Flux through a Time-periodic Gate
Monte Carlo Test of a Homogenization Result

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Abstract: We investigate via Monte Carlo numerical simulations and theoretical considerations the outflux of random walkers moving in an interval bounded by an interface exhibiting channels (pores, doors) which undergo an open/close cycle according to a periodic schedule. We examine the onset of a limiting boundary behavior characterized by a constant ratio between the outflux and the local density, in the thermodynamic limit. We compare such a limit with the predictions of a theoretical model already obtained in the literature as the homogenization limit of a suitable diffusion problem.

1 INTRODUCTION

A bunch of individuals moves at random inside a bounded region, say the *playground*. On the boundary of the playground there are one or more *doors* through which they can exit the playground itself. The time average flux of individuals exiting the playground will depend on the local density close to the doors. An interesting question is the following: suppose to know the rule governing the opening of the doors, what is the relation between the local individual density close to the doors and the outgoing flux?

This simple situation models many interesting phenomena on different space and time scales. We mention two examples: (i) the playground is a cell, the individuals are potassium ions, the door is a potassium channel (Hille, 2001; VanDongen, 2004), and the problem is that of computing the ionic current through the channel (Andreucci et al., 2011; Andreucci et al., 2012). This is a very important question in biology, indeed ionic channel are present in almost all living beings and play a key role in regulating the ionic concentration inside the cells.

(ii) The playground is a smoky room (imagine a fire in a cinema), the individuals are evacuees, the door is the door of the room, and the problem is that of computing at which rate the pedestrian are able to escape from the room itself (Schadschneider et al., 2009; Cirillo and Muntean, 2012; Cirillo and Muntean, 2013). In this case the interesting problem is that of understanding if the way in which the evacuees behave (for instance if they cooperate or not) has an influence on the outgoing flux magnitude.

In some situations, for instance when the outgoing flux is compensated by an incoming one, a stationary state with constant (in time) outgoing flux is achieved. In this case the ratio between the outgoing flux and the density close to the doors will be, obviously, a constant, which can be interpreted as the rate at which the individuals close to the doors succeed to exit the playground. This situation is also realized on a short time scale when the number of individuals in the region is large with respect to the number of them exiting the doors per unit of time.

A different situation is that in which no incoming flux is present. In this case the number of individuals inside the playground decreases and so does the typical outgoing flux. The natural question is that of understanding if some time averaged flux has a constant ratio with respect to the average local density close to the door (Andreucci and Bellaveglia, 2012). This question has been posed in (Andreucci and Bellaveglia, 2012) under the assumption that the doors open with a periodic schedule.

The setup considered in (Andreucci and Bellaveglia, 2012) is very basic and, hence, their result is absolutely general. A scalar field is defined on a d–dimensional open hypercube where the field evolves according to the diffusion equation. Homogeneous Neumann boundary conditions are assumed on the boundary of the hypercube excepting "small" circles lying on one of the $(d-1)$–hypercubic faces the

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boundary is made of. In those circles the boundary condition is time–dependent on a periodic schedule, more precisely the positive time axis is subdivided in disjoint intervals (periodic cycles) of equal length and any of such intervals is subdived into two disjoint parts. The boundary condition on the circles is then assumed to be homogeneous Dirichlet into the first part of each of these time intervals and homogeneous Neumann in the second part. (More general shapes than circles are actually considered in (Andreucci and Bellaveglia, 2012).)

If the field is interpreted as the density of individuals in the playgroud, the boundary condition in (Andreucci and Bellaveglia, 2012) can be described as follows: the boundary is always reflecting except for the small circles which are reflecting only in the second part of each of the time intervals considered above, while the individuals are allowed to exit the playground through these circles in the first part of each of these intervals. In other words the small circles are doors of the playground and those doors are open only in the first part of each of the time intervals.

The time periodic micro–structured boundary conditions suggest to approach the problem from the homogenization theory point of view (Bensoussan et al., 1978). With this approach in (Andreucci and Bellaveglia, 2012) it is proven that, provided the length of the open time is suitably small with respect to the length of the cycle, the ratio between the outgoing flux and the field on the small circles (the door) is not trivial, in the sense that it tends to a real number when the length of the periodic cycles tends to zero. This constant ratio is explicitely computed in (Andreucci and Bellaveglia, 2012) and is proven to depend on the way in which each time interval is subdivided into two parts, that is to say on the length of the open door and on that of the closed door time sub–intervals. This result is, in this context, an answer to the question that opened the paper, namely, to the question about the relation between the outgoing flux and the local density of individuals close to the exit.

The present paper has a two–fold aim. In the one–dimensional case we setup a Monte Carlo simulation aiming to (i) test numerically the homogenization limiting result (in the spirit for example of (Haynes et al., 2010)), (ii) compute the ratio between the outgoing flux and the local density close to the exit when the length of the periodic cycles is finite.

This project is realized by introducing a one–dimensional discrete space model on which independent particles perform symmetric random walks. The space is a finite interval on $\mathbb{Z}$ with a boundary point which is reflecting, whereas the other periodically changes its status from absorbing to reflecting and viceversa. We tune the parameters so that the discrete and the continuum space models have equivalent behaviors. Moreover, in the thermodynamics limit, namely, when the number of site of the discrete space model tends to infinity, the homogeneization result proven in the framework of the continuum space model is recovered. This is not proven rigorously, but it is demonstrated via heuristc arguments and Monte Carlo simulations.

The paper is organized as follows. In Section 2 we summarize the homogenization results found in (Andreucci and Bellaveglia, 2012) in the one–dimensional case. In Section 3 the discrete space model is introduced and its behavior is discussed on heuristic grounds. This model is studied via Monte Carlo simulations in Section 4, where all the numerical results are discussed. Section 5 is finally devoted to some brief conclusions.

2 A CONTINUUM SPACE MODEL

In this section we approach the problem via a continuum space model. We summarize, in the one–dimensional case, the results found in (Andreucci and Bellaveglia, 2012). We first introduce the mathematical model and then discuss its physical interpretation.

Pick the two reals $\tau \geq \sigma \geq 0$, the integer m, and the function $u_0 \in L^2([0,L])$. Set $T = (m+1)\tau$ and consider the boundary value problem consisting in the diffusion equation

$$u_t - Du_{xx} = 0 \quad \text{on } (0,L) \times (0,T) \tag{1}$$

with $D > 0$ the *diffusion coefficient*, the initial condition

$$u(x,0) = u_0(x) \quad \forall x \in (0,L) \tag{2}$$

and the boundary conditions

$$u_x(0,t) = 0 \;\; \forall t \in [0,T) \tag{3}$$

and

$$u(L,t) = 0 \;\; \forall t \in A \quad \text{and} \quad u_x(L,t) = 0 \;\; \forall t \in C \tag{4}$$

where

$$A = \bigcup_{k=0}^{m_\tau} [k\tau, k\tau + \sigma) \quad \text{and} \quad C = \bigcup_{k=0}^{m_\tau} [k\tau + \sigma, k\tau + \tau) \, .$$

According to the discussion in Section 1, the model above can be interpreted as follows: the field u is the density of individuals in the playground, m is the number of the door opening/closing cycles, τ is the length of each cycle, σ is the length of the time interval in each cycle during which the door is open, and, finally, A and C are, respectively, the parts of the global time interval $[0,T)$ when the door is open and closed.

In (Andreucci and Bellaveglia, 2012), via an homogenization approach, it has been proven the following convergence result in the limit $\tau \to 0$ for the solution of the boundary value problem (1)–(4) providing an answer to the question about the relation between the individual density $u(L,t)$ at the door and the outgoing flux $-Du_x(L,t)$.

Theorem 2.1. *Assume*

$$\exists \lim_{\tau\to 0} \frac{\sqrt{\sigma}}{\tau} =: \mu \geq 0 \tag{5}$$

and let u^τ be the solution of the boundary value problem (1)–(4)*. Then, as $\tau \to 0$, u^τ converges in the sense of $L^2([0,L]\times[0,T))$ to the solution u of the problem* (1), (2) *with boundary conditions*

$$u_x(0,t) = 0 \quad \forall t \in [0,T) \tag{6}$$

and

$$u_x(L,t) = -\frac{2\mu}{\sqrt{D\pi}} u(L,t) \quad \forall t \in [0,T). \tag{7}$$

Assume

$$\lim_{\tau\to 0} \frac{\sqrt{\sigma}}{\tau} = \infty; \tag{8}$$

then the solution of the boundary value problem (1)–(4) *converges to the solution of the problem* (1), (2) *with boundary condition*

$$u_x(0,t) = u(L,t) = 0 \ \forall t \in [0,T). \tag{9}$$

The physical meaning of the above theorem can be summarized as follows. If the length τ of each periodic unit (cycle) is small with respect to $\sqrt{\sigma}$ (see condition (8)), then, in the $\tau \to 0$ limit, the system behaves as if the door were always open, namely $u(L,t) = 0$. On the other hand, if τ is large with respect to $\sqrt{\sigma}$ (see condition (5) with $\mu = 0$), then, in the $\tau \to 0$ limit, the system behaves as if the door were always closed, namely $u_x(L,t) = 0$. Finally, if τ is of the same order of magnitude of $\sqrt{\sigma}$ (see condition (5) with $\mu > 0$), then, in the $\tau \to 0$ limit, the system behaves as if the door were open with the outgoing flux constrained to satisfy the condition $-Du_x(L,t) = (2\mu\sqrt{D/\pi})u(L,t)$.

2.1 A Glimpse of the Proof of Theorem 2.1

In order to explain the mathematical meaning of the convergence result stated in the theorem, we sketch the proof of the first part of Theorem 2.1. We refer the interested reader to (Andreucci and Bellaveglia, 2012) for more details. First of all we note that for the solution u^τ of the boundary value problem (1)–(4) it is not difficult to perform classical energy estimates and to prove compactness properties in time. Then, possibly by extracting subsequences, we have that a function u exists such that as $\tau \to 0$

$$u^\tau \text{ converges strongly in } L^2([0,L]\times[0,T)) \text{ to } u\,,$$

and

$$u_x^\tau \text{ converges weakly in } L^2([0,L]\times[0,T)) \text{ to } u_x\,.$$

Moreover, it is easily proven that u satisfies (1)–(3) in a standard weak sense. It is important to remark that, via these simple compactness considerations, it is not possible to say anything about the limiting boundary condition satisfied at $x = L$.

In order to identify such a limiting boundary condition, we consider the weak formulation of problem (1)–(4). We choose a smooth test function such that

$$\psi(x,t) = 0 \quad \text{for} \quad \begin{cases} x = 0 \text{ and } t \in (0,T) \\ x = L \text{ and } t \in A \\ x \in [0,L] \text{ and } t = T\,. \end{cases}$$

By multiplying (1) against ψ and by integrating by parts we get

$$-\int_0^T \int_0^L u^\tau \psi_t + \int_0^T \int_0^L Du_x^\tau \psi_x = \int_0^L u_0 \psi(x,0)\,. \tag{10}$$

Next we use the equation above with $\psi = \varphi w$, where $\varphi \in C^\infty([0,L]\times[0,T])$ is such that

$$\varphi(x,t) = 0 \quad \text{for} \quad \begin{cases} x = L \text{ and } t \in (0,T) \\ x \in [0,L] \text{ and } t = T \end{cases}$$

and w is chosen as follows.

The choice of the function w is the key ingredient of the proof. Identifying the properties that the function w has to satisfy in the setting of alternating pores is the main point of the paper (Andreucci and Bellaveglia, 2012), but the general idea of the definition of w was introduced by (Friedman et al., 1995) in a stationary case. We consider the interval $I_\tau = (L - \sqrt{D\tau}, L)$ and define w in $I_\tau \times (0,T)$ as the τ–periodic solution of the equation

$$w_t + Dw_{xx} = 0 \quad \text{on } I_\tau \times (0,T) \tag{11}$$

with boundary conditions

$$w(L,t) = 0 \ t \in A, \quad w_x(L,t) = 0 \ t \in C,$$

and, setting for the sake of notational simplicity $X(\tau) = L - \sqrt{D\tau}$,

$$w(X(\tau),t) = 1 \ t \in (0,T)\,.$$

Notice that we extend $w = 1$ for $x \in (0, X(\tau))$. In (Andreucci and Bellaveglia, 2012) it is proven that as $\tau \to 0$

$$w \text{ converges strongly to 1 in } L^2((0,L)\times(0,T))$$

and

$$w_x \text{ converges weakly to 0 in } L^2([0,L]\times[0,T))\,.$$

Moreover, it is also proven the following highly non–trivial property: as $\tau \to 0$

$$\int_0^T w_x(X(\tau),t)Du^\tau(X(\tau),t)\varphi(X(\tau),t) \to -\frac{2\mu}{\sqrt{D\pi}}\int_0^T Du(L,t)\varphi(L,t)\,. \quad (12)$$

Recall, now, equation (10) and notice that

$$-\int_0^T\int_0^L u^\tau\varphi w_t + \int_0^T\int_0^L Du_x^\tau w_x\varphi = -\int_0^T\int_0^L Du_x^\tau\varphi_x w + \int_0^T\int_0^L u^\tau\varphi_t w + \int_0^L u_0(x)w(x,0)\varphi(x,0)$$

Since w converges strongly to 1, we get that

$$-\int_0^T\int_0^L u^\tau\varphi w_t + \int_0^T\int_0^L Du_x^\tau w_x\varphi \xrightarrow{\tau\to 0} -\int_0^T\int_0^L Du_x\varphi_x + \int_0^T\int_0^L u\varphi_t + \int_0^L u_0(x)\varphi(x,0)\,. \quad (13)$$

We consider next the left hand side in (13) and compute its $\tau \to 0$ limit in a different way. First of all we note that

$$-\int_0^T\int_0^L u^\tau\varphi w_t + \int_0^T\int_0^L Du_x^\tau w_x\varphi = -\int_0^T\int_0^L u^\tau\varphi w_t + \int_0^T\int_0^L D(u^\tau\varphi)_x w_x - \int_0^T\int_0^L u^\tau w_x\varphi_x\,.$$

On the other hand, by using $(Du^\tau\varphi)$ as a test function for w in (11), and integrating by parts we obtain

$$-\int_0^T\int_{X(\tau)}^L (Du^\tau\varphi)\frac{w_t}{D} + \int_0^T\int_{X(\tau)}^L (Du^\tau\varphi)_x w_x = -\int_0^T w_x(X(\tau),t)Du^\tau(X(\tau),t)\varphi(X(\tau),t)\,.$$

Recalling, now, that $w=1$ for $x\in(0,X(\tau))$, from the two equations above we get

$$-\int_0^T\int_0^L u^\tau\varphi w_t + \int_0^T\int_0^L Du_x^\tau w_x\varphi = -\int_0^T w_x(X(\tau),t)Du^\tau(X(\tau),t)\varphi(X(\tau),t) - \int_0^T\int_0^L u^\tau w_x\varphi_x\,.$$

Recalling that w_x converges weakly to 0 in $L^2((0,L)\times(0,T))$ as $\tau\to 0$, by (12), the above equality yields

$$-\int_0^T\int_0^L u^\tau\varphi w_t + \int_0^T\int_0^L Du_x^\tau w_x\varphi \xrightarrow{\tau\to 0} \frac{2\mu}{\sqrt{D\pi}}\int_0^T Du(L,t)\varphi(L,t)\,. \quad (14)$$

By comparing (13) and (14) we finally get

$$\int_0^T\int_0^L[-Du_x\varphi_x + u\varphi_t] + \int_0^L u_0(x)\varphi(x,0) = \frac{2\mu}{\sqrt{D\pi}}\int_0^T Du(L,t)\varphi(L,t)$$

which is the weak formulation of the limiting boundary flux condition for u on $x=L$, given by

$$Du_x(L,t) = -\frac{2\mu}{\sqrt{D\pi}}Du(L,t) \qquad \text{for } t\in(0,T).$$

The theoretical approach just sketched will be commented upon also in the Conclusions.

3 A DISCRETE SPACE MODEL

We now approach the problem via a discrete space model. In this section we first define the model and then discuss heuristically the relation between the outgoing flux and the individual density close to the door. This problem will be investigated in the following section via Monte Carlo simulations.

We consider N one–dimensional independent random walkers on $\Lambda = \{\ell, 2\ell, \dots, n\ell\} \subset \ell\mathbb{Z}$ and denote by $t\in s\mathbb{Z}_+$ the time variable. We assume that each random walk is symmetric, only jumps between neighboring sites are allowed, that 0 is a reflecting boundary point, and that at the initial time the N walkers are distributed uniformly on the set Λ. Moreover, we pick the two integers $1\le\bar\sigma\le\bar\tau$, we partition the time space $s\mathbb{Z}_+$ in

$$A = \bigcup_{i=1}^{\infty}\{s(i-1)\bar\tau, \dots, s[(i-1)\bar\tau+\bar\sigma-1]\}$$

and

$$C = \bigcup_{i=1}^{\infty}\{s[(i-1)\bar\tau+\bar\sigma], \dots, s[i\bar\tau-1]\}\,,$$

and assume that the boundary point $(n+1)\ell$ is absorbing at times in A and reflecting at times in C.

More precisely, if we let $p(x,y)$ be the probability that the walker at site x jumps to site y we have that

$$p(\ell,\ell)=\frac{1}{2},\; p(x,x+\ell)=\frac{1}{2} \;\text{ for }\; x=\ell,\dots,(n-1)\ell,$$

and

$$p(x, x-\ell) = \frac{1}{2} \text{ for } x = 2\ell, \ldots, n\ell;$$

moreover

$$p(n\ell, n\ell) = \begin{cases} 0 & \text{at times in } A \\ 1/2 & \text{at times in } C \end{cases}$$

and

$$p(n\ell, (n+1)\ell) = \begin{cases} 1/2 & \text{at times in } A \\ 0 & \text{at times in } C. \end{cases}$$

Note that when the walker reaches the site $(n+1)\ell$ it is freezed there, so that this system is a model for the proposed problem in the following sense: each walker is an individual, the room is the set $\Lambda = \{\ell, \ldots, n\ell\}$, at the initial time there are N individuals in the room, each walker absorbed at the site $(n+1)\ell$ is counted as an individual which exited the room. We denote by $\mathbb{P}[\cdot]$ and $\mathbb{E}[\cdot]$ the probability and the average along the trajectories of the process.

In the framework of this model an estimator for the ratio between the outgoing individual flux and the typical number of individuals close to the door is given by

$$K_i = \frac{\mathbb{E}[F_i]/(s\overline{\tau})}{(\mathbb{E}[U_i]/\overline{\tau})/\ell} \qquad \text{for all } i \in \mathbb{Z}_+ \tag{15}$$

where F_i is the number of walkers that reach the boundary point $(n+1)\ell$ during the i–th cycle, U_i is the sum over the time steps in the i–th cycle of the number of walkers at the site ℓn.

We are interested into two main problems. The first question that we address is the dependence on time of the above ratio, in other words we wonder if this quantity does depend on i. The second problem that we investigate is the connection between the predictions of this discrete time model and those provided by the continuous space one introduced in Section 2. These two problems will be discussed in this section via heuristic estimates and in the next one via Monte Carlo simulations. Both analytic and numerical computations will be performed under the assumptions

$$\overline{\tau} \gg \overline{\sigma} \quad \text{and} \quad n > 2\overline{\sigma}. \tag{16}$$

The first hypothesis says that the time interval in which the right hand boundary point is absorbing is much smaller than that in which it is reflecting. In other words in each cycle the door is open in a very short time subinterval. The second assumption says that the length of the space interval is larger than $2\overline{\sigma}$ and this will ensure that particles being absorbed by the right hand boundary in a given cycle do not feel the presence of the left hand endpoint in that cycle.

3.1 The Estimator K_i is a Constant

Under the first of the two assumptions (16), it is reasonable to guess that during any cycle the walkers in the system are distributed uniformly in Λ, so that at each time and at each site of Λ the number of walker on that site is approximatively given by $\mathbb{E}[U_i]/\overline{\tau}$. Since $\overline{\sigma}$ is much smaller than $\overline{\tau}$, the mean number of walkers $\mathbb{E}[F_i]$ that reach the boundary point $(n+1)\ell$ during the cycle i is proportional to $\mathbb{E}[U_{i-1}]/\overline{\tau}$ and the constant depends only on $\overline{\sigma}$, so that we have

$$\mathbb{E}[F_i] = \frac{\alpha(\overline{\sigma})}{\overline{\tau}} \mathbb{E}[U_{i-1}]. \tag{17}$$

We also note that, since $\overline{\tau} \gg \overline{\sigma}$, we have that

$$n\frac{1}{\overline{\tau}}\mathbb{E}[U_i] = n\frac{1}{\overline{\tau}}\mathbb{E}[U_{i-1}] - \mathbb{E}[F_i]$$

By combining the two equations above we get that

$$K_i = K \equiv \Big[\frac{1}{\alpha(\overline{\sigma})} - \frac{1}{n}\Big]^{-1} \frac{1}{\overline{\tau}} \frac{\ell}{s} \tag{18}$$

showing that the estimator (15) does not depend on time, namely, it is equal to K for each i.

3.2 Estimating $\alpha(\overline{\sigma})$

As it will be discussed in the following subsection, we are interested in finding an estimate for $\alpha(\overline{\sigma})$ in the limit $\overline{\sigma}$ large.

First of all we give a very rough estimate of such a constant. As noted above, since we assumed, $\overline{\tau} \gg \overline{\sigma}$, it is reasonable to imagine that the walkers are distributed uniformly with density $\mathbb{E}[U_{i-1}]/\overline{\tau}$ when the i–th cycle begins (opening of the door). Hence, since the walkers are independent, we get

$$\mathbb{E}[F_i] = \frac{\mathbb{E}[U_{i-1}]}{\overline{\tau}} \times S,$$

where we denote by S the sum over the particles that at time $(i-1)\overline{\tau} - 1$ are less than $\overline{\sigma}$ sites from the absorbing boundary point of the probability that each of them reaches the absorbing boundary in the next $\overline{\sigma}$ time steps. Recalling (17), we have

$$\alpha(\overline{\sigma}) = S. \tag{19}$$

This representation allows an immediate rough estimate of the quantity $\alpha(\overline{\sigma})$. If $\overline{\sigma}$ is large, at time $\overline{\sigma}$ each walker space distribution probability can be approximated by a gaussian function with variance $\sqrt{2\overline{\sigma}}$ (Central Limit Theorem). Hence, the number of particles that reach in the following $\overline{\sigma}$ steps the boundary $(n+1)\ell$ is approximatively given by the number of walkers at the $\sqrt{2\bar{\sigma}}$ sites counted starting from the absorbing boudary point divided by 2. Hence, we find the estimate

$$\alpha(\bar{\sigma}) \approx \frac{1}{2}\sqrt{2\bar{\sigma}} = \sqrt{\frac{\bar{\sigma}}{2}}$$

suggesting that the quantity $\alpha(\bar{\sigma})$ depends on $\bar{\sigma}$ as $\sqrt{\bar{\sigma}}$.

We now discuss a more precise argument. In order to compute the right hand term in (19) we consider a particle performing a simple symmetric random walk on $\mathbb{Z}$ and denote by $\mathbb{Q}$ the probability along the trajectories of the process. Since we have assumed $n > 2\bar{\sigma}$, see (16), the probability that a particle in the original model starting at a position which is y site far from the absorbing boundary point, with $1 \le y \le \bar{\sigma}$, reaches such a point in a time smaller than or equal to $\bar{\sigma}$ is equal to the probability that the single symmetric walker on $\mathbb{Z}$ starting at 0 reaches the point y in a time smaller than or equal to $\bar{\sigma}$. Then, if we let T_y be the first hitting time to $y \in \mathbb{Z}$ for the simple symmetric walker on $\mathbb{Z}$ started at 0, from (19), we have that

$$\alpha(\bar{\sigma}) = \sum_{y=1}^{\bar{\sigma}} \mathbb{Q}[T_y \le \bar{\sigma}] = \sum_{y=1}^{\bar{\sigma}} \sum_{h=y}^{\bar{\sigma}} \mathbb{Q}[T_y = h] = \sum_{y=1}^{\bar{\sigma}} \sum_{h=y}^{\bar{\sigma}} \frac{y}{h} \mathbb{Q}[S_h = y]$$

where S_h denotes the position of the walker at time h and in the last equality we have used (Grimmet and Stirzaker, 2001, Theorem 14 in Section 3.10). Recalling, now, (Grimmet and Stirzaker, 2001, equation (2) in Section 3.10), we have that

$$\alpha(\bar{\sigma}) = \sum_{y=1}^{\bar{\sigma}} y \sum_{\substack{h=y:\\ h+y \text{ even}}}^{\bar{\sigma}} \frac{1}{h} \binom{h}{(h+y)/2} \frac{1}{2^h}. \tag{20}$$

We first remark that, since $\alpha(\bar{\sigma})$ is a double sum of positive terms, we have that $\alpha(\bar{\sigma})$ is an increasing function of $\bar{\sigma}$. In the next theorem we state two important properties of $\alpha(\bar{\sigma})$. The proof of the theorem will use the result stated in the following lemma.

Lemma 3.1. *Let $f : \mathbb{Z}_+ \to \mathbb{R}$ be a function such that the limit $\lim_{m\to\infty} f(m)$ does exist. Then,*

$$\lim_{m\to\infty} \frac{1}{\sqrt{m}} \sum_{i=1}^{m} \frac{1}{\sqrt{i}} f(i) = 2 \lim_{m\to\infty} f(m)$$

Proof. First note that

$$\lim_{m\to\infty} \frac{1}{\sqrt{m+1}-\sqrt{m}} \Big[\sum_{i=1}^{m+1} \frac{1}{\sqrt{i}} f(i) - \sum_{i=1}^{m} \frac{1}{\sqrt{i}} f(i) \Big] = \lim_{m\to\infty} \frac{1}{\sqrt{m+1}-\sqrt{m}} \frac{f(m+1)}{\sqrt{m+1}} = 2 \lim_{m\to\infty} f(m)$$

The statement follows by the Stolz-Cesàro theorem. □

Theorem 3.2. *The function $\alpha : \mathbb{Z}_+ \to \mathbb{R}$ satisfies*

$$\lim_{r\to\infty} \frac{\alpha(r)}{\sqrt{r}} = \sqrt{\frac{2}{\pi}}. \tag{21}$$

Proof. We assume r even; the case r odd can be treated similarly. In order to get (21) we rewrite (20) as

$$\alpha(r) = \alpha_{\mathrm{e}}(r) + \alpha_{\mathrm{o}}(r) \tag{22}$$

with

$$\alpha_{\mathrm{e}}(r) \equiv \sum_{k=1}^{r/2} (2k) \sum_{s=k}^{r/2} \frac{1}{2s} \binom{2s}{(2s+2k)/2} \frac{1}{2^{2s}}$$

and

$$\alpha_{\mathrm{o}}(r) \equiv \sum_{k=1}^{r/2} (2k-1) \times \sum_{s=k}^{r/2} \frac{1}{2s-1} \binom{2s-1}{(2s+2k-2)/2} \frac{1}{2^{2s-1}}$$

We shall prove that

$$\lim_{r\to\infty} \frac{\alpha_{\mathrm{e}}(r)}{\sqrt{r}} = \sqrt{\frac{1}{2\pi}}; \quad \lim_{r\to\infty} \frac{\alpha_{\mathrm{o}}(r)}{\sqrt{r}} = \sqrt{\frac{1}{2\pi}} \tag{23}$$

and hence (22) will imply (21).

We are then left with the proof of (23). We only prove the first of the two limits; the argument leading to the second one is similar. First of all we note that

$$\alpha_{\mathrm{e}}(r) = \sum_{k=1}^{r/2} \sum_{s=k}^{r/2} \frac{k}{s} \binom{2s}{s+k} \frac{1}{2^{2s}} = \sum_{s=1}^{r/2} \sum_{k=1}^{s} \frac{k}{s} \binom{2s}{s+k} \frac{1}{2^{2s}} = \sum_{s=1}^{r/2} \sum_{h=s+1}^{2s} \frac{h-s}{s} \binom{2s}{h} \frac{1}{2^{2s}}$$

Thus, by using the properties of the binomial coefficients we get

$$\alpha_{\mathrm{e}}(r) = -\sum_{s=1}^{r/2} \sum_{h=s+1}^{2s} \binom{2s}{h} \frac{1}{2^{2s}} + \sum_{s=1}^{r/2} \sum_{h=s+1}^{2s} \frac{h}{s} \binom{2s}{h} \frac{1}{2^{2s}} = -\sum_{s=1}^{r/2} \sum_{h=s+1}^{2s} \binom{2s}{h} \frac{1}{2^{2s}} + \sum_{s=1}^{r/2} \sum_{h=s+1}^{2s} \binom{2s-1}{h-1} \frac{1}{2^{2s-1}}$$

and, hence,

$$\alpha_{\mathrm{e}}(r) = -\sum_{s=1}^{r/2} \sum_{h=s+1}^{2s} \binom{2s}{h} \frac{1}{2^{2s}} + \sum_{s=1}^{r/2} \sum_{\ell=s}^{2s-1} \binom{2s-1}{\ell} \frac{1}{2^{2s-1}}$$

Now, by the Newton's binomial theorem we get

$$\alpha_e(r) = \sum_{s=1}^{r/2} \Big\{ -\frac{1}{2}\Big[1 - \frac{1}{2^{2s}}\binom{2s}{s}\Big] + \frac{1}{2}\Big\} = \sum_{s=1}^{r/2} \frac{1}{2^{2s+1}}\binom{2s}{s} \qquad (24)$$

which is a notable expression for α_e. The Stirling's approximation finally yields

$$\alpha_e(r) = \sum_{s=1}^{r/2} \frac{1}{2^{2s+1}} 2^{2s} \frac{1}{\sqrt{\pi}}\frac{1}{\sqrt{s}}[1+g(s)] = \frac{1}{2\sqrt{\pi}} \sum_{s=1}^{r/2} \frac{1}{\sqrt{s}}[1+g(s)]$$

where $g(s) \to 0$ as $s \to \infty$. Hence,

$$\lim_{r\to\infty} \frac{\alpha_e(r)}{\sqrt{r}} = \frac{1}{2\sqrt{\pi}} \lim_{r\to\infty} \frac{1}{\sqrt{r}} \sum_{s=1}^{r/2} \frac{1}{\sqrt{s}}[1+g(s)] = \frac{1}{2\sqrt{2\pi}} \lim_{t\to\infty} \frac{1}{\sqrt{t}} \sum_{s=1}^{t} \frac{1}{\sqrt{s}}[1+g(s)] \qquad (25)$$

The first of the two limits (23) finally follows from (25) and Lemma 3.1. ☐

Moreover, also relying upon the numerical simulations, we conjecture that there exists a positive integer r_0 such that

$$\frac{\alpha(r+1)}{\sqrt{r+1}} - \frac{\alpha(r)}{\sqrt{r}} > 0 \qquad (26)$$

for any integer $r \geq r_0$.

3.3 Comparison with the Continuum Space Model

In order to compare the results discussed above in this section with those in Section 2 referring to the continuous space model defined therein, we have to consider two limits. The parameter $\bar{\sigma}$ has to be taken large (recall, also, that we always assume $\bar{\tau} \gg \bar{\sigma}$, see (16)) so that, due to the Central Limit Theorem, the discrete and the continuous space model have similar behaviors provided the other parameters are related as $2Ds = \ell^2$. With this choice of the parameters, then, we expect that, provided the ratio σ/τ^2 is chosen properly, the discrete space model will give results similar to those predicted by the continuous space one with finite τ.

In (Andreucci and Bellaveglia, 2012), see Theorem 2.1, the relation between the outoing flux and the density close to the pore is worked out only in the limit $\tau \to 0$. We then have to understand how to implement such a limit in our discrete time model.

We perform this analysis in the critical case $\sigma = \mu^2\tau^2$. In order to compare the discrete and the continuum space models we first let

$$\ell = \frac{L}{n+1}. \qquad (27)$$

As already remarked above, from the Central Limit Theorem, it follows that the two models give the same long time predictions if $2Ds = \ell^2$; hence, the time unit is set to

$$s = \frac{\ell^2}{2D} = \frac{L^2}{2D(n+1)^2}. \qquad (28)$$

We then consider the random walk model introduced above by choosing $\bar{\sigma}$ and $\bar{\tau}$ such that the equality $\bar{\sigma}s = (\mu\bar{\tau}s)^2$ is satisfied as closely as possible (note that $\bar{\tau}$ and $\bar{\sigma}$ are integers). This can be done as follows: we fix L, n, μ, and $\bar{\sigma}$ and we then consider

$$\bar{\tau} = \Big\lfloor \frac{1}{\mu}\sqrt{\frac{\bar{\sigma}}{s}} \Big\rfloor = \frac{1}{\mu}\frac{n+1}{L}\sqrt{2D\bar{\sigma}} - \delta \qquad (29)$$

where $\lfloor\cdot\rfloor$ denotes the integer part of a real number and $\delta \in [0,1]$. With the above choice of the parameters, the behavior of the random walk model has to be compared with that of the continuum space model in Section 2 with period

$$\tau = s\bar{\tau} = \frac{1}{\mu}\frac{L\sqrt{\bar{\sigma}}}{(n+1)\sqrt{2D}} - \frac{L^2}{2D(n+1)^2}\delta. \qquad (30)$$

The equation (30) is very important in our computation, since it suggests that the homogenization limit $\tau \to 0$ studied in the continuum model should be captured by the discrete space model via the thermodynamics limit $n \to \infty$. We then expect that the estimator K has to converge to the constant $2\mu\sqrt{D}/\sqrt{\pi}$ in this limit.

This seems to be the case if we use the heuristic estimate of the constant K obtained above. Indeed, by (18) and (30), we have that

$$K = \Big[\frac{1}{\alpha(\bar{\sigma})} - \frac{1}{n}\Big]^{-1} \sqrt{\frac{2D}{\bar{\sigma}}}\mu \times \Big[1 + \frac{\delta\mu L}{\sqrt{2D\bar{\sigma}}}\frac{1}{n+1} + o\Big(\frac{1}{n+1}\Big)\Big] \qquad (31)$$

for the ratio between the outgoing flux and the local density close to the door, where $o(1/(n+1))$ is a function tending to zero faster than $1/(n+1)$ in the limit $n \to \infty$. In the next section we shall obtain such an estimate via a Monte Carlo computation, but here, by using (21), we get that

$$K \stackrel{n\to\infty}{\longrightarrow} \frac{\alpha(\bar{\sigma})}{\sqrt{\bar{\sigma}}}\sqrt{2D}\mu \stackrel{\bar{\sigma}\to\infty}{\longrightarrow} \sqrt{\frac{2}{\pi}}\sqrt{2D}\mu = 2\mu\sqrt{\frac{D}{\pi}}$$

which is the desired limit.

4 MONTE CARLO RESULTS

In this section we describe the Monte Carlo computation of the constant (15). This measure is quite difficult since in this problem the stationary state is trivial, in the sense that, since there is an outgoing flux through the boudary point $(n+1)\ell$ and no ingoing flux is present, all the particles will eventually exit the system itself.

Our problem can be rephrased as follows: both the outgoing flux and the local density at the door are two "globally decreasing" random variables, but their mutual ratio is constant in average. We then have to set up a procedure to capture this constant ratio.

For the time length of the open state, we shall consider the following values

$$\bar{\sigma} = 30, 50, 70, 100, 120, 150, 200\,.$$

For each of them, in order to perform the limit $\tau \to 0$, we shall consider

$$n = 200, 400, 600, 800, 1000, 1500, 3000, 5000, 10000$$

for the number of sites of the lattice Λ.

For each choice of the two parameters $\bar{\sigma}$ and n we shall run the process and compute at each cycle i the quantity

$$k_i = \frac{F_i/(\bar{\tau})}{U_i/(\bar{\tau})}$$

where, we recall, $\bar{\tau}$ is defined in (29) and F_i and U_i have been defined below (15).

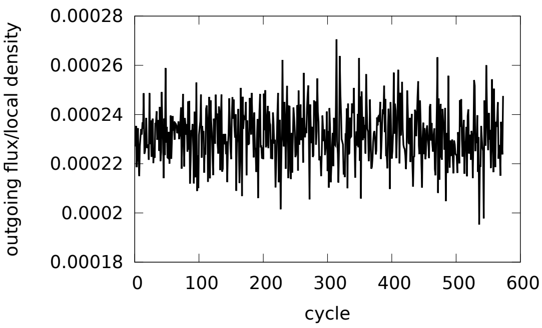

Figure 1: The quantity k_i is plotted vs. the cycle number i in the case $\bar{\sigma} = 30$ and $n = 5000$.

The quantity k_i is a random variable fluctuating with i, but, as it is illustrated in the Figures 1 and 2, it performs random oscillations around a constant reference value. We shall measure this reference value by computing the time average of the quantity k_i. We shall average k_i by neglecting the very last cycles which are characterized by large oscillations due to the smallness of the number of residual particles in the system.

The product of the reference value for the random variable k_i and the quantity ℓ/s, see the equations

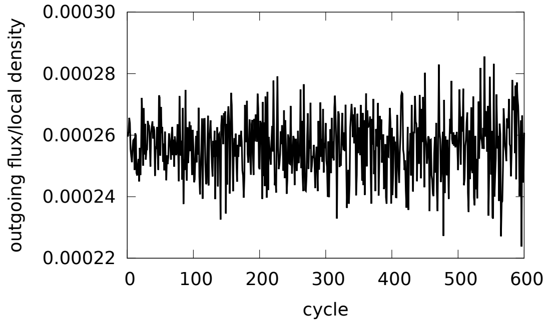

Figure 2: The quantity k_i is plotted vs. the cycle number i in the case $\bar{\sigma} = 200$ and $n = 5000$.

(15), (27) and (28), will be taken as an estimate for K. In other words the output of our computation will be the quantity

$$K = \frac{\ell}{s} \times (k_i \text{ time average})\,. \tag{32}$$

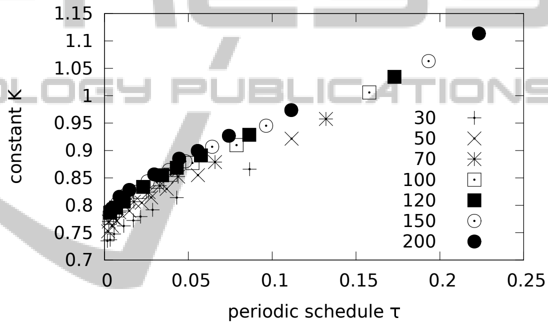

Figure 3: The Monte Carlo estimate of the constant K measured as in (32) vs. the periodic time schedule τ. Each series of data refers to the $\bar{\sigma}$ value reported on the right bottom part of the figure.

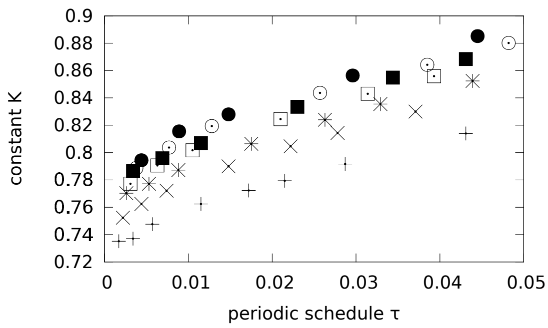

Figure 4: The same data as in figure 3 zoomed in the interval $[0, 0.05]$.

We perform the computation described above with $D = 1$, $L = \pi$, $\mu = 1/\sqrt{2}$; with this choice the continuum space model prediction for the ratio is $2\mu\sqrt{D}/\sqrt{\pi} = 0.798$.

Our numerical results are illustrated in Figures 3 and 4. We note that by increasing $\bar{\sigma}$ the numerical series tend to collapse to one limiting behavior.

Table 1: The parameter τ, computed via (30), for the specified values of $\bar{\sigma}$ and n.

		n								
		200	400	600	800	1000	1500	3000	5000	10000
$\bar{\sigma}$	30	0.0865	0.0431	0.0287	0.0215	0.0172	0.0115	0.0057	0.0034	0.0017
	100	0.1579	0.0787	0.0524	0.0393	0.0314	0.0210	0.0105	0.0063	0.0031
	200	0.2233	0.1114	0.0742	0.0556	0.0445	0.0296	0.0148	0.0089	0.0044

Table 2: Measured constant K for the specified values of $\bar{\sigma}$ and n.

		n								
		200	400	600	800	1000	1500	3000	5000	10000
$\bar{\sigma}$	30	0.8660	0.8140	0.7916	0.7794	0.7723	0.7624	0.7476	0.7371	0.7351
	100	1.0059	0.9099	0.8772	0.8559	0.8430	0.8245	0.8017	0.7906	0.7772
	200	1.1135	0.9738	0.9269	0.8994	0.8852	0.8564	0.8280	0.8155	0.7944

This is in agreement with what we proved in Section 3.2. Moreover, provided $\bar{\sigma}$ is large enough, for $\tau \to 0$ the measured constant tends to the theoretical value 0.798. For $\bar{\sigma} = 30, 100, 200$ we have also reported in Tables 1 and 2 the data plotted in Figure 3.

We can finally state that the Monte Carlo measure of the constant K is in very good agreement with the theoretical predictions discussed above.

We also note that, both the continuum space study outlined in Section 2 and the heuristic discussion of its discrete space counterpart given in Section 3 were just able to predict the value of the constant K in the limit $\tau \to 0$. No information was given on its behavior at finite τ.

The Monte Carlo computations, on the other hand, suggest that K increases with the periodic schedule τ. We cannot give, at this stage of our reasearch, a physical interpretation of this result. This is for sure a very interesting point in the framework of this problem, indeed, it is connected with the efficiency of the evacuation phenomenon in connection with the periodicity of the open/close door cycles.

5 CONCLUSIONS

We have studied via Monte Carlo simulations the outgoing flux through a “door” periodically alternating between open and closed states. We have shown that the discrete space random walk model exhibits the onset of the same limiting behavior as the continuum space model sketched in Section 2. The homogenization limit of the continuum space model corresponds to the thermodynamics limit in the discrete space one.

The first one of the goals stated in the Introduction, that is the numerical test of the homogenization result, has been in our opinion achieved (see the Figures and the comments in Section 4). We remark that we raised some problems in the theory of random walk which, albeit not tackled in this paper, seem to deserve a theoretical investigation (see Section 3.1).

As to our second goal of investigating the problem for finite τ, we have found clear evidence of a monotonic behavior in τ of the estimator K, which we deem believable in view of the just commented coherence shown by the Monte Carlo method with the theoretical Theorem 2.1.

In this connection we must remark that even from the short account of the main steps in the proof of Theorem 2.1, given in Section 2.1, it is quite clear that the monotonic behavior identified by the Monte Carlo approach is not easily amenable to investigation, or even discovery, by means of that theoretical approach.

As remarked in the previous Section, we do not presently provide a full insight in the origin and meaning of this behavior, which however is connected with our conjecture (26), and with the efficiency of the evacuation phenomenon as a function of τ. It is important to recall, finally, that at least in biological applications the efficiency of this mechanism is not the only concern. For example the alternating schedule of ion channels has been connected to the selection of a preferred ion species (VanDongen, 2004). Thus in general we expect τ to satisfy several different constraints coming from different features of the biological system.

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