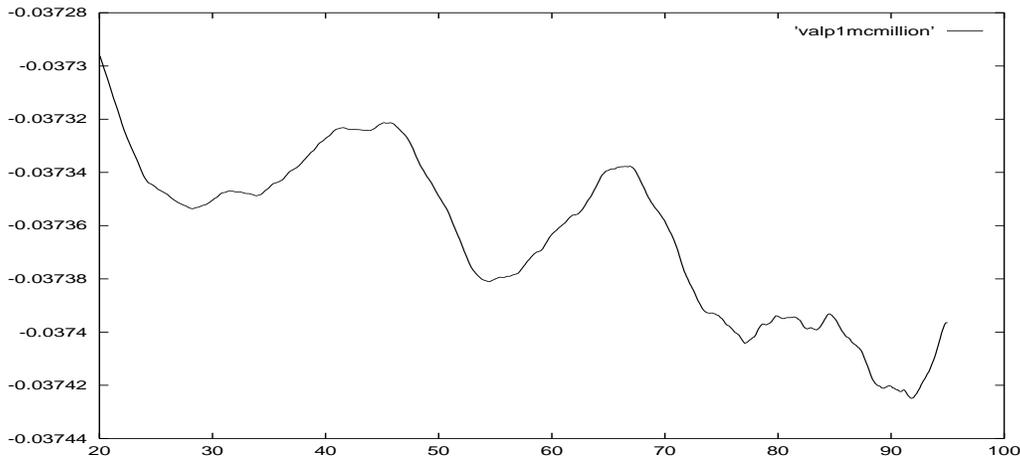


FIGURE 4.3. Least square approximation ($c = 1$) ; x -axis: t_p ; y -axis: $\alpha_0(t_p, t_p + 20, 400)$

4.6. Computation of the criticality factor by the interpolation method. For parameters chosen as above, the criticality factor is close to 1.0364019 (see Dahl and Sjostrand [5]). Using the interpolation method, we compute two approximate values of α_0 corresponding to two rough approximations of c resulting from a small number of simulations, e.g., $c_{min} = 1.036$ and $c_{max} = 1.037$.

For $c = c_{min}$, the following table shows that we can choose $\alpha_0 \simeq -4.13 \times 10^{-4}$.

t_1	binf	$\alpha_0 \min(t_1, t_2)$	bsup
50	-4.2810^{-4}	-4.1210^{-4}	-3.9410^{-4}
55	-4.2810^{-4}	-4.1310^{-4}	-3.9410^{-4}
60	-4.2810^{-4}	-4.1610^{-4}	-3.9610^{-4}

For $c = c_{max}$, the following table shows that we can choose $\alpha_0 \simeq 6.21 \times 10^{-4}$.

t_1	binf	$\alpha_0 \max(t_1, t_2)$	bsup
50	$6.05 \cdot 10^{-4}$	$6.22 \cdot 10^{-4}$	$6.38 \cdot 10^{-4}$
55	$6.02 \cdot 10^{-4}$	$6.21 \cdot 10^{-4}$	$6.39 \cdot 10^{-4}$
60	$5.9 \cdot 10^{-4}$	$6.19 \cdot 10^{-4}$	$6.4 \cdot 10^{-4}$

Using the secant method, the criticality factor can be approximated by

$$c_{min} - \alpha_0 \min \frac{c_{max} - c_{min}}{\alpha_0 \max - \alpha_0 \min} = 1.036399.$$

The accuracy is of order 10^{-5} since the reference value obtained by Dahl and Sjostrand [5] has an accuracy of order 10^{-8} .

4.7. Computation of the criticality factor by the least squares method. We now use the least squares method to approximate c . We use $c_{min} = 1.03639$ and $c_{max} = 1.03641$. Figures 4.4 and 4.5 show the time evolution of the principal eigenvalue corresponding to these two values of c . We observe that the estimators of the principal eigenvalue are stable on the time interval (40, 55). After time 55, the statistical error of the Monte Carlo method becomes too large because the event ($\tau^D > t$) becomes too rare. We thus use the approximations of the principal eigenvalue obtained at time $t = 55$, namely -1.08×10^{-5} and

1.01×10^{-5} . The opposite signs of these eigenvalues confirm that the criticality factor is located in the interval $[1.03639, 1.03641]$. Using the secant method as above, we now obtain $c \simeq 1.0364003$. The accuracy now is of order 10^{-6} . To obtain this result the CPU time on a DEC 600 MHz computer has been around 10 hours. This cost is high for a one-dimensional problem. However it would not increase rapidly with the dimension of the problem.

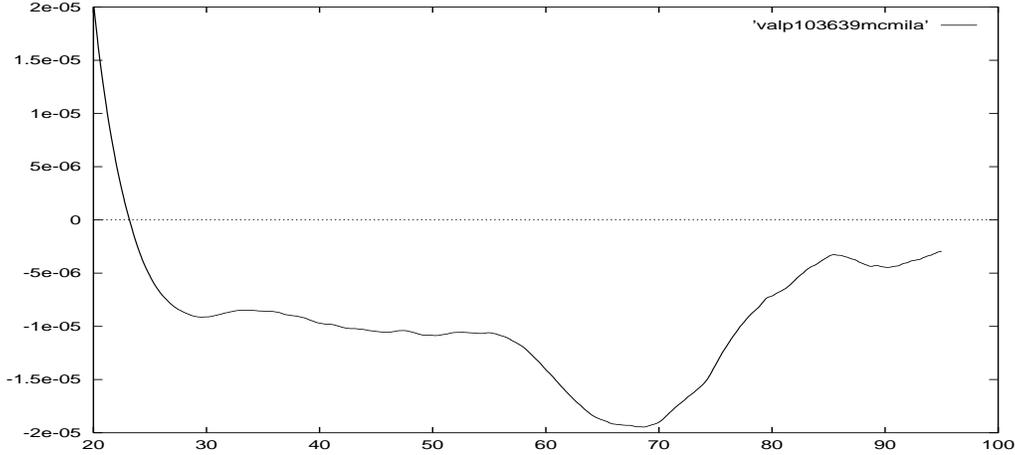


FIGURE 4.4. Least squares approximation ($c = 1.03639$) ; x -axis: t_p ; y -axis: $\alpha_0(t_p, t_p + 20, 400)$

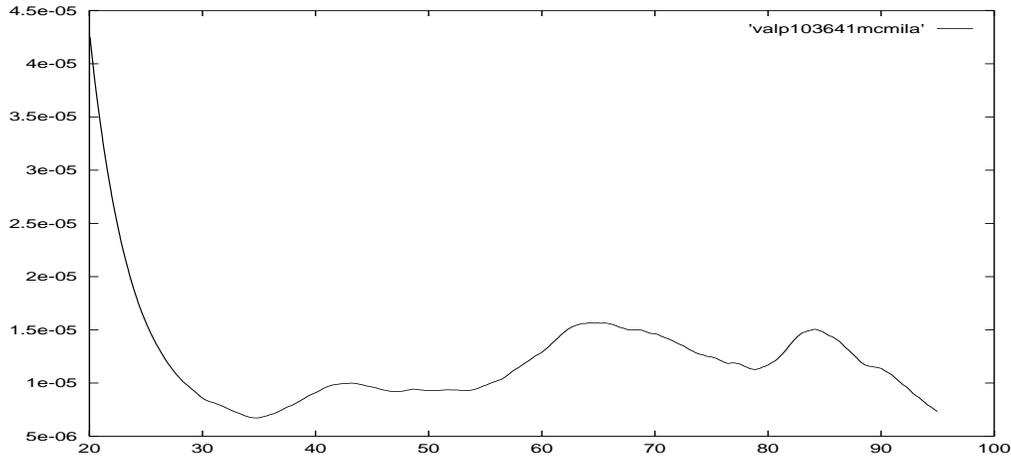


FIGURE 4.5. Least squares approximation ($c = 1.03641$) ; x -axis: t_p ; y -axis: $\alpha_0(t_p, t_p + 20, 400)$

5. NUMERICAL EXPERIMENTS FOR TWO EXTENDED LEHNER–WING MODELS

5.1. An anisotropic model.

5.1.1. *The physical model.* We now consider a model more general than the Lehner-Wing model where the anisotropy is taken into account. We have to solve the Cauchy problem

$$\frac{\partial u}{\partial t} = -v \frac{\partial u}{\partial x} + (c - 1)u(t, x, v) + \frac{c}{2} \int_V (1 + 3\mu v v') u(t, x, v') dv',$$

with an initial condition $u(0, x, v) = u_0(x, v)$ and absorption boundary conditions. The constant μ represents the average of the cosines of the angles of deviation at the collision. As in Dahl and Sjostrand [5] we choose μ in the interval $[0, 0.3]$. As explained above, we choose $u_0 \equiv 1$. The density of the velocity after a collision

now is $f(v') = \left(\frac{1 + 3\mu vv'}{2}\right)$, where v is the velocity before the collision. Let $a = 3\mu v$. The simulation of the velocity is achieved by

$$\frac{-1 + \sqrt{1 - 2a + a^2 + 4aU}}{a},$$

where U is uniformly distributed on $[0, 1]$ (this can be checked by inverting the distribution function of f).

5.1.2. *Numerical results.* We choose $\mu = 0.1$. The critical value computed by Dahl and Sjostrand is 1.0932421. We compute the principal eigenvalue at time $t = 50$ for $c = 1.09323$ and $c = 1.09325$. We respectively obtain $\alpha_0 = -1.1 \times 10^{-5}$ and $\alpha_0 = 7 \times 10^{-6}$. The criticality factor is approximated by $c \simeq 1.0392422$. The error is of order 10^{-6} . We have found similar accuracies for various values of μ , which confirms the efficiency of this method.

5.2. Multiplying spheres.

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

$$\frac{\partial u}{\partial t} = -v \nabla_x u(t, x, v) + (c - 1)u(t, x, v) + c \left(\frac{1}{4\pi} \int_{S_2} u(x, z_1, t) dz_1 - u(t, x, z) \right),$$

with an initial condition $u(0, x, v) = u_0(x, v)$ and absorption boundary conditions. The velocity domain is the unit sphere S_2 and the spatial domain is the ball centered at O of radius d .

5.2.2. *Simulation of the velocities on the unit sphere.* The density of the velocities on the unit sphere S_2 is

$$f(\theta, \varphi) = \frac{1}{2} \sin(\theta) \mathbb{I}_{[0, \pi]}(\theta) \frac{1}{2\pi} \mathbb{I}_{[0, 2\pi]}(\varphi).$$

To simulate a random variable with density

$$g(\theta) = \frac{1}{2} \sin(\theta) \mathbb{I}_{[0, \pi]}(\theta),$$

we simulate

$$Z = 2 \arcsin(\sqrt{U}),$$

where U has a uniform distribution on $[0, 1]$. The three components of the velocity are

$$v_x = \sin(\theta) \sin(\varphi), v_y = \sin(\theta) \cos(\varphi), v_z = \cos(\theta),$$

where the density of θ is g , and φ has a uniform distribution on $[0, 2\pi]$.

5.2.3. *Numerical results.* We choose $d = 8$. The criticality factor computed by Dahl and Sjostrand is $c = 1.1384602$. We approximate it using the least squares method to compute the principal eigenvalue, and we use 2 billions trajectories. The principal eigenvalues corresponding to $c_{min} = 1.1384$ and $c_{max} = 1.1385$ respectively are -8×10^{-5} and 5×10^{-5} . The secant method then leads to $c \simeq 1.138462$. Again the accuracy is of order 10^{-6} .

6. STUDY OF A BIDIMENSIONAL INHOMOGENEOUS PROBLEM

The above Lehner–Wing model and its variants were one dimensional. Thus, in these cases, deterministic methods are certainly much more efficient than Monte Carlo methods. However our Monte Carlo method provides a satisfactory accuracy on the criticality factor.

In this section and in the next one, we aim to show that our method still leads to a good approximation of the $keff$ coefficient in multidimensional situations where the cost and the complexity of deterministic methods render Monte Carlo methods attractive and competitive, even if the number of simulations often needs to be large to obtain a good accuracy (our various choices for this number are made in terms of the desired accuracy according to the confidence intervals described in Subsection 2.3.2). In addition, the programming of Monte Carlo methods on these problems is much easier than the programming of deterministic methods.

We notice that, in the examples below, to our knowledge, no theoretical result allows us to be sure that the principal eigenvalue exists and is simple. Indeed, the fission cross section Σ_f is inhomogeneous and locally equal to 0; in addition, the velocity domain includes 0.

6.1. **The physical model.** We now consider a variant of the Khalil test case [13]. It has been suggested to P. Seumen Tonou [20] by Xavier Warin. The eigenvalue problem is

$$L\Psi = \frac{1}{\lambda}F\Psi,$$

where the operators L and F are defined by

$$Lu(x, y, \mu, \phi) = \mu \frac{\partial u}{\partial x} + \sqrt{1 - \mu^2} \cos(\phi) \frac{\partial u}{\partial y} + \Sigma_{\text{tcs}}(x, y)u - \frac{\Sigma_s(x, y)}{4\pi} \int_{-1}^1 \int_0^{2\pi} u(x, y, \mu, \phi) d\mu d\phi,$$

and

$$Fu(x, y) = \frac{\nu(x, y)\Sigma_f(x, y)}{4\pi} \int_{-1}^1 \int_0^{2\pi} u(x, y, \mu, \phi) d\mu d\phi.$$

The domain D is divided into five zones. Each zone is characterized by its total cross section Σ_{tcs} and its scattering cross section Σ_s . The splitting zones are also characterized by their fission cross section Σ_f which indicates the possibility of a fission at point (x, y) . The average number of neutrons by fission at (x, y) is $\nu(x, y)$.

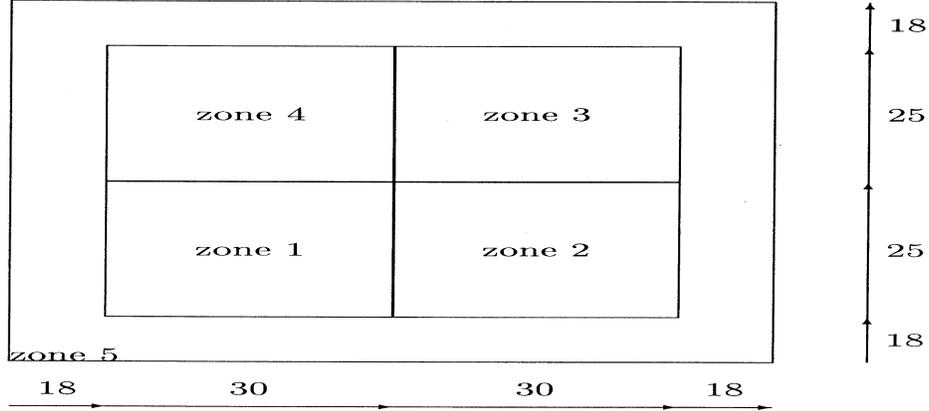


FIGURE 6.1. The physical domain

The dimensions of zone 1 are 30×25 , etc. The characteristics of the zones are listed in the following table.

Zone	$\nu\Sigma_f$	Σ_{tcs}	Σ_s
1	0.079	0.6	0.53
2	0	0.48	0.20
3	0.043	0.70	0.66
4	0	0.65	0.50
5	0	0.90	0.89

6.2. **The stochastic representation of the Cauchy problem.** The Cauchy problem is

$$\frac{\partial u}{\partial t} = b(\mu, \phi) \cdot \nabla_{x,y} u + c(x, y)u + \gamma(x, y) \int \int_V (u(x, y, \eta, \zeta, t) - u(x, y, \mu, \phi, t)) \pi(x, y, \eta, \zeta) d\eta d\zeta,$$

with

$$b(\mu, \phi) = (-\mu, -\sqrt{1 - \mu^2} \cos(\phi)),$$

$$c(x, y) = \nu(x, y)\Sigma_f(x, y) + \Sigma_s(x, y) - \Sigma_{\text{tcs}}(x, y),$$

$$\gamma(x, y) = \nu(x, y)\Sigma_f(x, y) + \Sigma_s(x, y),$$

$$\pi(x, y, \eta, \zeta) = \frac{1}{4\pi} \mathbb{I}_{[-1,1] \times [0,2\pi]}(\eta, \zeta).$$

The Feynman–Kac formula writes

$$u(x, y, \mu, \phi, t) = \mathbb{E}_{x,y,\mu,\phi} \left[\mathbb{I}_{\tau^D > t} u_0(X_t, V_t) \exp \left(\int_0^t c(X_s, V_s) ds \right) \right].$$

6.3. Variance reduction.

6.3.1. *The computational domain.* As for homogeneous models, a Monte Carlo method is used to compute

$$g_E(t) = \frac{1}{\text{vol}(E)} \int_E u(x, y, \mu, \phi, t) dx dy d\mu d\phi$$

for $E \subset D$. The most natural choice is $E = D$. A better choice in terms of variance-reduction is the most splitting zone, that is, the zone 1, since the function u takes small values in the other zones. In view of the characteristics of the model, an even better choice is the bottom left quarter of this zone. This observation is confirmed by our numerical experiments.

6.3.2. *The choice of the initial condition.* In view of the expansion (2.2) it is best to choose u_0 equal to an eigenfunction of the principal eigenvalue. To get a rough approximation of this eigenfunction, one can either use a deterministic method (see Warin [22]) or a Monte Carlo method with a relatively small number of particles (see Brockway et al. [2]). The numerical experiments confirm that this technique is efficient.

6.4. **Computation of the criticality factor.** We combine the techniques presented in the two preceding subsections and we use the least-square method to approximate the principal eigenvalue. We simulate 600 millions trajectories. Figs. 6.2 and 6.3 respectively correspond to $\lambda = 1.0095$ and $\lambda = 1.0085$, and represent the time evolution of the estimator of the principal eigenvalue.

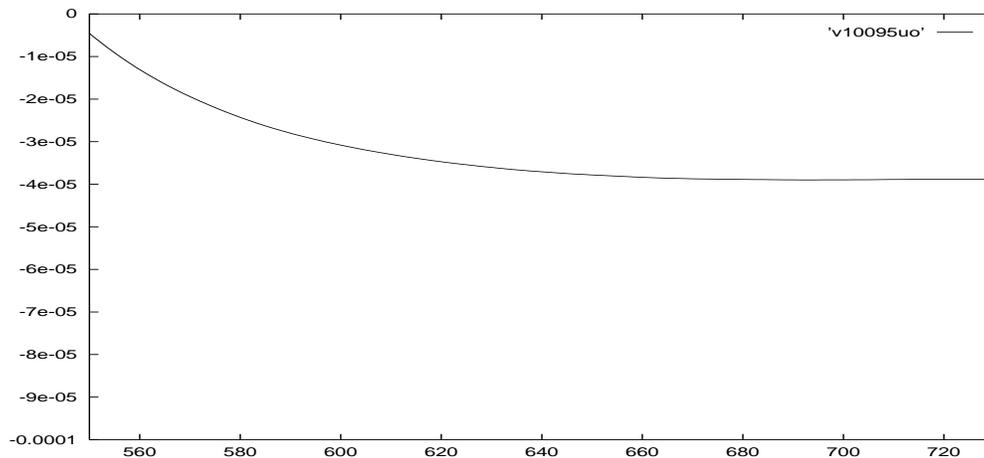


FIGURE 6.2. Least square approximation ($\lambda = 1.0095$) ; x -axis: t_p ; y -axis: $\alpha_0(t_p, t_p + 20, 400)$

Using the secant method again and the two approximate values -3.9×10^{-5} and 3.1×10^{-5} of the principal eigenvalue, we find $keff \simeq 1.00894$. Compared to the reference value 1.00890 provided by Xavier Warin at the Électricité de France, the error is 4×10^{-5} .

7. A THREE-DIMENSIONAL PROBLEM

7.1. **The physical model.** Now consider the operators L et F defined as

$$Lu(x, v) = v \nabla_x u(t, x, v) + \Sigma_{\text{tcs}}(x, v) u(t, x, v) - \frac{\Sigma_s(x, v)}{4\pi} \int_{S_2} u(t, x, v') dv',$$

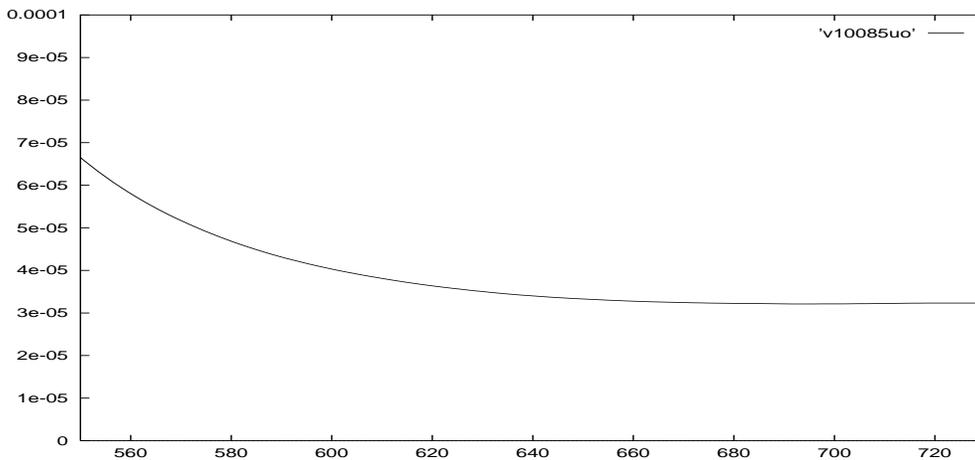


FIGURE 6.3. Least square approximation ($\lambda = 1.0085$) ; x -axis: t_p ; y -axis: $\alpha_0(t_p, t_p + 20, 400)$

and

$$Fu(x, v) = \frac{\nu(x, y)\Sigma_f(x, v)}{4\pi} \int_{S_2} u(t, x, z) dz.$$

The domain D is three dimensional: the two first spatial coordinates lie in the 2-D domain of the preceding subsection, and the third spatial coordinate lies in the interval $[0, 66]$. We again divide the domain into 5 zones with the same characteristics as above.

7.2. The stochastic representation. The Cauchy problem writes

$$\frac{\partial u}{\partial t} = b(v) \cdot \nabla_x u + c(x, v)u + \gamma(x, v) \left\{ \int_{S_2} (u(x, v_1, t) - u(t, x, v)) \pi(x, v_1) dv_1 \right\}$$

with

$$\begin{aligned} b(v) &= (-v_x, -v_y, -v_z), \\ c(x, v) &= \nu(x, v)\Sigma_f(x, v) + \Sigma_s(x, v) - \Sigma_{\text{tcs}}(x, v), \\ \gamma(x, v) &= \nu(x, v)\Sigma_f(x, v) + \Sigma_s(x, v), \\ \pi(x, v) &= \frac{1}{4\pi} \mathbb{I}_{S_2}(v). \end{aligned}$$

7.3. Numerical results. Our numerical experiment is performed for $\lambda = 0.971$ and $\lambda = 0.972$. The corresponding approximate principal eigenvalues are, respectively, 3.9×10^{-5} and -3.4×10^{-5} . Using the secant method, the approximate value of the k_{eff} coefficient is 0.97146 whereas the reference value is 0.97142 (see Warin [22]), so that the error is around 4×10^{-5} .

8. CONCLUSION

We have developed and studied a probabilistic method to obtain both theoretical and numerical results on the principal eigenvalues of neutron transport operators. An accurate study of the law of the Markov process related to this transport operator allowed us, for homogeneous models, to establish a probabilistic representation of the principal eigenvalue. The crucial point was to find both lower and upper bounds for the transition density of this process. One should be able to extend our technique and results to more general homogeneous transport operators.

The numerical method has been tested on various homogeneous and inhomogeneous models. For all of these problems, we have obtained very good accuracy for the principal eigenvalue and the criticality parameters. Our Monte Carlo method has two main drawbacks compared to deterministic methods. In spite of various variance reduction techniques, CPU times are long to obtain good accuracy of criticality factors. Furthermore, our method does not compute an approximation of the critical eigenfunction. However this last point can be considered as an important advantage. As we do not need to compute this critical

eigenfunction, the complexity of our method depends weakly on the dimension of the problem. For some inhomogeneous 2D and 3D problems we have observed similar CPU times.

The probabilistic approach presented here does not allow one to obtain approximate eigenfunctions. Nevertheless further extensions and improvements of the method are possible. For example, we can also consider even more difficult problems where the velocity of the neutrons is not normalized. No additional discretization is required (which would not be true if we were to use a deterministic method). The only difference consists in changing the law of the velocities after a collision. Another advantage of the Monte Carlo method is that it provides an approximation of the principal eigenvalue, which allows one to see whether the reactor is supercritical or subcritical. Some refinements of the variance reduction techniques can be developed, such as weighted least-squares estimators or biasing methods. We also emphasize that, as any other Monte Carlo method, our method can take advantage of parallel computing. Finally, the method can be applied for the numerical computation of the principal eigenvalue of elliptic operators in high dimensions or in complex domains. The situation would then be very similar to the homogeneous transport problem, except that an additional error appears which is due to the discretization of the stochastic differential equation. These studies are in progress.

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