

## On a Monte Carlo method for neutron transport criticality computations

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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.

*Keywords:* neutron transport equations; principal eigenvalue; criticality; Monte Carlo method; Feynman–Kac formula; variance reduction.

### 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  $\mathbb{R}_+ \times D \times V$ , for the equation

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

where the neutron transport operator  $T$  is defined as

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

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  $\Sigma_s$  and the fission cross section  $\Sigma_f$  which characterize the physical properties of the nuclear reactor which is usually highly heterogeneous (Bussac *et al.*, 1978). The boundary conditions depend on the behaviour of the neutrons at the

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boundary. In this paper, we focus on the specific criticality transport equation

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

where

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

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  $\Sigma_{\text{tcs}}$ ,  $\Sigma_s(x, z, v)$  and  $\Sigma_f$  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  $\mathcal{T}^\lambda$  is real and simple, and that its eigenfunction is positive: see, e.g. Mika (1971). Let  $\alpha_0^\lambda$  be the principal eigenvalue of the operator  $\mathcal{T}^\lambda$ . If  $\alpha_0^\lambda = 0$ , there is a perfect balance between the production and the absorption of the neutrons. The corresponding  $\lambda$  is often 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  $\alpha_0^\lambda$ . Furthermore, under weak hypotheses,  $\alpha_0^\lambda$  is a decreasing function of  $\lambda$  which tends to  $+\infty$  when  $\lambda$  tends to 0 and is negative for  $\lambda$  large enough (see, e.g. Dautray & Lions, 1988).

In criticality studies, one desires to compute the value of  $\lambda$  for which the principal eigenvalue  $\alpha_0^\lambda$  of the operator  $\mathcal{T}^\lambda$  is as close to zero as possible. Therefore, one must find the largest value  $\lambda$  such that there exists a solution  $\Psi$  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 (1968). For other criticality analyses see, e.g. Bardos *et al.* (1984).

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

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

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 (1981), Planchard (1995), Karp (1998), Warin (1993). With these methods, a good approximation may be difficult to achieve, especially for 3D 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.* (1998) and Kalos (1981). Monte Carlo methods are used to approximate  $\alpha_0^\lambda$ ,  $\lambda$  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 Kalos, 1981). Monte Carlo methods are also used to approximate the keff coefficient; this consists of solving the sequence of equations

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

by means of a stochastic particle method: see, e.g. Brockway *et al.* (1985). Here, we propose a new Monte Carlo method which avoids the numerical resolution of partial differential equations 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  $\alpha_0^\lambda$  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  $\alpha_0^\lambda$ . 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 Section 1, we aim to approximate by a Monte Carlo method the principal eigenvalue of the operator  $\mathcal{T}$  in order to determine the keff 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 (1988) and Mokhtar-Kharroubi (1997).

### 2.1 A deterministic representation of the principal eigenvalue

We recall some properties of  $\mathcal{T}$  (see Chapters 1 and 21 in Dautray & Lions, 1988). 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  $\alpha_0$  which is real and simple. Moreover, there exists  $\beta < \alpha_0$  such that

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

where  $P_0$  is the projector in  $L^2(D \times V)$  on the eigenspace associated to  $\alpha_0$  (see Dautray & Lions, 1988, Chapter 21, Section 3, proof of Proposition 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

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

REMARK 2.1 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  $\Sigma_s$  and  $\Sigma_f$  do not depend on  $x$  (see Dautray & Lions, 1988, Chapter 21, Section 3).

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

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

It results from (2.2) that

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

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

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

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

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

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

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

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  $(n+1)$ th 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:

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

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

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

with  $\zeta_0 = x$ , and the function  $\Theta$  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. Dautray *et al.*, 1989).

**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

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

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, i.e.

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

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

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

where  $\tau^D$  is the first exit time of  $(X_t)$  from  $D$ . See, e.g. Dautray *et al.* (1989) and Bensoussan *et al.* (1979).

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,

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

### 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

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

In view of (2.4) and (2.10), one may thus compute  $\alpha_0$  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  $\beta$  is very close to  $\alpha_0$ . However, this difficulty occurs with any other numerical method.

2.3.2 *Interpolation method.* We deduce from (2.2) that, for all subdomain  $E$  of the domain  $D \times V$ , there exists a real number  $K_0$  such that, for all  $t$  large enough,

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

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  $\alpha_0$ , 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  $\frac{\sigma_1}{g_1 \sqrt{N}} \ll 1$  we obtain

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

We thus have

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

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  $\alpha_0$  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  $\alpha_0$  which, according to our numerical experiments, seems more accurate than the previous ones.

Before analysing numerically the above refinements of the direct Monte Carlo simulations (see Sections 4–7 below), we consider a homogeneous 1D model which allows us to express  $\alpha_0$  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  $\alpha_0$  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. Note 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, 1988).

#### 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  $\alpha_j$ 's are the eigenvalues of  $\mathcal{L}$  arranged in decreasing order and the  $\Psi_j$ 's are the corresponding eigenfunctions. Using this method, Kac (1951) 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 (1985) considers a general elliptic operator  $\mathcal{L}$  with Dirichlet boundary conditions in a bounded domain  $D$  in  $\mathbb{R}^k$ . Let  $\tau^D$  be the first exit time from  $D$  of the stochastic process  $X_t^x$  whose generator is  $\mathcal{L}$ . The principal eigenvalue  $\alpha_0$  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 (1985) and Friedman (1976). These proofs deeply use the fact that  $\mathcal{L}$  is the generator of a diffusion process. As we are concerned with generators of transport processes, we follow another method developed by Kifer (1988). 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: e.g. consider the model studied in Section 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  $\rho$  be a real number. Consider bounded domains  $D$  and  $V$ , and the Cauchy problem in  $\mathbb{R}_+ \times D \times V$ :

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

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 Section 2.2.2 on  $b$ ,  $\Theta$  and  $\Pi^{x,v}$  hold in force. In view of (2.8) one has

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

where  $\tau^D$  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  $b$ ,  $\Theta$  and  $\Pi^{x,v}$  satisfy the hypotheses listed in Section 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  $\beta_\rho$  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 Section 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 3.1** 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

$$\mathbb{E}_{x,v}[f(X_t, V_t)\mathbb{I}_{\tau^D > t}] = \mathbb{E}_{x,v}[f(X_t^D, V_t^D)] = \int_V \int_D p^D(t, (x, v), (x_1, v_1)) f(x_1, v_1) dx_1 dv_1$$

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

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

and

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

Finally, suppose that

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

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

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

(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 3.1** Under the assumptions made in Section 2.1, in view of the expansion (2.2) and using (3.6), we have

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

A Monte Carlo approximation of  $\alpha_0$  can thus consist in approximating the distribution function of  $\tau^D$  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 (1988, Chap. 3). Fix  $(x, v)$  in  $D$  and let  $t > T$ . We have

$$\mathbb{P}_{x,v}(\tau^D > t) = \int_V \int_D p^D(t, (x, v), (x_1, v_1)) dx_1 dv_1.$$

From the Markov property it follows that

$$\mathbb{P}_{x,v}(X_t^D \in D) = \int_V \int_D p^D(T, (x, v), (x_1, v_1)) \mathbb{P}_{x_1, v_1}(\tau^D > t - T) dx_1 dv_1,$$

which implies the following two inequalities:

$$\mathbb{P}_{x,v}(X_t^D \in D) \geq \operatorname{ess\,inf}_{(x_1, v_1) \in A} p^D(T, (x, v), (x_1, v_1)) \iint_A \mathbb{P}_{x_2, v_2}(\tau^D > t - T) dx_2 dv_2 \quad (3.8)$$

and

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

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

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

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

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

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 1D model

The aim of this section is to show how the hypotheses of Theorem 3.1 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 1D model. Nevertheless, our presentation involves the main ingredients to handle multidimensional homogeneous models as well.

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

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

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

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

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

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

Note 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 (1988, Chapter 21).

We now prove that the hypotheses of Theorem 3.1 are satisfied, i.e. inequalities (3.3), (3.4) and (3.5) hold. 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 (3.12) without boundary conditions, i.e. when  $D = \mathbb{R}$ . We still assume that  $c > 0$ .

LEMMA 3.2 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  $p_0(\zeta, v)$  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  $p(t, \zeta, v)$  in  $L^\infty(\mathbb{R} \times V_\delta)$  and

$$\forall t > 0, \quad \text{ess sup}_{\zeta \in \mathbb{R}} \int_{V_\delta} p(t, \zeta, v) dv \leq \text{ess sup}_{\zeta \in \mathbb{R}} \int_{V_\delta} p(0, \zeta, v) dv. \quad (3.15)$$

*Proof.* The existence of the density is a standard result on transport jump processes (see Dautray & Lions, 1988, Chap. 3). In order to get the bound from above, we observe that the density  $p(t, \zeta, v)$  is a weak solution to the Fokker–Planck equation in  $\mathbb{R}_+ \times \mathbb{R} \times V_\delta$

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

with initial condition

$$p(0, \zeta, v) = p_0(\zeta, v).$$

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  $p(t, \zeta, v)$  as the solution of the integral equation

$$p(t, \zeta, v) = p_0(\zeta + vt, v) \exp(-ct) + \frac{c}{2(1-\delta)} \int_0^t \int_{V_\delta} p(s, \zeta + v(t-s), v') \exp(c(s-t)) dv' ds$$

(see Dautray *et al.*, 1989, Chapter 3, Section 3.2.1). Gronwall’s lemma implies that  $p(t, \zeta, v)$  is bounded and thus integrable w.r.t.  $v$ . A second application of Gronwall’s lemma then leads to (3.15).  $\square$

We now consider problems satisfying (3.13).

**PROPOSITION 3.1** 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

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

**REMARK 3.2** We emphasize that, in the above statement and in the proof below, the specific form of the velocity domain  $V_\delta$  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

$$\begin{aligned} & \mathbb{P}_{x,v}((X_T, V_T) \in B_0, S_2 \leq T) \\ &= \mathbb{E} \iint_G \mathbb{P}_{x+\theta_1 v + \theta_2 v_1, v_2}((X_{T-\theta_1-\theta_2}, V_{T-\theta_1-\theta_2}) \in B_0) c^2 e^{-c(\theta_1+\theta_2)} d\theta_1 d\theta_2, \end{aligned}$$

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  $V_\delta$ . Let  $(\theta_1, \theta_2)$  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 3.2 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

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

Fix  $\theta_1, \theta_2$  and  $\theta_3$  in  $\tilde{G}$ . In view of Lemma 3.2, 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  $C_\delta \inf\left(\frac{1}{\theta_2}, \frac{1}{\theta_3}\right)$  for some  $C_\delta$  which does not depend on the  $\theta_i$ 's. Observe that this bound from below is a function of  $(\theta_2, \theta_3)$  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  $C_\delta$  we get

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

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

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

(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

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

*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

$$\begin{aligned} \mathbb{P}_{x,v}(\tau^D > t) &\geq \mathbb{P}_{x,v}(X_t^D \in D, t_A \leq S_1 \leq t_D) \\ &= \mathbb{E} \int_{t_A}^{t_D} \mathbb{P}_{x+s_1v, Y}(X_{t-s_1}^D \in D) \psi_{S_1}(s_1) ds_1, \end{aligned}$$

where  $Y$  is uniformly distributed on the velocity space and

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

We obviously have

$$\mathbb{P}_{x+s_1v, Y}(X_{t-s_1}^D \in D) \geq \mathbb{P}_{x+s_1v, Y}(X_t^D \in D) \text{ a.s.,}$$

and therefore

$$\mathbb{P}_{x,v}(\tau^D > t) \geq \frac{1}{2(1-\delta)} \mathbb{E} \int_{V_\delta} \int_{t_A}^{t_D} \mathbb{P}_{x+s_1v, v_1}(X_t^D \in D) \psi_{S_1}(s_1) ds_1 dv_1.$$

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  $x_1 = x + s_1v$ , 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,

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

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

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

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

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

$$\exists \beta > 0, \quad \mathbb{P}_{x,v} \left( X_T^D \in (y - \varepsilon, y + \varepsilon), V_T^D \in \left( u - \frac{\varepsilon}{2T}, u + \frac{\varepsilon}{2T} \right) \right) > \beta \varepsilon^2$$

for all  $(x, v) \in D \times V$  and  $(y, u) \in A$  and all  $\varepsilon$  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  $\gamma_1$  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 towards  $y$  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 collision-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  $\gamma_2$  and  $\eta$  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

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

We thus have

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

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

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

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

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

An integration provides

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

where

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

The previous expression is bounded from below by

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

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

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

where

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

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

$$\int_0^1 \cdots \int_0^1 \mathbb{I}_{q - \frac{\varepsilon}{\Theta} \leq x_\Delta + \sum_{j=\Theta}^{N-\Delta} x_j y_j \leq q + \frac{\varepsilon}{\Theta}} dx_1 \cdots dx_{N-1} dy_2 \cdots dy_{N-1}.$$

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

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

There exists  $\zeta > 0$  such that

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

is strictly positive. For such a  $\zeta > 0$  we have

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

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

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

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  $\Psi_S$  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 (Dautray & Lions, 1988, Chapter 18) and is also called multiplying slabs (Dahl & Sjostrand, 1979). 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 Dautray & Lions (1988, Chapter 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

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

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, i.e. 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

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

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 centre 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. Figure 1 shows the time evolution of the direct approximation  $\bar{a}_0(t) := \frac{1}{t} \log(g_E(t))$  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 five of our  $10^6$  simulated trajectories is  $\tau^D$  larger than 400) and, in addition, we have to compute the logarithm of this probability.

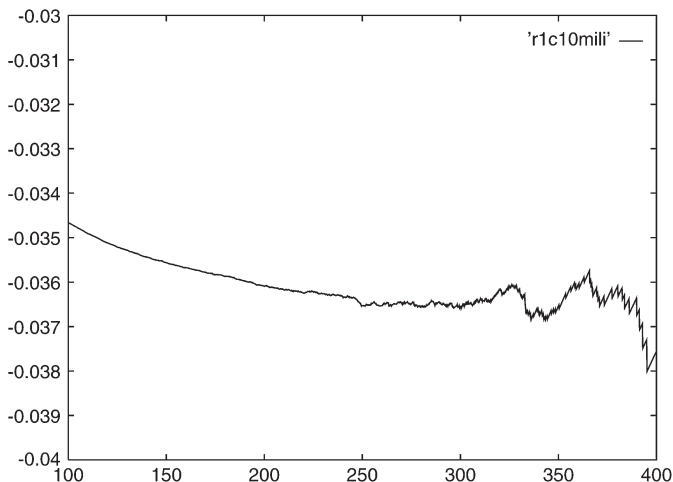


FIG. 1. Direct method;  $x$ -axis:  $t$ ;  $y$ -axis:  $\bar{a}_0(t)$ .

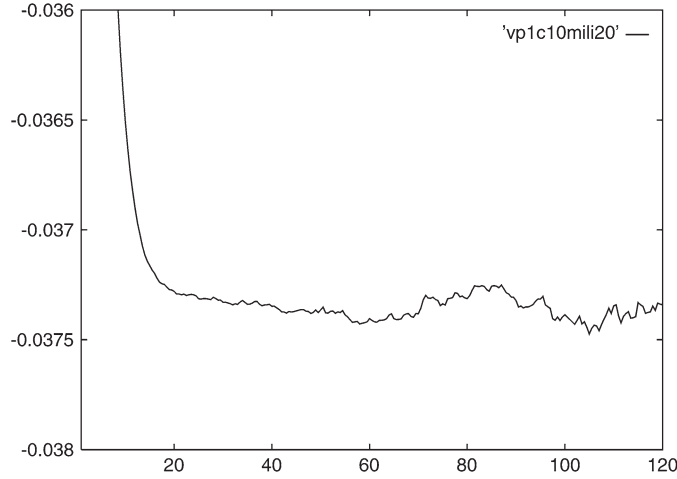


FIG. 2. Interpolation method; x-axis:  $t_1$ ; y-axis:  $\alpha_0(t_1, t_1 + 20)$ .

TABLE 1 *Approximation of the Principal Eigenvalue by the Interpolation Method*

$t_1$	$b_{\text{inf}}$	$\alpha_0(t_1, t_2)$	$b_{\text{sup}}$
50	$-3.7361 \times 10^{-2}$	$-3.7344 \times 10^{-2}$	$-3.7326 \times 10^{-2}$
55	$-3.7360 \times 10^{-2}$	$-3.7341 \times 10^{-2}$	$-3.7322 \times 10^{-2}$
60	$-3.7364 \times 10^{-2}$	$-3.7344 \times 10^{-2}$	$-3.7321 \times 10^{-2}$

#### 4.4 Approximation of the principal eigenvalue by the interpolation method

We now consider the interpolation method of Section 2.3.2. Figure 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  $-0.0374$ .

Table 1 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 ( $b_{\text{inf}}, b_{\text{sup}}$ ).

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  $\alpha_0$  by  $\alpha_0(50, 70)$ . We note that the length of the confidence interval is around  $4 \times 10^{-5}$ , 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 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 Section 4.3. Compared to the interpolation method, the least-squares method appears to be much more accurate. Actually, it

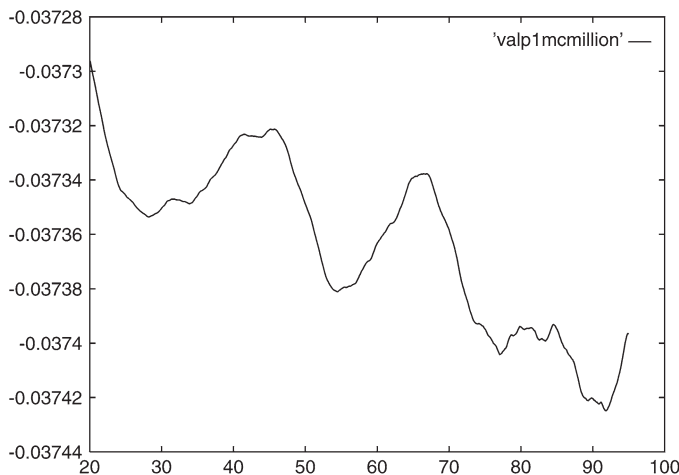


FIG. 3. Least-square approximation ( $c = 1$ );  $x$ -axis:  $t_p$ ;  $y$ -axis:  $\alpha_0(t_p, t_p + 20, 400)$ .

provides an approximation of the principal eigenvalue within  $[-0.0374, -0.0373]$ , which means that the accuracy is of order  $10^{-4}$ .

#### 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, 1979). Using the interpolation method, we compute two approximate values of  $\alpha_0$  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  $c = c_{\min}$ , Table 2 shows that we can choose  $\alpha_0 \simeq -4.13 \times 10^{-4}$ .

For  $c = c_{\max}$ , Table 3 shows that we can choose  $\alpha_0 \simeq 6.21 \times 10^{-4}$ .

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 (1979) has an accuracy of order  $10^{-8}$ .

TABLE 2 *Approximation of the Criticality Factor by the Interpolation Method;  $c = c_{\min}$*

$t_1$	$b_{\inf}$	$\alpha_{0 \min}(t_0, t_1)$	$b_{\sup}$
50	$-4.28 \times 10^{-4}$	$-4.12 \times 10^{-4}$	$-3.94 \times 10^{-4}$
55	$-4.28 \times 10^{-4}$	$-4.13 \times 10^{-4}$	$-3.94 \times 10^{-4}$
60	$-4.28 \times 10^{-4}$	$-4.16 \times 10^{-4}$	$-3.96 \times 10^{-4}$

TABLE 3 *Approximation of the Criticality Factor by the Interpolation Method;  $c = c_{\max}$*

$t_1$	$b_{\inf}$	$\alpha_{0\max}(t_0, t_1)$	$b_{\sup}$
50	$6.05 \times 10^{-4}$	$6.22 \times 10^{-4}$	$6.38 \times 10^{-4}$
55	$6.02 \times 10^{-4}$	$6.21 \times 10^{-4}$	$6.39 \times 10^{-4}$
60	$5.9 \times 10^{-4}$	$6.19 \times 10^{-4}$	$6.4 \times 10^{-4}$

#### 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 and 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  $-1.08 \times 10^{-5}$  and  $1.01 \times 10^{-5}$ . 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 h. This cost is high for a 1D problem. However, it would not increase rapidly with the dimension of the problem.

## 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  $\mu$  represents the average of the cosines of the angles of deviation at the collision. As in Dahl & Sjostrand (1979) we choose  $\mu$  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  $f(v') = \frac{1+3\mu v v'}{2}$ , 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  $\mu$ , which confirms the efficiency of this method.

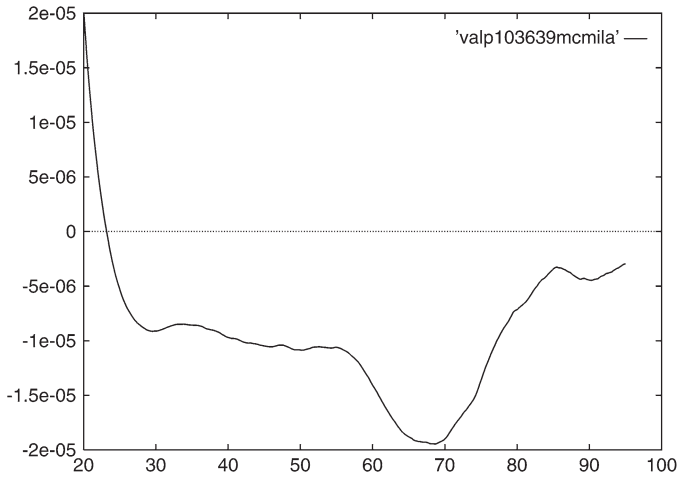


FIG. 4. Least-squares approximation ( $c = 1.03639$ );  $x$ -axis:  $t_p$ ;  $y$ -axis:  $\alpha_0(t_p, t_p + 20, 400)$ .

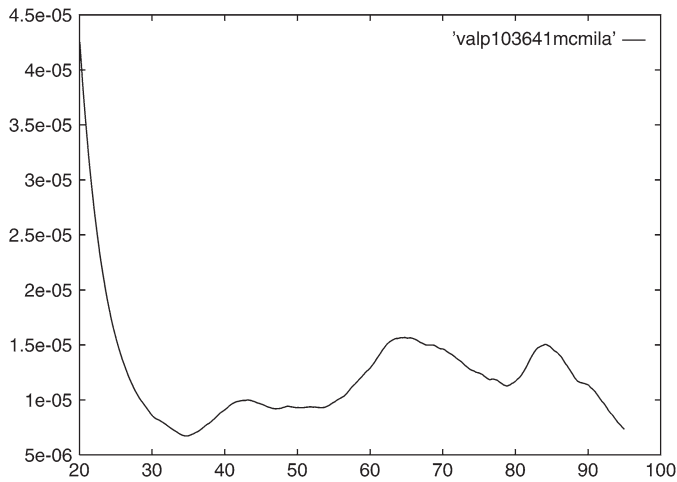


FIG. 5. Least-squares approximation ( $c = 1.03641$ );  $x$ -axis:  $t_p$ ;  $y$ -axis:  $\alpha_0(t_p, t_p + 20, 400)$ .

## 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 centred at the origin 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

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

To simulate a random variable with density

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

we simulate

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

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

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

where the density of  $\theta$  is  $g$ , and  $\varphi$  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 billion trajectories. The principal eigenvalues corresponding to  $c_{\min} = 1.1384$  and  $c_{\max} = 1.1385$ , respectively, are  $-8 \times 10^{-5}$  and  $5 \times 10^{-5}$ . 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 1D. 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 Section 7, 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 Section 2.3.2). In addition, the programming of Monte Carlo methods for these problems is much easier than the programming of deterministic methods.

We note 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  $\Sigma_f$  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 (Khalil, 1986). It has been suggested to Seumen Tonou (1997) by Xavier Warin at the Électricité de France. The eigenvalue problem is

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

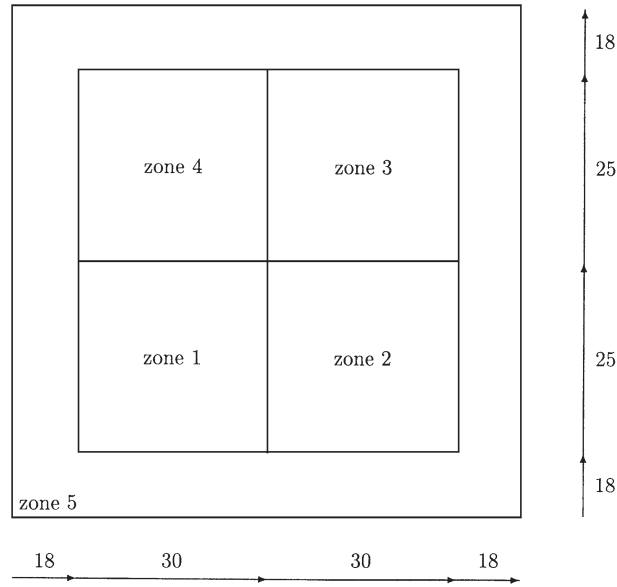


FIG. 6. The physical domain.

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 physical domain  $D$  (see Fig. 6) is divided into five zones. Each zone is characterized by its total cross section  $\Sigma_{\text{tcs}}$  and its scattering cross section  $\Sigma_s$ . The splitting zones are also characterized by their fission cross section  $\Sigma_f$  which indicates the possibility of a fission at point  $(x, y)$ . The average number of neutrons by fission at  $(x, y)$  is  $\nu(x, y)$ .

The dimensions of zone 1 are  $30 \times 25$ , etc. The characteristics of the zones are listed in Table 4.

TABLE 4 Characteristics of the zones

Zone	$\nu \Sigma_f$	$\Sigma_{\text{tcs}}$	$\Sigma_s$
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

$$\begin{aligned} \frac{\partial u}{\partial t} &= b(\mu, \phi) \cdot \nabla_{x,y} u + c(x, y)u \\ &+ \gamma(x, y) \iint_V (u(x, y, \eta, \zeta, t) - u(x, y, \mu, \phi, t)) \pi(x, y, \eta, \zeta) d\eta d\zeta, \end{aligned}$$

with

$$\begin{aligned} b(\mu, \phi) &= (-\mu, -\sqrt{1 - \mu^2} \cos(\phi)), \\ c(x, y) &= v(x, y) \Sigma_f(x, y) + \Sigma_s(x, y) - \Sigma_{\text{tcs}}(x, y), \\ \gamma(x, y) &= v(x, y) \Sigma_f(x, y) + \Sigma_s(x, y), \\ \pi(x, y, \eta, \zeta) &= \frac{1}{4\pi} \mathbb{I}_{[-\Delta, \Delta] \times [\Gamma, \Theta\pi]}(\eta, \zeta). \end{aligned}$$

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 zone with the highest number of splittings, i.e. 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 corresponding to the principal eigenvalue. To get a rough approximation of this eigenfunction, one can use either a deterministic method (see Warin, 1993) or a Monte Carlo method with a relatively small number of particles (see Brockway *et al.*, 1985). The numerical experiments confirm that this technique is efficient.

### 6.4 Computation of the criticality factor

We combine the techniques presented in Sections 6.3.1 and 6.3.2 and we use the least-square method to approximate the principal eigenvalue. We simulate 600 million trajectories. Figures 7 and 8, respectively, correspond to  $\lambda = 1.0095$  and  $\lambda = 1.0085$ , and represent the time evolution of the estimator of the principal eigenvalue.

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

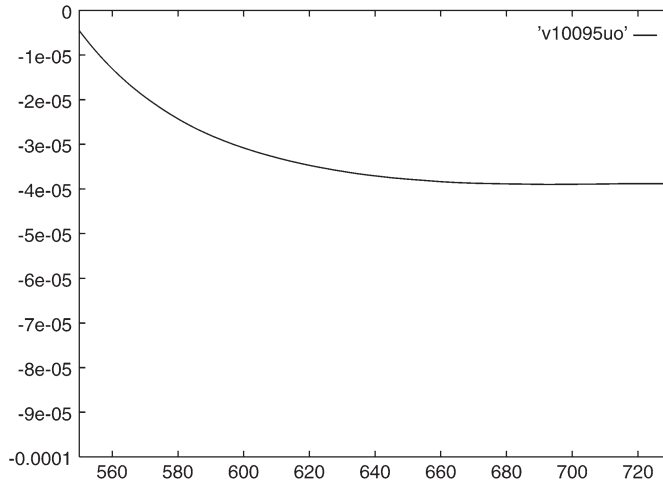


FIG. 7. Least-square approximation ( $\lambda = 1.0095$ ); x-axis:  $t_p$ ; y-axis:  $\alpha_0(t_p, t_p + 20, 400)$ .

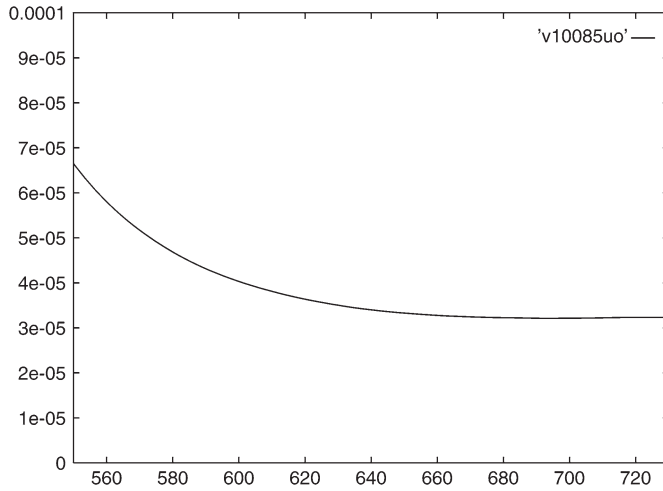


FIG. 8. Least-square approximation ( $\lambda = 1.0085$ ); x-axis:  $t_p$ ; y-axis:  $\alpha_0(t_p, t_p + 20, 400)$ .

## 7. A 3D problem

### 7.1 The physical model

Now consider the operators  $L$  and  $F$  defined as

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

and

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

The domain  $D$  is 3D: the two first spatial coordinates lie in the 2D domain of Section 6.4, and the third spatial coordinate lies in the interval  $[0, 66]$ . We again divide the domain into five zones with the same characteristics as above.

### 7.2 The stochastic representation

The Cauchy problem writes

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

with

$$\begin{aligned} b(v) &= (-v_x, -v_y, -v_z), \\ c(x, v) &= v(x, v) \Sigma_f(x, v) + \Sigma_s(x, v) - \Sigma_{\text{tcs}}(x, v), \\ \gamma(x, v) &= v(x, v) \Sigma_f(x, v) + \Sigma_s(x, v), \\ \pi(x, v) &= \frac{1}{4\pi} \mathbb{I}_{S_0}(v). \end{aligned}$$

### 7.3 Numerical results

Our numerical experiment is performed for  $\lambda = 0.971$  and  $\lambda = 0.972$ . The corresponding approximate principal eigenvalues are, respectively,  $3.9 \times 10^{-5}$  and  $-3.4 \times 10^{-5}$ . Using the secant method, the approximate value of the keff coefficient is 0.97146 whereas the reference value is 0.97142 (see Warin, 1993), so that the error is around  $4 \times 10^{-5}$ .

## 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 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.

### Acknowledgements

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