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# On the possibility of track length based Monte-Carlo algorithms for stationary drift-diffusion systems with sources and sinks

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The problem of constructing Monte-Carlo solutions of drift-diffusion systems corresponding to Fokker-Planck equations with sources and sinks is revisited. Firstly, a compact formalism is introduced for the specific problem of stationary solutions. This leads to identification of the dwell time as the key quantity to characterize the system and to obtain a proper normalization for statistical analysis of numerical results. Secondly, the question of appropriate track length estimators for drift-diffusion systems is discussed for a 1D model system. It is found that a simple track length estimator can be given only for pure drift motion wihout diffusion. The stochastic nature of the diffusive part cannot be appropriately described by the path length of simulation particles. Further analysis of the usual situation with inhomogeneous drift and diffusion coefficients leads to an error estimate based on particle trajectories. The result for limits in grid cell size and time step used for the construction of Monte-Carlo trajectories resembles the Courant-Friedrichs-Lewy and von Neumann conditions for explicit methods.

## I. INTRODUCTION

The Monte-Carlo approach is a well-known and widely used method for the numerical solution of time-dependent and stationary problems [1–5]. Its particular strength is in the flexible incoporation of complex multi-dimensional geometries, its straightforward implementation in computer codes and its algorithmic robustness. Although sometimes based on intuition most applications are based on rigorous mathematical relations between systems of partial differential equations, corresponding Green's functions and stochastic processes. Many examples of such applications are based on Fokker-Planck models for drift-diffusion dynamics and its equivalent in the theory of stochastic differential equations. To mention only a few: codes in plasma physics research for studies on kinetic impurity transport [6–8] , for neutral particle transport [9**?** –11] and for plasma fluid transport [12] are based on certain variants of Fokker-Planck models including sources and sinks. Usually these codes are optimized for the treatment of stationary systems and all together they suffer from statistical noise due to limited CPU time which limits the number stastistical samples. The search for a solution to this problem, i. e. increasing the algorithmic efficiency and reducing the noise, has a long history and led to the design of so-called estimators [13] which allow to gain more information out of the computational effort than simpler and perhaps more intuitive methods. One example of such a device is the track length estimator, which does not only accounts for certain locations of simulation particles, but rather considers the finite path length of simulation particles to evaluate the particle distributions in the computational volume and thereby reduces the statistical noise in the numerical solution. Although well established for many years in simulations of neutrons and neutral particle transport it is surprising that its implementation in diffusion problems is not that well discussed nor documented. Questions in this context concern a proper normalization of numerical solutions, error estimates and a rigorous mathematical derivation of sometimes intuitively obvious methods. In this paper we want to contribute to the discussion of implementing a track length estimator in drift-diffusion problems closely related to the research fields mentioned above. To introduce notation and mathematical framework the problem at hand is sketched briefly in section II. The formalism leads immediately to the dwell time of the physical system as the key quantity for constructing a time stepping algorithm. In section III the general framework is applied to the Fokker-Planck equation. Well known facts on its corresponding stochastic differential equations and Green's functions are used to discuss the particular Monte-Carlo approach for its solution. Without loss of generality, basic results are derived for the particular case of a homogeneous 1D problem. Based on this, in section IV the concept of the track length as a mean to estimate the dwell time is discussed. After a few general comments on simulations of diffusive motion, the analysis of the more important inhomogeneous 1D case in section V shows that requirements on accuracy of the stochastic approach excludes simple track length estimators for diffusive problems and leads essentially to restrictions on time step and spatial resolution recovering the Courant-Friedrichs-Lewy and von Neumann conditions for explicit finite difference methods. In the concluding section VI a short summary of the findings is given.

## II. CONSTRUCTION OF MONTE-CARLO PATHS, DWELL TIME AND NORMALIZATION

In the context of particle transport, collision processes and fluid flow the Monte-Carlo approach can be considered roughly as a sampling of random paths of simulation particles according to certain rules determining jumps or discrete steps in a computational volume. The distribution of these particles resulting from a given particle

ensemble at the beginning of the simulation then represents the solution for a particular quantity of interest. A random path in configuration space can be described by a probability density $P_m^+(\mathbf{x}_m|\mathbf{x}_0;t_m)$ representing a path of a single particle starting at location $\mathbf{x}_0$ and moving to location $\mathbf{x}_m$ with $m$ steps passing the intermediate locations $\mathbf{x}_1$, $\mathbf{x}_2$,...,$\mathbf{x}_{m-1}$. The time corresponding to the step from $\mathbf{x}_{i-1}$ to $\mathbf{x}_i$ is denoted by $\Delta_i$, the total time needed for the entire path is denoted by $t_m{=}\sum_{i=1}^m \Delta_i$. Each step is a random event guided by some transition probability density $p^+(\mathbf{x}_i|\mathbf{x}_{i-1};\Delta_i)$. The notation $p^+$ labels a step where the particle really arrives at $\mathbf{x}_i$, whereas the opposite event, where the particle disappears during the step, is taken into account by a transition probability $p^-(\mathbf{x}_i|\mathbf{x}_{i-1};\Delta_i)$. The sum of those describes the certain event that the particle does a step. This is written as

$$p(\mathbf{x}|\mathbf{y};\Delta) = p^+(\mathbf{x}|\mathbf{y};\Delta) + p^-(\mathbf{x}|\mathbf{y};\Delta) \tag{1}$$

and

$$\int_\Omega p(\mathbf{x}|\mathbf{y};\Delta)\, d\mathbf{x} = 1 \tag{2}$$

and means that a particle existing at $\mathbf{y}$ will definitely do a step during a time increment $\Delta$ towards some location in the volume $\Omega$, but perhaps it will get lost. Therefore, the probability of a particle still existing after $m$ steps can be described by

$$P_m^+(\mathbf{x}_m|\mathbf{x}_0;t_m) = \prod_{i=1}^m p^+(\mathbf{x}_i|\mathbf{x}_{i-1};\Delta_i) \tag{3}$$

The representation by a product of probabilities requires the Markov assumption, i. e. each step is independent of the previous steps. Therefore, the event that a particle does $m-1$ steps and gets lost at the $m$th step is

$$\begin{aligned} P_m^-(\mathbf{x}_m|\mathbf{x}_0;t_m) &= p^-(\mathbf{x}_m|\mathbf{x}_{m-1};\Delta_m)\times \\ &\quad\times P_{m-1}^+(\mathbf{x}_{m-1}|\mathbf{x}_0;t_m-\Delta_m) \end{aligned} \tag{4}$$

Next the path probabilities are connected to ensembles of particles by assuming that the probability of finding a particle at $\mathbf{x}_0$ at time $t_0$ can be described by a probability distribution function $f^+(\mathbf{x}_0,t_0)$ obeying

$$\int_\Omega f^+(\mathbf{x}_0,t_0)\, d\mathbf{x}_0 = 1 \tag{5}$$

The particle density $n$ of the ensemble at time $t_0$ is obtained by multiplication with the total number $N$ of particles in the volume $\Omega$

$$n(\mathbf{x}_0,t_0) = N\, f^+(\mathbf{x}_0,t_0) \tag{6}$$

Thus, the distribution function

$$\begin{aligned} &f^+(\mathbf{x}_m,t_m) \\ &\quad= \int_\Omega\!\ldots\!\int_\Omega P_m^+(\mathbf{x}_m|\mathbf{x}_0;t_m)\, f^+(\mathbf{x}_0,t_0)\, d\mathbf{x}_{m-1}\ldots d\mathbf{x}_0 \end{aligned} \tag{7}$$

gives the distribution of particles $n(\mathbf{x}_m,t_m) = N\, f^+(\mathbf{x}_m,t_m)$ in the volume after $m$ time steps. The resulting integral equation

$$f^+(\mathbf{x}_m,t_m) = \int_\Omega p^+(\mathbf{x}_m|\mathbf{x}_{m-1};\Delta_m)\, f^+(\mathbf{x};t_{m-1})\, d\mathbf{x} \tag{8}$$

identifies the transition probabilities as propagators for the distribution function during the random path. To simplify notation and for subsequent discussions a general propagator for the Monte-Carlo chain is introduced by

$$\begin{aligned} &G^+(\mathbf{x}_m|\mathbf{x}_j;t_m) \\ &\quad= \int_\Omega\!\ldots\!\int_\Omega P_m^+(\mathbf{x}_m|\mathbf{x}_j;t_m-t_j)\, d\mathbf{x}_{m-1}\ldots d\mathbf{x}_{j+1} \end{aligned} \tag{9}$$

This definition allows to write

$$f^+(\mathbf{x}_m,t_m) = \int_\Omega G^+(\mathbf{x}_m|\mathbf{x}_j;t_m-t_j)\, f^+(\mathbf{x}_j,t_j)\, d\mathbf{x}_j \tag{10}$$

Similarly a propagator for the termination of the path is defined by

$$\begin{aligned} &G^-(\mathbf{x}_m|\mathbf{x}_j;t_m) \\ &\quad= \int_\Omega\!\ldots\!\int_\Omega P_m^-(\mathbf{x}_m|\mathbf{x}_j;t_m-t_j)\, d\mathbf{x}_{m-1}\ldots d\mathbf{x}_{j+1} \end{aligned} \tag{11}$$

and a corresponding distribution function $f^-$

$$f^-(\mathbf{x}_m,t_m) = \int_\Omega G^-(\mathbf{x}_m|\mathbf{x}_j;t_m-t_j)\, f^+(\mathbf{x}_j,t_j)\, d\mathbf{x}_j \tag{12}$$

which represents the loss probability distribution for particles at the $m$th step. Due to the normalization condition of Eq. 2 a recursive relation for the distribution functions $f^+$ and $f^-$ can be found

$$\int_\Omega f^+(\mathbf{x},t_m)\, d\mathbf{x} = \int_\Omega f^+(\mathbf{x},t_{m-1})\, d\mathbf{x} - \int_\Omega f^-(\mathbf{x},t_m)\, d\mathbf{x} \tag{13}$$

and it follows

$$\int_\Omega f^+(\mathbf{x},t_m)\, d\mathbf{x} + \sum_{i=1}^m \int_\Omega f^-(\mathbf{x},t_i)\, d\mathbf{x} = 1 \tag{14}$$

which simply expresses the fact that a particle is still present in the volume $\Omega$ after $m$ steps or was lost at an intermediate step. The distribution function $f^-(\mathbf{x},t)$ allows to derive easily certain statistical averages along the chain. For example, the average dwell time $\tau_m$ of

a particle, i. e. the average duration of particles along chains with $m$ steps, is given by

$$\tau_m = \frac{\sum_{i=1}^{m} \int_\Omega t_i \, f^-(\mathbf{x}, t_i)\, d\mathbf{x}}{\sum_{i=1}^{m} \int_\Omega f^-(\mathbf{x}, t_i)\, d\mathbf{x}} = \frac{\sum_{i=1}^{m} \sum_{k=1}^{i} \int_\Omega \Delta_i \, f^-(\mathbf{x}, t_i)\, d\mathbf{x}}{\sum_{i=1}^{m} \int_\Omega f^-(\mathbf{x}, t_i)\, d\mathbf{x}} \tag{15}$$

In appendix A the average dwell time $\tau$ for a system with finite Monte-Carlo chains is derived in the continous limit. It is shown that the dwell time is given by the cumulative distribution function $F^+(\mathbf{x})$

$$\tau = \int_\Omega \int_0^\infty f^+(\mathbf{x}, t)\, dt\, d\mathbf{x} \equiv \int_\Omega F^+(x)\, d\mathbf{x} \tag{16}$$

For completeness and to point out the relation to numerical procedures we show also the evaluation of Eq. 15 using discrete sums. However, in contrast to the continous case, for this purpose it is necessary to require that all time steps are equal, i. e. $\Delta_k = \Delta$ and $t_k = k\Delta$ for $1 \leq k \leq m$. Then one can use Eq. 14 and the relations

$$\begin{aligned} &\sum_{i=1}^{m} \sum_{k=1}^{i} \int_\Omega f^-(\mathbf{x}, t_k)\, d\mathbf{x} \\ &\quad = \sum_{i=1}^{m} (m + 1 - i) \int_\Omega f^-(\mathbf{x}, t_i)\, d\mathbf{x} \\ &\quad = m - \sum_{i=1}^{m} \int_\Omega f^+(\mathbf{x}, t_i)\, d\mathbf{x} \end{aligned} \tag{17}$$

to find

$$\begin{aligned} &\frac{\tau_m}{\Delta} \sum_{i=1}^{m} \int_\Omega f^-(\mathbf{x}, t_i)\, d\mathbf{x} \\ &\quad = (m+1) \sum_{i=1}^{m} \int_\Omega f^-(\mathbf{x}, t_i)\, d\mathbf{x} \\ &\qquad -m + \int_\Omega \sum_{i=1}^{m} f^+(\mathbf{x}, t_i)\, d\mathbf{x} \end{aligned} \tag{18}$$

Assuming now an upper limit $M$ for the number of Monte-Carlo steps, i. e. $f^+(\mathbf{x}, t_m) = 0$ for $m \geq M$ one finds

$$\tau_M = \Delta \int_\Omega \sum_{i=0}^{M} f^+(\mathbf{x}, t_i)\, d\mathbf{x} \equiv \Delta \int_\Omega F_M^+(\mathbf{x}, t_M)\, d\mathbf{x} \tag{19}$$

Note, that the cumulative distribution function $F_M^+(\mathbf{x}, t_M)$ for the discrete case does not have the dimensions as its equivalent $F^+(x)$ in the continous case, which is an integral over time. This is the reason for the time step $\Delta$ appearing in Eq. 19. However, the Eq. 19 is actually a basic result to provide a link between the physical system and numerical models. The cumulative particle number

$$N_M = \sum_{i=1}^{M} \int_\Omega n(\mathbf{x}, t_i)\, d\mathbf{x} = N \int_\Omega F_i^+(\mathbf{x}, t_i)\, d\mathbf{x} \tag{20}$$

represents the number of particles in the stationary system, where all path lengths are present simultaneously. And this is identical to the outcome of standard numerical approaches where a number of $N^*$ particles is launched and their particular trajectories are tracked via markers at their respective positions at each time step $\Delta$ until they are lost, i. e. reached a maximum number of steps. The term markers just denotes the actual position of particle and its tracking is usually done by increasing a counter for each grid cell in the discrtized computational domain by one (perhaps multiplied with a specific weight). Consequently, this means that the sum of all the markers for all particles $N_M^* = \sum_{i=1}^{M} N^*(t_M)$ in the simulation (labeled by the asterisk) is an estimate for the stationary situation. On the other hand, the dwell time $\tau_M$ is an intrinsic characteristic of the physical system under consideration and is linked to the ratio of stationary particle number $N_M$ and source feeding via $N$ particles per time $\Delta$.

$$\frac{\tau_M}{\Delta} = \frac{N_M}{N} = \frac{N_M^*}{N^*} \tag{21}$$

The Eq. 21 provides the necessary normalization condition for the analysis of Monte-Carlo chains of stationary systems: the number of physical particles $N_M$ can be obtained by the simple scaling $N_M/N = N_M^*/N^*$, where $N$ is given by the known physical source strength, $N^*$ is the number of simulation particles and $N_M^*$ is the outcome of the numerical construction and superposition of Monte-Carlo paths. This approach is straightforward and gives accurate results as long as the chosen particle number and step size is sufficient to obtain good statistical estimates. This is quite often not easy to ensure. For this reason in the next section the marker method, where the dwell time is computed directly, will be compared with the track length method, which has been proven to be more efficient in some applications [9; 13]. But, here we will focus on its possible application for drift-diffusion systems described by Fokker-Planck models.

## III. FOKKER-PLANCK EQUATION AND GREEN'S FUNCTIONS

The multi-dimensional Fokker-Planck equation with sources and sinks can be written

$$\frac{\partial f}{\partial t} = -\boldsymbol{\nabla}\cdot\left[\mathbf{V}\,f - \frac{1}{2}\,\boldsymbol{\nabla}\cdot(\mathbf{D}\,f)\right] + S_+ - S_- \tag{22}$$

It describes the temporal evolution of a scalar function $f$ transported by a convection with drift velocity $\mathbf{V}$ and conduction guided by a diffusion tensor $\mathbf{D}$. Sources are summarized by $S_+$ and sinks by $S_-$, respectively. The Fokker-Planck equation naturally appears in the context of passive scalar transport like Brownian motion. And, even though it is a linear equation it plays an important role in linearized methods for non-linear fluid dynamics and similar problems. Here we consider Eq. 22 as an evolution equation for the particle distribution function $f^+$ discussed in the previous section, but this does not affect any other interpretation. A very appealing feature of the Fokker-Planck equation is that for constant $\mathbf{V}$ and $\mathbf{D}$ its Green's function is known and that its importance for stochastic processes has been studied intensively. We refer to these fundamentals just by recalling two basic facts: (1) The Green's function for Eq. 22 without sources and sinks is given by

$$G(\mathbf{x},t) = \sqrt{\frac{|\mathbf{D}^{-1}|}{8\pi^3 t}}\exp\left[-\frac{(\mathbf{x}-\mathbf{V}t)\cdot\mathbf{D}^{-1}\cdot(\mathbf{x}-\mathbf{V}t)}{2t}\right] \tag{23}$$

and it is fulfilling the integral relation

$$f(\mathbf{x}+\Delta\mathbf{x}, t+\Delta t) = \int\limits_{\mathbf{\Omega}} G(\Delta\mathbf{x},\Delta t)\,f(\mathbf{x},t)\,d\mathbf{x} \tag{24}$$

(2) The basic recipe for constructing a Monte-Carlo chain to obtain a discrete representation of a solution of Eq. 22 reads

$$\Delta\mathbf{x} = \mathbf{V}\,\Delta t + \mathbf{B}\cdot\boldsymbol{\xi}\,\sqrt{\Delta t} \tag{25}$$

where $\boldsymbol{\xi}$ is a vector whose components are three independent Gaussian random numbers with mean 0 and variance 1. The tensor $\mathbf{B}$ fulfills $\mathbf{D} = \mathbf{B}\cdot\mathbf{B}^{\mathrm{T}}$. The basic correspondence between these two aspects is that the Green's function can be regarded as probability distribution of the step $\Delta\mathbf{x}$ and the construction rule of Eq. 25 provides exactly this Gaussian distribution. For details on this a vast amount of literature exists, see e. g. [14; 15] and references therein.

As for us, we continue with the discussion of the dwell time introduced in the previous section as the basic quantity for the evaluation of Monte-Carlo chains. For this purpose and to keep the math as simple as possible we restrict ourselves on a prototypical 1D problem

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x}(V\,f) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(D\,f) - \alpha\,f + S_+ - S_- \tag{26}$$

Here, $V$ and $D$ are constant drift and diffusion coefficients, $S_+$ and $S_+$ are unspecified source and sink terms and $\alpha$ is a decay rate introducing an additional loss process, e. g. ionization processes, radioactive decay or absorption processes. It is a strength of the Monte-Carlo method, that usually the source and sink terms $S_+$ and $S_-$ can be treated by starting and terminating chains at particular locations. Therefore, we exclude the sources and sinks contained in $S_+$ and $S_-$ in the temporal evolution of $f$. The remaining transport piece and decay process can be computed via

$$f(x,t+\Delta) = \int\limits_{-\infty}^{\infty} G(x-y,\Delta)\,f(y,t)\,dy \tag{27}$$

where

$$G(x-y,\Delta) = \frac{e^{-\alpha\Delta}}{\sqrt{2\,\pi\,D\,\Delta}}\exp\left[-\frac{(x-y-V\,\Delta)^2}{2\,D\,\Delta}\right] \tag{28}$$

is the relevant Green's function of Eq. 26 with properties

$$\int\limits_{-\infty}^{+\infty} G(x-y,\Delta)\,dx = \int\limits_{-\infty}^{+\infty} G(x-y,\Delta)\,dy = e^{-\alpha\Delta} \tag{29}$$

and

$$\int\limits_{-\infty}^{\infty} G(x-y,\Delta_2)\,G(y-z,\Delta_1)\,dy = G(x-z,\Delta_1+\Delta_2) \tag{30}$$

Comparison of Eq. 27 with Eq. 8 shows that the Green's function $G(x-y,\Delta)$ can be regarded as the transition probability density $p^+(x|y;\Delta)$ guiding the Monte-Carlo steps. Similarly the loss probability is given by $p^-(x|y;\Delta) = (1-e^{-\alpha\Delta})\,G(x-y,\Delta)$. Note, that for pure drift motion the Green's function becomes

$$p^+(x|y;\Delta) = G(x-y,\Delta) = \delta(x-y-V\,\Delta)\,e^{-\alpha\Delta} \tag{31}$$

with $\delta(x-y-V\,\Delta)$ being the Dirac delta function. Now we are in the position to evaluate certain expressions of section II. One finds

$$\int\limits_{-\infty}^{\infty} f^+(x,t_m)\,dx = e^{-\alpha t_m} \tag{32}$$

and

$$\int\limits_{-\infty}^{\infty} f^-(x,t_m)\,dx = \left(e^{-\alpha\Delta_m}-1\right)\,e^{-\alpha t_m} \tag{33}$$

The dwell time $\tau_m$ for the 1D problem reads

$$\tau_m = \frac{\displaystyle\sum_{i=1}^{m}\sum_{k=1}^{i}\Delta_k \int\limits_{-\infty}^{\infty} f^-(x,t_i)\,dx}{\displaystyle\sum_{i=1}^{m}\int\limits_{-\infty}^{\infty} f^-(x,t_i)\,dx} \tag{34}$$

and - as elucidated in appendix A - in the continous limit with measure $\mu(t) = 1 - e^{\alpha t}$ (see appendix A) this provides the compact result

$$\tau_m = \frac{\int_0^{t_m} \alpha\, t\, e^{-\alpha t}\, dt}{\int_0^{t_m} \alpha\, e^{-\alpha t}\, dt} = \frac{1}{\alpha} - \frac{t_m\, e^{-\alpha t_m}}{1 - e^{-\alpha t_m}} \tag{35}$$

Now we come to the question of average track length $\lambda_m$. As mentioned above, the reason to use this quantity in estimating a particle distribution is - as for any other choice of estimator - to get more information from the time stepping and to use a larger time step. We start with the general discrete expression similar to the definition of $\tau_m$ in Eq. 15

$$\lambda_m = \frac{\sum_{i=1}^{m} \int_\Omega \sum_{k=1}^{i} |\mathbf{x}_k - \mathbf{x}_{k-1}|\, f^-(\mathbf{x}, t_i)\, d\mathbf{x}}{\sum_{i=1}^{m} \int_\Omega f^-(\mathbf{x}, t_i)\, d\mathbf{x}} \tag{36}$$

For the prototypical 1D problem considered here one finds by the use of Eqs. 27-30 that

$$\begin{aligned} &\int_{-\infty}^{\infty} |x_k - x_{k-1}|\, f^-(x, t_i)\, dx \\ &\qquad = L(\Delta_k) \int_{-\infty}^{\infty} f^-(x, t_i)\, dx \qquad \text{for } 1 \le k \le i \end{aligned} \tag{37}$$

where $L(\Delta)$ is the average length of a jump for a drift-diffusive time step $\Delta$

$$\begin{aligned} L(\Delta) &= \int_{-\infty}^{\infty} \frac{|x|}{\sqrt{2\pi D\Delta}} \exp\left[-\frac{(x - V\Delta)^2}{2D\Delta}\right] dx \\ &= \sqrt{\frac{2D\Delta}{\pi}} \exp\left(-\frac{V^2\Delta}{2D}\right) + V\Delta \operatorname{erf}\left(V\sqrt{\frac{\Delta}{2D}}\right) \end{aligned} \tag{38}$$

Finally, the average track length $\lambda_m$ in the 1D case is given as

$$\lambda_m = \frac{\sum_{i=1}^{m} \sum_{k=1}^{i} L(\Delta_k) \int_{-\infty}^{\infty} f^-(x, t_i)\, dx}{\sum_{i=1}^{m} \int_{-\infty}^{\infty} f^-(x, t_i)\, dx} \tag{39}$$

note that $L(\Delta_k) \to |V|\, \Delta_k$ for $D \to 0$ and then $\lambda_m = |V|\, \tau_m$. This limit forms the basis for the use of track length in many applications with pure drift. Without any diffusion the average track length is synonymous with the dwell time and this fact gives reason to sample path increments instead of counting markers during construction of Monte-Carlo path. Of course an increase of the numerical efficiency has to be checked for the specific problem at hand. Sometimes the simple marker method might be more efficient, even if smaller time steps are necessary. However, for finite diffusion coefficient $D > 0$ the extension of the track length method encounters certain problems which will be discussed in more detail in the next section.

## IV. DWELL TIME VS TRACK LENGTH

The dwell time has been shown to be the basic quantity for normalizing and evaluating numerical Monte-Carlo chains in section II. This led to the normalization condition Eq. 21. Expressions have been derived for the dwell time $\tau_m$, Eq. 34, and the average path length $\lambda_m$, Eq. 39, in a 1D drift-diffusion system. The question initiating the present analysis was: by which means the track length $\lambda$ might be useful in replacing the time consuming computation of the dwell time $\tau$ by markers. At first glance the answer might look simple: due to the fact that $L(\Delta_i)$ is known analytically and that it depends only on the time step $\Delta_i$ (the case, where $L(\Delta_i)$ depends also varies spatially, will be part of the discussion in the next section) the comparison of Eqs. 15 and 34 with Eqs. 36 and 39 lead to the idea that it might be enough to sample the scaled path

$$\Phi_i = \frac{|x_i - x_{i-1}|}{L(\Delta_i)}\, \Delta_i \tag{40}$$

because

$$\frac{\sum_{i=1}^{m} \int_{-\infty}^{\infty} \sum_{k=1}^{i} \frac{|x_k - x_{k-1}|}{L(\Delta_k)}\, \Delta_k f^-(x, t_i)\, dx}{\sum_{i=1}^{m} \int_{-\infty}^{\infty} f^-(x, t_i)\, dx} = \tau_m \tag{41}$$

As noted before, for pure drift motion the average step length is just $L(\Delta_k) = |V|\Delta_k$. Therefore, the numerical procedure of sampling $\Phi_i$ consists of sampling $|x_i - x_{i-1}|/|V|$ for all particles and all paths. Then it is clear that the resulting cumulative distribution represents the dwell time. For a diffusive step it is not that obvious due to the random character of the step expressed in the construction of Eq. 25 which reads in the 1D case

$$\Delta x = V\Delta t + \sqrt{D\Delta t}\, \gamma \tag{42}$$

Here, $\gamma$ is a random number with zero mean and variance 1. Indeed, the special nature of the Fokker-Planck model does not allow to introduce an effective velocity $L(\Delta)/\Delta$ to be used to scale the step length $|x_i - x_{i-1}|$.

The problem is illustrated by Fig. 1 for a particle passing two cell faces. The advantage of a track length estimator would lie in the possibility to evaluate pieces of a single particle step when particles jump over more than one grid cell in the computational domain. The grid cells are just serving for counting markers during Monte-Carlo time stepping and to obtain a discrete representation of the solution of interest. The idea is to distribute dwell times to different grid cells according to a proper splitting of the distance between to subsequent locations, i.e. $\Delta = \Delta_1 + \Delta_2$. This would allow large time steps, because the single step is retroactively splitted into several steps. Therefore, having computed a step $x \to z$ for a

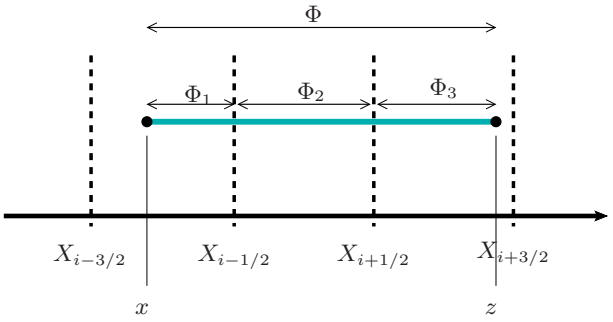


FIG. 1 Sketch of a particle step during time step $\Delta$ from location $x$ to location $z$. Here two cell boundaries at $X_{i-1/2}$ and $X_{i+1/2}$ are passed with a single step. The estimator $\Phi$ covers the entire step. The evaluation of the Monte-Carlo trajectories needs the determination of the components $\Phi_1$, $\Phi_2$ and $\Phi_3$ for proper sampling.

given time step $\Delta$ which passes, e. g. a single grid cell boundary at point $y$, a unique splitting of the estimator $\Phi$ is needed to evaluate

$$\Phi = \frac{|z-x|}{L(\Delta)}\Delta = \frac{|y-x|}{L(\Delta_1)}\Delta_1 + \frac{|z-y|}{L(\Delta_2)}\Delta_2 = \Phi_1 + \Phi_2 \quad (43)$$

However, this requires $L(\Delta) = L(\Delta_1) + L(\Delta_2)$. For the non-diffusive case $D = 0$ this is fulfilled, but unfortunately one finds by inspection of Eq. 38 that for finite diffusion coefficient $D$

$$L(\Delta_1) + L(\Delta_2) > L(\Delta_1 + \Delta_2) \quad (44)$$

for any finite $\Delta_1$ and $\Delta_2$. Moreover, when considering the sum of average path lengths for $m$ steps with time increment $\Delta$ one finds that

$$\sum_{k=1}^{m} L(k\Delta) = \sum_{k=1}^{m} \sqrt{\frac{2Dk\Delta}{\pi}}\exp\left(-\frac{V^2 k\Delta}{2D}\right) + \sum_{k=1}^{m} Vk\Delta\,\mathrm{erf}\left(V\sqrt{\frac{k\Delta}{2D}}\right) \quad (45)$$

is a monotonically increasing function of the number of steps $m$ if the total time $m\Delta$ is kept constant. The total length diverges for $m \to \infty$. Then $\sum_{k=1}^{m} L(k\Delta) \to \infty$. This shows that the length $L(\Delta)$ is not a useful quantity to describe the path of a diffusing particle during a prescribed time interval $\Delta$. The explanation for these peculiarities is that the line segment between two points in stochastic diffusive steps does not tell us anything about intermediate locations of a particle. It could have been anywhere with a finite probability. In other words, sampling the path length or the estimator $\Phi$ does not allow to obtain the dwell time as it was possible by marker counting via Eq. 21. Therefore, a proper normalization is not provided. The only exception is the pure drift which is deterministic and allows retroactive analysis of the straight line segment connecting two subsequent locations. But even this is not ensured if $V$ is not constant everywhere and certain errors occur if the time step is chosen too large. this will be discussed in more detail in the next section.

## V. THE 1D INHOMOGENEOUS CASE

In the previous section it has been found that an overall picture of the dwell time being of central importance for the Monte-Carlo sampling can not be extracted from segments of the particle trajectories if diffusion is present. Rather, the trajectories represent only probabilities. This is illustrated in Fig. 2 where the dwell time $T_i$ for a single time step $\Delta$ is shown as a function of the location $x_0$ where a particle has started. The dwell time $T_i(x_0)$ of a particle starting at position $x_0$ for each particular grid cell is introduced by

$$T_i(x_0) = \int_{X_{i-1/2}}^{X_{i+1/2}} \int_0^{\Delta} G(x - x_0, t)\, dt\, dx \quad (46)$$

where $X_{i-1/2}$ and $X_{i+1/2}$ denote the location of the $i$th cell boundaries. A dwell $T_i(x_0) \approx \Delta$ means that the possible jumps of a particle started at a particular $x_0$ are most likely inside the $i$th cell. A lower value means that the probability for detours into other cells is significant. It can be seen that particles starting in a particular cell in general have a finite dwell time in certain regions of the neighboring cells. This has to be taken into account when a particle step is to be weighted properly. Actually, it is needed to consider the dwell time for each cell separately to gain information for the proper weighting of the Monte-Carlo sampling. On the other hand this means that the full Green's function integral Eq. 46 is evaluated and this is what the Monte-Carlo algorithm is supposed to do. The situation becomes even worse when the inhomogeneous case with spatially varying velocity $V(x)$ and diffusion $D(x)$ is considered. Then the Green's function is not even known and the Monte-Carlo stepping is justified only for regions with constant $V$ and $D$, as usual in discretized computational volumes. But this leads directly to the requirement that the overlap in dwell

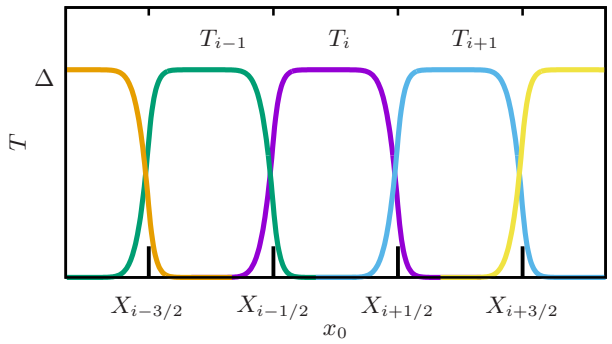


FIG. 2 Sktech of the dwell time $T_k$ for different cells as a function of the particle's starting position $x_0$. The time step is $\Delta$ and the dwell time can reach this value inside the cells if most possible steps are essentially inside a particular cell. But when the particle starts closer to the cell boundaries its dwell time in the neighboring cell is non-zero due to possible stochastic detours. The plots were obtained numerically by using the parameters $V$=2 m/s, $D$=1 m$^2$/s, $X_{i-3/2}$=-1, $X_{i-1/2}$=2, $X_{i+1/2}$=5, $X_{i+3/2}$=8, $\alpha$=0 and time step $\Delta$=0.1 s.

times $T_i$ over cell boundaries as sketched in Fig. 2 should be as small as possible as it introduces numerical errors. To quantify the error one might estimate the width $b$ of the overlap in Fig. 2 where the dwell time $T_i$ drops from $\Delta$ to 0. With the definition

$$b\left|\frac{\partial T_i}{\partial x_0}\right| = \Delta \tag{47}$$

and $|\partial T_i/\partial x_0|$ taken at a cell boundary, a measure for the error $E$ can be introduced by $b/\Delta_x$, $\Delta_x = X_i - X_{i-1}$. The requirement $b/\Delta_x \ll 1$ gives the condition

$$E = \frac{\Delta}{\Delta_x}\left|\frac{\partial T_i}{\partial x_0}\right|_i^{-1} \ll 1 \tag{48}$$

where $|\partial T_i/\partial x_0|_i$ is the minimum of $|\partial T_i/\partial x_0|$ at positions $X_{i-1/2}$ and $X_{i+1/2}$. The detailed expressions for those derivatives are given in appendix B. It is important to note that for $\alpha = 0$ the following limits of Eq. 48 can be found: For $V \neq 0$ and $D \to 0$

$$E_{D=0} = |V|\frac{\Delta}{\Delta_x} \ll 1 \tag{49}$$

and for $V \to 0$ and $D > 0$

$$E_{V=0} = \sqrt{\frac{\pi D}{2\Delta}}\frac{\Delta}{\Delta_x} \ll 1 \tag{50}$$

which are well known from stability analysis of finite difference schemes [16]. But here the conditions result from requirements on accuracy for the otherwise numerically stable Monte-Carlo procedure The term stable in this context is used in the sense that no instabilities occur in the straightforward sampling along particle trajectories. Of course the application for linearized models of non-linear systems might suffer from the usual numerical difficulties with respect to unstable modes. The Fig. 3 illustrates the condition of Eq. 48 in comparison with the limiting cases of Eqs. 49 and 50.

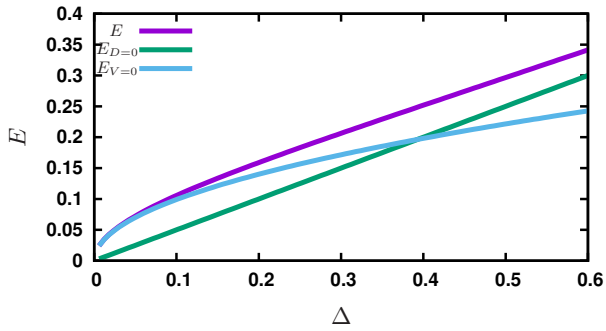


FIG. 3 Sketch of the error estimates $E$, $E_{V=0}$ and $E_{D=0}$ defined in Eqs. 48, 49 and 50. The general error estimate $E$ combines the limiting cases $E_{V=0}$ and $E_{D=0}$ and is more restrictive for the choice of a time step $\Delta$. The plots were obtained numerically by using the parameters $V$=2 m/s, $D$=1 m$^2$/s, $\Delta_x$=4 and $\alpha$=0.

## VI. CONCLUSION

The problem of Monte-Carlo time stepping algorithms for Fokker-Planck equations has been reconsidered. The basic aim in finding numerical solutions of stationary problems is in the numerical estimation of the dwell time. This can be obtained by the standard procedure of launching an ensemble of simulation particles and tracking their entire paths by counting markers in a discretized grid. The ratio of the cumulative number of particles and the number of launched particles per time step provides the dwell time and a proper normalization to connect the simulation results with the physical system under consideration. The path length sampling has been considered as a possible alternative for the time consuming counting of markers. This is obviously a simple and efficient method for free flight problems, like for neutral particles or neutrons in many applications, where the motion is dominated by drift and therefore deterministic. However, it is shown that the stochastic nature of the diffusive piece in the transport excludes the use of simple track length sampling because the path length of diffusion trajectories is not a well defined quantity and not appropriate to represent the dwell time. As long as no other track length based estimator is found - and in this work no proposal is given - the stepping algorithm is restricted to the usual marker method. An additional analysis of the inomogeneous 1D problem allowed to derive further restrictions on the construction of Monte-Carlo trajectories which shows that the well known Courant-Friedrichs-Lewy condition for explicit finite difference schemes has to be taken into account also for the marker based Monte-Carlo schemes.

**Acknowledgments**

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## APPENDIX A: Dwell time and other averages in the continous limit

The dwell $\tau_m$ has been defined in section II by the discrete expression Eq. 15

$$\tau_m = \frac{\sum_{i=1}^{m} \int_\Omega t_i \, f^-(\mathbf{x}, t_i)\, d\mathbf{x}}{\sum_{i=1}^{m} \int_\Omega f^-(\mathbf{x}, t_i)\, d\mathbf{x}} \tag{A1}$$

Assuming that all requirements of measure theory and Lebesgue integration are met one might introduce a probability measure $\mu$

$$\begin{aligned} \mu(t_m) &= \sum_{i=1}^{m} \int_\Omega f^-(\mathbf{x}, t_i)\, d\mathbf{x} \\ &= 1 - \int_\Omega f^+(\mathbf{x}, t_m)\, d\mathbf{x} \equiv \int_0^{t_m} \mu'(t)\, dt \end{aligned} \tag{A2}$$

with density $\mu'$

$$\mu'(t) = -\int_\Omega \frac{\partial f^+(\mathbf{x}, t)}{\partial t}\, d\mathbf{x} \tag{A3}$$

Then the dwell time $\tau_m$ in the continous limit is written as

$$\tau_m = \int_0^{t_m} t \, \frac{\mu'(t)}{\mu(t_m)}\, dt \tag{A4}$$

This can be evaluated via

$$\begin{aligned} \int_0^{t_m} t\, \mu'(t)\, dt &= -\int_\Omega \int_0^{t_m} t \frac{\partial f^+(\mathbf{x}, t)}{\partial t}\, dt\, d\mathbf{x} \\ &= -t_m \int_\Omega f^+(\mathbf{x}, t_m)\, d\mathbf{x} + \int_\Omega \int_0^{t_m} f^+(\mathbf{x}, t)\, dt\, d\mathbf{x} \end{aligned} \tag{A5}$$

to obtain

$$\begin{aligned} &\tau_m - \tau_m \int_\Omega f^+(\mathbf{x}, t_m)\, d\mathbf{x} \\ &\quad = \int_\Omega \int_0^{t_m} f^+(\mathbf{x}, t)\, dt\, d\mathbf{x} - t_m \int_\Omega f^+(\mathbf{x}, t_m)\, d\mathbf{x} \end{aligned} \tag{A6}$$

The stationarity of the problem considered here requires that $f^+(\mathbf{x}, t_m) = 0$ for $t_m > t_M$, with a finite time $t_M$ giving the upper limit for a Monte-Carlo chain. Then one finds for $\tau = \lim_{t_m \to \infty} \tau_m$

$$\tau = \int_\Omega \int_0^\infty f^+(\mathbf{x}, t)\, dt\, d\mathbf{x} \equiv \int_\Omega F^+(x)\, d\mathbf{x} \tag{A7}$$

In a similar way one can derive the chain average $\omega_m$ of a quantity $w = w(t)$

$$\omega_m = \frac{\sum_{i=1}^{m} \int_\Omega w(t_i)\, f^-(\mathbf{x}, t_i)\, d\mathbf{x}}{\sum_{i=1}^{m} \int_\Omega f^-(\mathbf{x}, t_i)\, d\mathbf{x}} \tag{A8}$$

with the continous limit

$$\omega = \int_\Omega \int_0^\infty \frac{\partial w}{\partial t}\, f^+(\mathbf{x}, t)\, dt\, d\mathbf{x} \tag{A9}$$

## APPENDIX B: Evaluation of derivatives in the time stepping error

The definition of Eq. 46 for the dwell time $T_i$ in the $i$th cell

$$T_i = \int_{X_{i-1/2}}^{X_{i+1/2}} \int_0^\Delta G(x - x_0, t)\, dt\, dx \tag{B1}$$

gives

$$\frac{\partial T_i}{\partial x_0} = \int_0^\Delta G(X_{i-1/2} - x_0, t)\, dt - \int_0^\Delta G(X_{i+1/2} - x_0, t)\, dt \tag{B2}$$

This can be evaluated using the relation

$$\begin{aligned} \int_0^\Delta G(x, t)\, dt = \frac{1}{2v'} \exp\left(\frac{vx}{D} - \frac{v'|x|}{D}\right) \left[1 + \operatorname{erf}\left(\frac{v'\Delta - |x|}{\sqrt{2D\Delta}}\right)\right] \\ - \frac{1}{2v'} \exp\left(\frac{vx}{D} + \frac{v'|x|}{D}\right) \left[1 - \operatorname{erf}\left(\frac{v'\Delta + |x|}{\sqrt{2D\Delta}}\right)\right] \end{aligned}$$

(B3)

where

$$v' = \sqrt{2\alpha D + v^2} \tag{B4}$$

Defining $\Delta_x = X_{i+1/2} - X_{i-1/2}$ one finds for $x_0 = X_{i-1/2}$

$$\begin{aligned}\left.\frac{\partial T_i}{\partial x_0}\right|_{X_{i-1/2}} &= \frac{1}{v'}\,\mathrm{erf}\left(\frac{v'\Delta}{\sqrt{2D\Delta}}\right) \\ &-\frac{1}{2v'}\exp\left(\frac{v\Delta_x}{D} - \frac{v'\Delta_x}{D}\right)\left[1 + \mathrm{erf}\left(\frac{v'\Delta - \Delta_x}{\sqrt{2D\Delta}}\right)\right] \\ &+\frac{1}{2v'}\exp\left(\frac{v\Delta_x}{D} + \frac{v'\Delta_x}{D}\right)\left[1 - \mathrm{erf}\left(\frac{v'\Delta + \Delta_x}{\sqrt{2D\Delta}}\right)\right]\end{aligned} \tag{B5}$$

and at $x_0 = X_{i+1/2}$ the derivative is

$$\begin{aligned}\left.\frac{\partial T_i}{\partial x_0}\right|_{X_{i+1/2}} &= -\frac{1}{v'}\,\mathrm{erf}\left(\frac{v'\Delta}{\sqrt{2D\Delta}}\right) \\ &+\frac{1}{2v'}\exp\left(-\frac{v\Delta_x}{D} - \frac{v'\Delta_x}{D}\right)\left[1 + \mathrm{erf}\left(\frac{v'\Delta - \Delta_x}{\sqrt{2D\Delta}}\right)\right] \\ &-\frac{1}{2v'}\exp\left(-\frac{v\Delta_x}{D} + \frac{v'\Delta_x}{D}\right)\left[1 - \mathrm{erf}\left(\frac{v'\Delta + \Delta_x}{\sqrt{2D\Delta}}\right)\right]\end{aligned} \tag{B6}$$

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