Numerical solutions of first-exit-time problems

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We study the effective numerical solution of first-exit-time problems in any number of dimensions with an arbitrary boundary. We show how a full discretization of the diffusive process, both in space and time, gives accurate results, allowing a clean mathematical analysis and the realization of fast and compact algorithms.

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I. INTRODUCTION

The numerical simulation of stochastic equations faces two major problems. On one hand there is always a statistical error in any measured quantity; this can be reduced arbitrarily at the cost of more and more simulating time. On the other hand most simulation algorithms introduce a systematic error, parametrized for instance by the time step h used in the integration of the stochastic equations, and an extrapolation for $h \to 0$ is required to estimate the exact value.

We agree with the general philosophy pointed out in [1]: the use of higher-order algorithms is not as good as it seems. This necessary extrapolation cannot be done at too large h otherwise the systematic error is no longer under control. The same extrapolation in the case of a low-order algorithm is faster since we can use a relatively large h. Furthermore, in the situations where the trajectory itself is important, higher-order algorithms can pose new, unexpected problems. An interesting example is the so-called first-exit-time problem [2, 3]: in this case the difficulty is that one has to know exactly when a trajectory has crossed a given boundary. The most naive algorithm implies an $O(\sqrt{h})$ error on the first exit time T. An improvement has been proposed [4] to overcome this bad order of convergence. However, this solution results in a slow algorithm and cannot be extended easily to the general situation of an arbitrary boundary in any number of dimensions d.

We propose here a method in which both space and time are discretized following the general ideas of [5, 6]. This solves the problem of the boundary very simply in the univariate case and with minor changes in the general multivariate case. The full discretization that we perform has two important features. From the point of view of simulation the algorithm is very fast and compact; it uses only uniform random numbers [7] and only for making choices. In particular, in the univariate case, the algorithm needs integer arithmetic only and can store quickly the hard core of the computation (namely, the various components of the driving force) before starting the main iteration. From the point of view of the analysis, it allows us to write down a simple discrete equation whose mathematical rigor is not questionable and which can be studied in a very clean way since the systematic error is under control.

The plan of the paper is the following: in Sec. II we describe our fully discretized approach; in Sec. III we discuss the univariate mean first-exit-time problem; in Sec. IV we examine the particular problems posed by an arbitrary boundary and, finally, in Sec. V, we present the results obtained within particular models. Appendix A works out in full detail a simple soluble case exploring the problems posed by higher-order algorithms, while Appendix B illustrates an interesting relation between the discrete approach to the mean first-exit-time problems and a solution of the Poisson equation in terms of random walks.

II. FROM CONTINUUM TO DISCRETE DYNAMICS

We want to study the stochastic process in R^d corresponding to the equation

$$\dot{x}_i(t) = f_i(x) + \xi_i(t), \tag{1}$$

where $\xi_i(t)$ is a Gaussian noise satisfying

$$\langle \xi_i(t) \rangle = 0,$$
$$\langle \xi_i(t)\xi_j(t') \rangle = 2D\delta_{ij}\delta(t-t'),$$

with all higher correlation functions determined by the Gaussian character of the noise. We have no problems of interpretation of the above stochastic equation and the Fokker-Planck equation obeyed by the distribution

$$P(x,\,t) = \langle \delta(x - x(t)) \rangle \tag{2}$$

is

$$\partial_t P(x,t) = \hat{L}\, P(x,t), \tag{3}$$

where $\hat{L}$ is the Fokker-Planck operator

$$\hat{L} = D\frac{\partial^2}{\partial x_i \partial x_i} - \frac{\partial}{\partial x_i}\,[f_i(x)\cdots] \tag{4}$$

whose adjoint $\hat{L}^\dagger$ determines the temporal evolution of the average of all the quantities

$$\frac{d}{dt}\langle \Phi(x) \rangle = \langle \hat{L}^\dagger \Phi(x) \rangle. \tag{5}$$

Our strategy will be the following: we shall discretize both time and space with *a priori* independent steps h and Δ. We shall show that it is possible to relate h and Δ with a sort of Einstein relation in order to look at the discrete Fokker-Planck equation in terms of the probabilities of making discrete jumps.

The important point is that the probabilistic interpretation links together the two limits $h \to 0$ and $\Delta \to 0$ and we can keep easily under control the continuum limit. Writing derivatives using finite differences relations,

$$f'(x) = \frac{1}{2\Delta}\,[f(x+\Delta) - f(x-\Delta)] + O(\Delta^2) \tag{6}$$

and

$$f''(x) = \frac{1}{\Delta^2}\,[f(x+\Delta) - 2f(x) + f(x-\Delta)] + O(\Delta^2), \tag{7}$$

we obtain immediately the equation

$$\begin{aligned} P(x, t+h) &= P(x,t) + h\hat{L}_\Delta P(x,t) + O(h^2) \\ &= a_i^+(\Delta_i^- x) P(\Delta_i^- x, t) + a^0(x) P(x) \\ &\quad + a_i^-(\Delta_i^+ x) P(\Delta_i^+ x, t), \end{aligned} \tag{8}$$

where the coefficients $a_i^k(x)$ can be interpreted as the probabilities of making a jump of k Δ steps in the ith direction. This requires that the $a_i^k(x)$ lie in the interval (0, 1) and their sum to be 1. The mesh step Δ is the same for all the directions; the notation is

$$\Delta_i^\pm x = (\ldots, x_i \pm \Delta, \ldots). \tag{9}$$

The explicit expression for the probabilities is the following:

$$\begin{aligned} a^0(x) &= 1 - \frac{2hDd}{\Delta^2}, \\ a_i^\pm(x) &= \frac{hD}{\Delta^2} \pm \frac{h}{2\Delta} f_i(x). \end{aligned}$$

We can easily check that the correct continuum limit is recovered if and only if $h \sim \Delta^2$, the precise proportionality being determined by the requirement of having the greatest time step possible compatible with the probabilistic realization of the above discretization so to accelerate the simulation. We find that our discrete version of the Einstein relation is

$$h = \frac{\Delta^2}{2Dd}. \tag{10}$$

Then

$$a^0(x) = 0, \tag{11}$$

$$a_i^\pm(x) = \frac{1}{2d}\left(1 \pm \frac{\Delta}{2D} f_i(x)\right). \tag{12}$$

We remark that for a localized motion (corresponding to a peaked equilibrium distribution) these can be always interpreted as probabilities if h and consequently Δ are taken small enough.

The simulation of the above algorithm is very simple: at each step one has to choose a jump from a discrete set of moves. The choice is made with probabilities depending on the force. In one-dimensional problems, as we shall see, these probabilities can be stored before starting the simulation so that the algorithm turns out to be very compact and fast. In $d > 1$ the boundary poses new problems to be discussed below and this storing is not possible anymore.

In the one-dimensional case, one can write a second-order algorithm (Fokker-Planck equation correct up to terms $h^2 \sim \Delta^4$) in the compact form

$$\begin{aligned} a^\pm(x) &= e^{V(x)}\,[F(x \pm \tfrac{1}{2}\Delta)]^{-1}, \\ a^0(x) &= 1 - a^+(x) - a^-(x), \end{aligned} \tag{13}$$

where $f(x) = -V'(x)$ and

$$\begin{aligned} F(x) = \exp\frac{V(x+\Delta/2)}{D} &+ 4\exp\frac{V(x)}{D} \\ &+ \exp\frac{V(x-\Delta/2)}{D}. \end{aligned} \tag{14}$$

This algorithm satisfies the detailed balance condition and thanks to the ergodicity of the random walk, ensures the exact convergence to the equilibrium distribution $e^{-V(x)/D}$. In greater detail, the structure of Eq. (13) ensures the correct equilibrium distribution while the particular choice of $F(x)$ is needed to achieve second order in precision. In Sec. V we shall compare this method to the first-order algorithm.

One possible extension of the second-order formula to the $d > 1$ case is given by the following equation:

$$\begin{aligned} \exp\left(h\sum_{i=1}^d \hat{L}_i\right) = \left(\prod_{i=1}^d \exp\frac{h}{2}\hat{L}_i\right)\left(\prod_{i=1}^d \exp\frac{h}{2}\hat{L}_{d+1-i}\right) \\ + O(h^3), \end{aligned} \tag{15}$$

which is readily obtained from the formula

$$\begin{aligned} \exp\left(\frac{h}{2}\hat{A}\right)\exp(h\hat{B})\exp\left(\frac{h}{2}\hat{A}\right) \\ = \exp[h(\hat{A}+\hat{B}) + O(h^3)]. \end{aligned} \tag{16}$$

Here $\hat{L}_i$ is the Fokker-Planck operator in the ith direction.

The algorithm corresponding to Eq. (15) is very simple. As a first step, we order once and for all the first d integers forming the sequence $\sigma = \{i_1, i_2, \ldots, i_d\}$. Then, we make a one-dimensional update of all the possible directions moving forward along σ. Finally, the same sweep is repeated, but moving backward along σ, as one can see in Eq. (15).

The result is a full update which follows the Fokker-Planck evolution up to the second order and which satisfies exactly the detailed balance condition. As an illustrative example, let us consider $d = 2$, then we can choose $\sigma = \{1, 2\}$ and the formula

$$\exp[h(\hat{L}_x + \hat{L}_y)] = \left(\exp\frac{h}{2}\hat{L}_x \exp\frac{h}{2}\hat{L}_y\right) \times \left(\exp\frac{h}{2}\hat{L}_y \exp\frac{h}{2}\hat{L}_x\right) + O(h^3) \tag{17}$$

must be read as a progressive update in the order $x \to y \to y \to x$ with step $h/2$. Further analysis and numerical investigations on these kind of algorithms are in preparation [8].

III. APPLICATION TO MEAN FIRST-EXIT-TIME PROBLEMS

We describe briefly the mean first-exit-time problem. We consider the diffusion from a given starting point in the presence of an assigned boundary: the quantity to be determined is the mean time needed for the diffusing variable to reach the boundary. The use of a naive algorithm like the Euler one to discretize the Langevin equation shows where the difficulty is. Consider the evolution from x_0 dictated by

$$x_{n+1} = x_n + hf(x_n) + \sqrt{2Dh}\xi_n, \tag{18}$$

where ξ_n are uncorrelated normalized Gaussian random numbers. Assume that absorbing barriers exist at $|x| = L$. The equation reproduces the correct equilibrium distribution

$$P(x) = e^{-V(x)/D}, \quad f(x) = -V'(x) \tag{19}$$

apart from terms $O(h)$; nevertheless, the mean first-exit-time has a $O(\sqrt{h})$ intrinsic error due to the uncertainty in the time of crossing the boundary. This error is estimated by the time needed in a Brownian random walk to cover the distance Δ and by the Einstein relation, this is $\sim \sqrt{h}$. In [4] it is shown that it is possible to keep track of the diffusing "particles" that cross the boundary but that are not detected. Anyway, the algorithm needs the expensive evaluation of an exponential and cannot be easily generalized to nontrivial boundaries. The discretization of space eliminates this uncertainty since we know exactly when a jump crosses the boundary.

As the multivariate case presents some subtleties, let us first consider $d = 1$ as a useful example. Given a random walk on a one-dimensional lattice, let $P(L, \tau | y)$ be the probability of reaching a boundary situated at $x = L$ in a time $t = \tau h$ starting from $x = y$. It is easy to convince oneself that P satisfies the equation

$$P(L, \tau + 1 | x) = a^+(x)P(L, \tau | \Delta^+ x) + a^-(x)P(L, \tau | \Delta^- x), \tag{20}$$

which expresses the composition of probabilities and is readily understood in terms of discrete jumps. The first exit time in units of h is clearly given by

$$T(x) = \sum_{\tau=1}^{\infty} P(L, \tau | x)\tau \tag{21}$$

and translating the sum by one time step

$$T(x) = \sum_{\tau=0}^{\infty} P(L, \tau + 1 | x)(\tau + 1) = a^+(x)T(\Delta^+ x) + a^-(x)T(\Delta^- x) + 1, \tag{22}$$

which again can be given a simple interpretation in terms of probabilities. Note that we have obtained directly a numerical method for the exact determination of the mean first exit time. The vector $T_n = T(n)$ (T_n being the mean first exit time from the nth site) can be found exactly as the solution of the tridiagonal problem

$$K_{mn}T_n = w,$$

$$K_{mn} = \delta_{mn} - a_n^+ \delta_{m+1,n} - a_m^- \delta_{m,n+1}, \quad m \neq 1, \quad n \neq N \tag{23}$$

$$w = (0, 1, \ldots, 1, 0)^T,$$

where we impose the boundary condition

$$T_n = 0 \tag{24}$$

on an absorbing barrier and

$$T_n = 1 + T_{n+1} \tag{25}$$

on a reflecting barrier bounding the right side.

These relations correspond to the continuum equations

$$\hat{L}^\dagger T = -1, \tag{26}$$

where the adjoint operator is

$$\hat{L}^\dagger = D\frac{\partial^2}{\partial x_i \partial x_i} + f_i(x)\frac{\partial}{\partial x_i} \tag{27}$$

and the boundary conditions on absorbing and reflecting boundaries are

$$T(x_{\text{abs}}) = 0, \quad T'(x_{\text{ref}}) = 0, \tag{28}$$

but note how easily and intuitively we have recovered them on the lattice. Some remarks are in order: in the univariate problem, the boundary structure is totally trivial since a barrier is just a point.

The first-order algorithm which involves only one-step jumps has no problems, provided one chooses the lattice

such that one of the sites is exactly on the boundary. This is always possible and no $O(\sqrt{h})$ error occurs.

For a higher-order algorithm, like the one obtainable by a straightforward extension of the first order described here, the situation is different. Generally speaking, one has to consider multiple jumps and it is impossible, in general, to avoid an uncertainty in the crossing time. This is shown in more detail in Appendix A where we show how this mechanism works in the solvable case of the Wiener process.

IV. $D > 1$ AND ARBITRARY BOUNDARY

According to our general idea, let us focus on the problem of finding a fast $O(h)$ accurate algorithm in the multivariate case with arbitrary boundary. In more than one dimension the problem of the boundary becomes very important since its geometrical structure is in general not trivial. If we replace the true physical boundary with a discretized version, we introduce, in general, an $O(\Delta)$ error which means as usual an $O(\sqrt{h})$ error on the mean first exit time. One could think to solve this problem by modifying the mesh and putting the boundary's edge exactly on it. This cancels the $O(\sqrt{h})$ error in the discretization of the boundary, but introduces a comparable error in the discretization of the Fokker-Planck operator. If we consider the discretization of the Laplace operator obtained by writing second derivatives as finite differences on asymmetric intervals, for instance using

$$f''(x) \simeq 2\left(\frac{1}{a(a+b)} f(x+a) - \frac{1}{ab} f(x) + \frac{1}{b(a+b)} f(x-b) \right) \tag{29}$$

with $a, b = O(\Delta)$, expanding the right-hand side we get the left-hand side apart from a $O(\Delta)$ correction due to the asymmetry of the interval. This $O(\sqrt{h})$ contribution vanishes only if $a = b$. This means that covering a region bounded by a nonstraight line using asymmetric rectangular lattices or triangular ones is not the solution.

The conclusion is that we are not able to construct a *static* lattice covering an arbitrary region without introducing an $O(\sqrt{h})$ error in the approximation of the boundary or in the discretization of the Fokker-Planck operator. Here *static* means that it is fixed once and for all before starting the simulation. From the point of view of simulation, *staticity* means the possibility of storing the bulk of the computation, that is, computing only once the forces.

If we do not require the lattice to be static, we can use an adaptive algorithm. A simple first-order one is the following: consider a domain $D \subset R^d$ and its boundary ∂D.

(1) Start with a point P and a space step Δ.

(2) Set

$$\delta = \min_i(\Delta, \mathcal{D}_i(P, \partial D)), \tag{30}$$

where $\mathcal{D}_i$ is the distance computed in the ith direction and set

$$h = \frac{\delta^2}{2Dd}. \tag{31}$$

(3) Choose a direction i and move backward or forward the point P with probabilities

$$a_i^{\pm}(P) = \frac{1}{2d}\left(1 \pm \frac{\delta}{2D} f_i(P)\right). \tag{32}$$

(4) Go back to (2) if the boundary has not been reached.

This dynamic algorithm has the obvious disadvantage that it is not possible to store previously a table of the forces, but on the other hand, it is quite general since it works for an arbitrary boundary in any dimension d. Anyway, it is clear that one can rely on the discrete algorithm with fixed step size taking advantage of its speed and fitting a polynomial in $\sqrt{h}$ to the mean first exit times at different step size.

As an example we shall simulate numerically the mean first exit time in radially symmetric two-dimensional (2D) processes driven by the force $f(\rho)$. Assuming an absorbtive boundary at $\rho = R$, the mean first exit time solves the equation

$$\frac{D}{\rho}\frac{d}{d\rho}\left(\rho \frac{dT}{d\rho}\right) + f(\rho)\frac{dT}{d\rho} = -1 \tag{33}$$

with the boundary conditions

$$T'(0) = T(R) = 0. \tag{34}$$

The condition $T'(0) = 0$ follows from requiring $T(0) < \infty$, the point $\rho = 0$ being a reflecting barrier for the random motion.

In the Wiener case $f(\rho) \equiv 0$ and the solution is simply

$$T(\rho) = \frac{1}{4D}(R^2 - \rho^2). \tag{35}$$

In the Ornstein-Uhlenbeck process, which describes a particle bounded by the elastical force $f(\rho) = -k\rho$, one finds

$$T(0) = \frac{1}{2k}\left[\mathrm{Ei}\left(\frac{kR^2}{2D}\right) - \gamma_E - 2\ln\left(\frac{kR^2}{2D}\right)\right], \tag{36}$$

where the exponential integral function $Ei(z)$ is defined by

$$\mathrm{Ei}(z) = \mathrm{P}\int_{-\infty}^{z} \frac{e^t}{t} dt, \tag{37}$$

where P denotes principal value. In particular, if $k = 1$, $R = 1$, and $D = 1/2$,

$$T(0) = \tfrac{1}{2}[\mathrm{Ei}(1) - \gamma_E] = 0.658\,951. \tag{38}$$

V. NUMERICAL RESULT

In this section we want to show with explicit examples the accuracy and speed of the discrete algorithms described above. To this end, we make a comparison with the first-order Euler scheme in three cases of the Wiener, Ornstein-Uhlenbeck, and Ginzburg-Landau model in one dimension. The results with the Euler algorithm are

taken from [7]. The data shown are obtained with 10^6 realizations of the stochastic process and their values agree with the ones obtained by inversion of the mean first-time matrix as explained in Sec. III while the statistical error is negligible. Let us call Discrete 1 the first-order discrete algorithm and Discrete 2 the second-order one, Eq. (13). The ratio of the speeds is

$$\frac{t_{\text{Euler}}}{t_{\text{Discrete 1}}} \sim 8, \quad \frac{t_{\text{Euler}}^{\text{improved}}}{t_{\text{Discrete 1}}} \sim 12, \tag{39}$$

where the improvement refers to the Strittmatter solution to deal with the $\sqrt{h}$ error term. The greater precision of the discrete algorithm due to the absence of the $\sqrt{h}$ term is evident from Figs. 1, 2 and 3. In Figs. 4 and 5 we show also the almost constant results from the algorithm Discrete 2.

We are going to fit the mean first exit times at different values of h with an appropriate polynomial in $\sqrt{h}$ or h and compare the results with the theoretical value obtained by analytical computation. These fits are shown as solid lines in Figs. 1, 2 and 3.

In the Wiener process the fits give

$$\begin{aligned} T_{\text{theor}} &= 1.0, \\ T_{\text{Euler}} &= 0.9951 + 1.3\sqrt{h}, \\ T_{\text{Discrete 1}} &= 1.0, \\ T_{\text{Discrete 2}} &= 1.0. \end{aligned}$$

In the Ornstein process with $D = 0.5$ we obtain

$$\begin{aligned} T_{\text{theor}} &= 1.445\,246, \\ T_{\text{Euler}} &= 1.4460 + 2.3\sqrt{h}, \\ T_{\text{Discrete 1}} &= 1.4453 - 0.43h, \\ T_{\text{Discrete 2}} &= 1.44524 + 0.30h^2. \end{aligned}$$

Finally, in the Ginzburg-Landau process with $D = 0.1$ we have

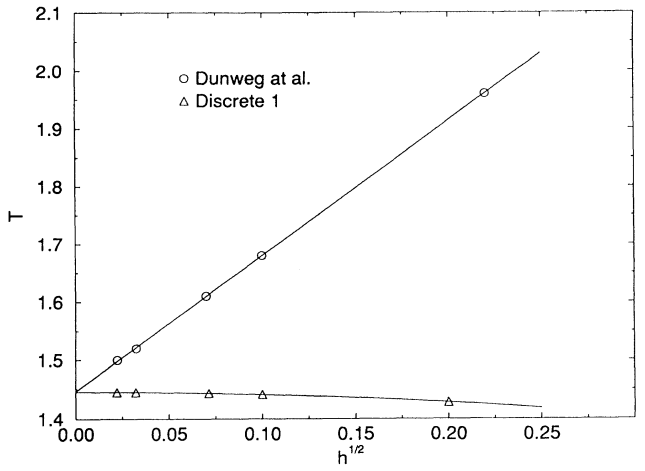

FIG. 2. First exit time for the Ornstein-Uhlenbeck process.

$$\begin{aligned} T_{\text{theor}} &= 30.821\,30, \\ T_{\text{Euler}} &= 30.899 + 16.89\sqrt{h}, \\ T_{\text{Discrete 1}} &= 30.820 + 10.90h, \\ T_{\text{Discrete 2}} &= 30.8213 + 0.32h^2. \end{aligned}$$

In the case of the Discrete 2 algorithm, it is impressive to see how small the correction term is, especially for the Ginzburg-Landau process.

We have tested the adaptive algorithm in the case of the 2D Ornstein-Uhlenbeck model on the disk making again a comparison with the Euler algorithm. The points obtained at $D = 0.5$ are shown in Fig. 6 and the fit gives

$$\begin{aligned} T_{\text{theor}} &= 0.658\,951, \\ T_{\text{Euler}} &= 0.6594 + 1.00\sqrt{h}, \\ T_{\text{Discrete 1}} &= 0.6589 - 0.29h. \end{aligned}$$

Here the discrete result is obtained by direct simulation since no exact inversion is possible with the adaptive algorithm. The error bars are negligible compared to the

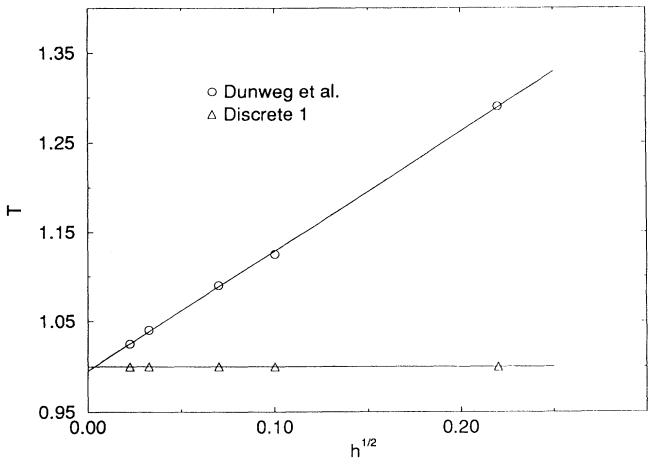

FIG. 1. First exit time for the Wiener process.

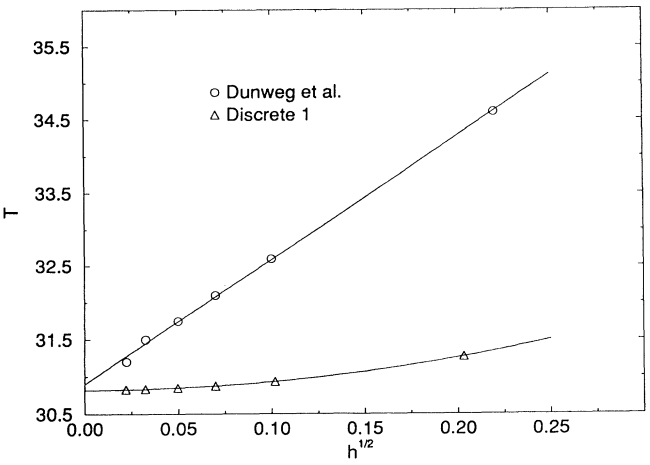

FIG. 3. First exit time for the Ginzburg-Landau process.

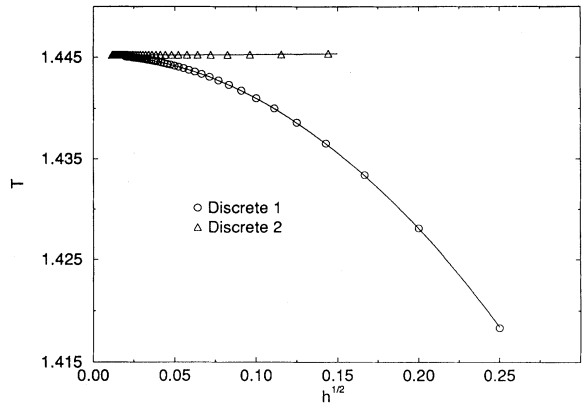

FIG. 4. Discrete 1 vs Discrete 2 algorithm results in the Ornstein-Uhlenbeck process.

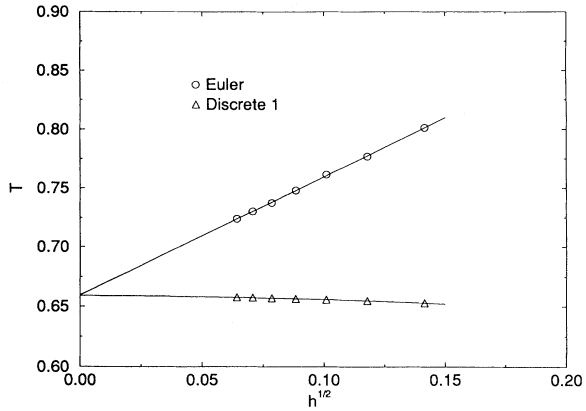

FIG. 6. Results obtained with the adaptive algorithm in a 2D Ornstein-Uhlenbeck process.

size of the symbols. The ratio of the speeds is

$$\frac{t_{\text{Euler}}}{t_{\text{Discrete}}} \sim 6.5, \quad \frac{t_{\text{Euler}}}{t_{\text{Discrete naive}}} \sim 9.5. \tag{40}$$

Also given is the ratio for the "Discrete naive" algorithm, namely, the discrete first-order algorithm with fixed step sizes in which the storing of the forces is allowed.

Finally we have computed the exact solution of the tridiagonal problem for the first-order treatment of the Ginzburg-Landau potential

$$V(x) = -\tfrac{1}{2}x^2 + \tfrac{1}{4}x^4 \tag{41}$$

for a diffusing particle starting at $x = 1.0$ and with different values of the diffusion coefficient. In Table I we report the results of the fit with a linear function $T = T_0 + T_1 h$, considering different values of the diffusion constant D.

VI. CONCLUSIONS

In this work we have shown how to devise and implement algorithms for the integration of stochastic differential equations based on the discretization of both the simulation time and the configuration space. The "Einstein relation" linking the two discretizations allows us to connect the limits of continuum and zero time step, and this results in a very fast and accurate method of simulation: the systematic errors are well under control and the speed of the algorithm permits good statistical precision.

We have applied this method to the determination of mean first exit times; in this problem not only the equilibrium distribution is important, but also the trajectory itself. Numerical results confirm the expected improvement over existing algorithms.

Since the algorithm is computationally efficient, the first-order discretization is enough, and the high statistical accuracy attained permits us to extract easily the results in the simultaneous continuum and $\tau \to 0$ limit, using standard fitting procedures.

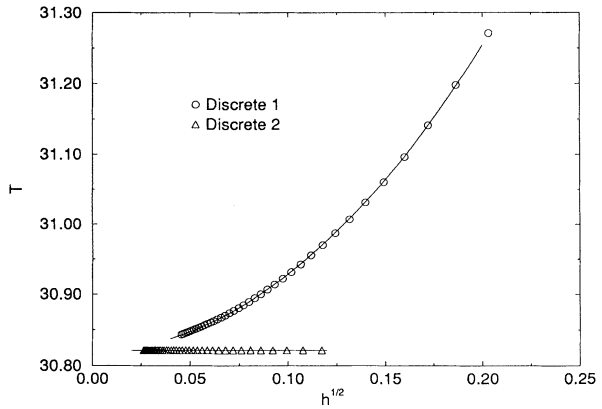

FIG. 5. Discrete 1 vs Discrete 2 algorithm results in the Ginzburg-Landau process.

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APPENDIX A: MEAN FIRST EXIT TIME FOR THE WIENER PROCESS

In the continuum the mean first exit time for the Wiener process satisfies the equation

TABLE I. Results of the fit with a linear function $T = T_0 + T_1 h$ with different values of diffusion constant D.

D	Theor.	T_0	T_1
0.10	30.821	30.82	10.96
0.09	40.728	40.73	17.76
0.08	57.478	57.48	32.08
0.07	89.195	89.20	66.15
0.06	159.87	159.9	165.2
0.05	361.90	361.9	562.6
0.04	1238.4	1238	3040
0.03	9739.6	9739	4.395×10^4
0.02	6.1606×10^5	6.162×10^5	6.294×10^6

$$DT''(x) = -1,$$
$$T(0) = T(1) = 0.$$

and the trivial solution is

$$T(x) = \frac{1}{2D}x(1-x). \tag{A1}$$

The interesting point to stress is that this exact solution satisfies at all orders the discrete equation for $T(x)$. A straightforward extension of the approach described in the main text gives with an $O(h^2)$ precision the following second-order equation for the lattice mean first-passage time

$$T_n = (1 - \tfrac{5}{4}\xi + \tfrac{3}{4}\xi^2) + \tfrac{2}{3}\xi(1 - \tfrac{3}{4}\xi)(T_{n+1} + T_{n-1}) + \tfrac{1}{24}\xi(3\xi - 1)(T_{n+2} + T_{n-2}).$$

Here, the parameter ξ is an arbitrary constant which generalizes the Einstein relation linking space and time through the relation

$$h = \xi\frac{\Delta^2}{2Dd}. \tag{A2}$$

The equilibrium action is corrected by $O(h^3)$ terms, which are absent if we choose ξ to reduce this solution to the algorithm of Eq. (13).

Now, the point is that the jump dynamics solves the above equation with the *effective* boundary conditions

$$T_{-1} = T_0 = T_a = T_{a+1} = 0, \quad a\Delta = 1 \tag{A3}$$

since we consider the jumping particle outside the region if at a certain time step it is on the boundary or one step beyond it. The naive discretization of the continuum solution does not satisfy these boundary conditions. Using standard techniques for the solution of recurrency equations with constant coefficients, we find the most general solution of the above equation

$$T_n = \frac{1}{\xi}n(a-n) + \sum_{i=1}^{4} c_i\rho_i^n, \tag{A4}$$

where ρ_i are the four solutions of the equation

$$(\rho - 1)^2\left(\rho^2 + 2\frac{3\xi - 7}{1 - 3\xi}\rho + 1\right) = 0, \tag{A5}$$

namely

$$\rho = 1, 1, \omega, \omega^{-1} \tag{A6}$$

with

$$\omega = \frac{3\xi - 7 + 2\sqrt{3(4-3\xi)}}{3\xi - 1}. \tag{A7}$$

The relevant interval in which a probabilistic interpretation of the equation for the first exit time is possible is

$$\tfrac{1}{3} < \xi < \tfrac{4}{3} \tag{A8}$$

in which $\omega(\xi)$ decreases monotonically from 0 to -1. Since $\rho = 1$ is a double root the most general solution which respects the symmetry

$$n \to a - n \tag{A9}$$

is

$$T_n = \frac{1}{\xi}n(a-n) + c_1 + c_2(\omega^n + \omega^{a-n}). \tag{A10}$$

Imposing the boundary conditions one finds

$$c_1 = -\frac{1}{\xi}(a+1)\frac{\omega(1+\omega^a)}{(1-\omega)(1-\omega^{a+1})},$$
$$c_2 = \frac{1}{\xi}(a+1)\frac{\omega}{(1-\omega)(1-\omega^{a+1})}. \tag{A11}$$

We must distinguish at this point three cases.

(1) $\frac{1}{3} < \xi < \frac{4}{3}$. In this interval $|\omega| < 1$ so that as $a \to \infty$, with no reference to the parity of a we get

$$c_1 \to \frac{1}{\xi}(1+a)\frac{\omega}{\omega - 1},$$
$$c_2 \to \frac{1}{\xi}(1+a)\frac{\omega}{1-\omega}.$$

The error in the computation of $T(0) = hT_{a/2}$ is then

$$h\delta T_{a/2} = \frac{h}{\xi}(a+1)\frac{\omega}{\omega-1}(1 - 2\omega^{a/2}) \sim \frac{a\omega}{\xi(\omega-1)} = \frac{\Delta}{D}\frac{\omega}{\omega-1} \tag{A12}$$

and this is $O(\sqrt{h})$ since $\Delta \sim h^{1/2}$.

(2) $\xi = \frac{1}{3}$. There are no steps with length 2 so that the discrete solution is the one of the first-order algorithms which is

$$T_n = 3n(a-n), \tag{A13}$$

namely, going back to the continuum, the exact one.

(3) $\xi = \frac{4}{3}$. This is the most interesting case since its sensibility upon the boundary condition shows the lattice version of the $\sqrt{h}$ problem.

The ρ parameter in the general solution of the recurrent equation now takes the values

$$\rho = 1, 1, -1, -1. \tag{A14}$$

If we are to preserve the left-right symmetry of the problem, we must have the same number of sites on the left and on the right of $x = 1/2$ so that we must consider the case $a = 2N$ of an even lattice. Then, the flip symmetry $n \to a - n$ gives after having imposed the boundary conditions

$$T_n = \tfrac{3}{4}n(2N-n) + \tfrac{3}{8}(2N+1)[1 - (-1)^n]. \tag{A15}$$

Now we must take care of the parity of N. The point $x = 1/2$ always corresponds to the site $n = N$ and we find for the error in the computation of the first exit time

$$h\,\delta T_N = \begin{cases} 0 & N \text{ even} \\ \dfrac{3h}{4}(2N+1) \sim \sqrt{h} & N \text{ odd}, \end{cases} \tag{A16}$$

which is just what one gets from the numerical simulations.

APPENDIX B: SOURCES

An interesting application of the jump-dynamics approach is related to the following result. Consider a region $\mathcal{D}$ (one dimensional for simplicity, but this is not a limitation) with absorbing boundary. The Kolmogorov backward equation [3] for the probability of being at x_k at time $t+1$, starting from x_n in the free Wiener motion, is

$$P(x_k, t+1 \mid x_n) = \tfrac{1}{2}P(x_k, t \mid x_{n+1}) + \tfrac{1}{2}P(x_k, t \mid x_{n-1}). \tag{B1}$$

We construct the lattice version of the continuum quantity

$$\varphi(x) = D\int_0^\infty dt \int_{\mathcal{D}} d\xi\, P(\xi, t \mid x)\rho(\xi) \tag{B2}$$

which is

$$\varphi_n = \tilde{D}\sum_{t=0}^{\infty}\sum_k P(x_k, t \mid x_n)\rho_k, \tag{B3}$$

where the adimensional number $\tilde{D}$, assuming $h = \Delta^2/2D$, is

$$\tilde{D} = D\frac{h}{\Delta^2} = \tfrac{1}{2}. \tag{B4}$$

It follows that

$$\varphi_{n+1} - 2\varphi_n + \varphi_{n-1} = \sum_{t,k}\{P(x_k, t+1 \mid x_n) - P(x_k, t \mid x_n)\}\rho_k \to -\rho_n \tag{B5}$$

as $N \to \infty$ since the boundary is absorbing and

$$P(x_k, 0 \mid x_n) = \delta_{kn}. \tag{B6}$$

So φ_n is the discretization of the solution $\varphi(x)$ of the Poisson equation

$$\Delta\varphi = -\rho \tag{B7}$$

with zero Dirichlet boundary conditions by construction, since absorbing boundary means

$$y \in \partial\mathcal{D} \Rightarrow \forall x, \quad P(x, t \mid y) = 0. \tag{B8}$$

On the other hand, it is clear that φ_n can be obtained computing the first exit time from x_n with the local time step $hD\rho(x)$ and this is an alternative way of solving the Poisson equation. We remark that this result can be proved from the more general results on abstract Markov chains associated to Liouville operators [9].

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