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EXPONENTIALLY FAST MONTE CARLO SIMULATIONS FOR NON-EQUILIBRIUM SYSTEMS

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Abstract: A new numerical technique is demonstrated and shown to reduce exponentially the time required for Monte Carlo simulations of non-equilibrium systems. The quasi-stationary probability distribution is computed for two model systems, and the results are compared with the asymptotically exact theory in the limit of extremely small noise intensity. Singularities of the non-equilibrium distributions are revealed by the simulations.

Keywords: *stochastic, non-equilibrium, probability distribution, Monte Carlo simulation*

1. INTRODUCTION

Fluctuations in systems away from thermal equilibrium represnt a problem of long standing in statistical physics [Onsager and Machlup, 1953]. Well known examples of systems in which non-equilibrium fluctuations play a particularly important role include e.g. lasers [Keay et al., 1995], proteins [Serpersu and Tsong, 1983], Josephson junctions [Kautz, 1996], and chemical reactions [Smelyanskiy et al., 1999b]. In particular, activated processes are of big importance. Noise induced escape means a transition from one state to another, which e.g. in chemical system describes a reaction [Smelyanskiy et al., 1999b; Huber and Kim, 1996]. In non-equilibrium systems, where symmetries of detailed balance are broken, no general methods exist for the calculation of even basic quantities like the probability distribution. This is a case where numerical and asymptotic theoretical methods for investigating the probability distribution are of particular importance.

In the limit of small noise intensity, $D \to 0$ [Ventcel and Freidlin, 1970; McKane, 1989; Dykman, 1990; Smelyanskiy et al., 1999b], asymptotic theoretical approaches, such as WKB-like or path-integral methods, can be used. The theory suggests that a solution to the problem of non-equilibrium fluctuations requires an understanding of the dynamics of deviations from the steady state [Onsager and Machlup, 1953] and an analysis of singularities in the non-equilibrium potential [Graham and Tel, 1984; Smelyanskiy et al., 1997]. Some ideas have recently been proposed for how to extend the existing ($D \to 0$ limit) theory to encompass the case of still small but finite noise intensity [Smelyanskiy et al., 1999a; Lehmann et al., 2000; Bandrivskyy et al., 2003].

Monte Carlo simulation provides the main numerical technique used to verify such theoretical predictions, and to analyse the behavior of the dynamical system under study. The theory gives an asymptotically exact solution only in the $D \to 0$ limit. In contrast, D in the numerical simulations is necessarily finite. Typically, the time required for Monte Carlo simulations grows exponentially as $D \to 0$. This meant that theoretical predictions of interesting singular structures, and of the non-equilibrium probability distribution [Graham and Tel, 1984; Jauslin, 1987], for long remained untested either experimentally or by numerical simulation. Furthermore, there has been no clear understanding of how the picture changes as the noise intensity becomes finite.

Earlier attempts to speed up the simulations focussed mainly on finding optimal fluctuational paths and rates of transition in between stable states of a system (e.g. efficient transition path sampling [Dellago et al., 1999] and dynamics importance sampling [Woolf, 1998], which follow the earlier suggestion of [Pratt, 1986]). In [Crooks and Chandler, 2001] the path sampling method was adapted to non-equilibrium systems. Based on the same idea, the umbrella sampling technique was suggested to estimate the probability to reach any point of phase space of an equilibrium system starting from a fixed initial state [Dellago et al., 1999]. An idea how to improve sampling by splitting up the probability packets was suggested in [Huber

and Kim, 1996]. So far, however, no general algorithm has been suggested for non-equilibrium systems, able to provide both the whole probability distribution and also dynamical information, e.g. optimal fluctuational paths, for small noise intensities.

We now introduce a numerical method that enables the time required for Monte Carlo simulations to be reduced by an exponentially large factor. It is applicable to generic two-dimensional non-equilibrium systems, does not require any *a priori* knowledge about the system apart from its dynamical equations of motion, and it allows the quasi-stationary probability distribution to be computed directly over the whole phase space. Using this method, we reveal singular behavior of the non-equilibrium distribution and show that it is in quantitative agreement with the asymptotic theory. The central idea is to perform the simulations in sequential steps.

We construct the quasi-stationary distribution in stages, patching together intermediate results, starting from the minimum of the potential and gradually moving away from it. We find that the time required for the simulations at each step is reduced by an exponentially large factor as compared to the standard technique: if the time necessary for a conventional Monte Carlo simulation technique is T, our modified method would require only time

$$T_m \approx NT \exp^{-(N-1)\frac{\Delta\Phi}{D}},$$

where N is the number of steps involved and $\frac{\Delta\Phi}{D}$ is distance in logarithm of the probability between them. Given that T is exponentially large, the benefit in reduced processing time can be very substantial. The result of simulations for Duffing system (Fig.3, for $D = 0.02$) can be practically directly compared with a result given by an ordinary technique. It took us around 15 minutes to simulate the whole distribution shown in Fig.3 (for $D = 0.02$) with our fast technique, and it takes around four days of standard Monte Carlo simulation to obtain comparable statistics close to the boundary of attraction.

We explain the underlying principle of the method in Sec. 2, testing it by application to a very simple equilibrium stochastic system where all the results are already known. Then, in Sec. 3 we apply it to two much-studied non-equilibrium systems and compare the numerical results with the corresponding theoretical predictions. Finally, we summarise our conclusions in Sec. 4.

2. THE FAST MONTE CARLO SIMULATIONS TECHNIQUE

To illustrate the technique, we consider an overdamped Brownian particle moving in a bistable Duffing potential $U(x) = -x^2/2 + x^4/4$. The corresponding Langevin equation is

$$\dot{x} = -U'(x) + \xi(t), \tag{1}$$

where $\xi(t)$ is zero-mean white Gaussian noise with intensity D and moments

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(0) \rangle = 2D\delta(t).$$

The form of the probability distribution is completely defined by the potential $U(x)$, and is of the Boltzmann type $\rho(x) \propto \exp(-U(x)/D)$. As in the case of a non-equilibrium system (where the probability distribution is not defined by a potential) a standard Monte Carlo technique can be used to deduce $\rho(x)$. Numerical integration of the Langevin equation (1), assuming the system to be located initially at one of the potential minima x_m, gives the discrete probability distribution $\rho(x)$, peaked at x_m. The potential can be deduced as $\Phi(x) \propto -D \ln \rho(x)$. If the noise intensity is very small, the system fluctuates in a close vicinity of x_m and large deviations from it are extremely rare. The conventional Monte Carlo method cannot be used to study the dynamics of optimal escape paths, or the properties of the probability distribution far from the potential minima: the statistics required cannot in practice be collected within a realistic time when the noise intensity is within the range of interest, i.e. small but finite. We have overcome this problem by starting from the distribution already obtained near x_m.

We fix two probability levels ρ_i and ρ_f, lying well within the region where the numerical ρ is accurate, with $\rho_f < \rho_i$ corresponding to two levels in the potential Φ_i and Φ_f, and two coordinates x_i and x_f, as shown in Fig. 1. We require the levels ρ_i and ρ_f to be fairly different, such that the corresponding x_i and x_f are sufficiently separated: the distance between them must exceed $\sqrt{Dh}$, where h is the integration time step used in the Monte Carlo simulation, and must also exceed the discretization step Δx in the discrete probability distribution. All simulations were carried out following the procedure described by Mannella [2000].

The next simulation step is started from the level Φ_i (putting the system at $x = x_i$ as its initial condition). If the system starts to evolve along a fluctuational trajectory (towards the boundary of attraction) we just follow its natural dynamics according to (1) and collect the statistics for building the probability distribution in a usual way. If the system starts with a relaxation trajectory (towards x_m), or when it crosses the boundary x_i due to relaxation some time later, we stop the simulation and reinject the system back to the initial state x_i.

In this way we simulate the full dynamics of the system at higher levels of the potential $\Phi(x) > \Phi_i$ (in the region of coordinate space $x > x_i$ for this particular case). Thus, in the subsequent simulation step we follow only those fluctuations that have already attained a certain level in the potential Φ_i, without waiting for this exponentially slow event to happen. In this way, a new piece of the probability distribution is built with a time saving $\sim \exp \Phi_i/D$ compared to a simulation starting from the potential minimum x_m. The upper curve of Fig.1 shows the new piece of the potential $\Phi_2(x)$, as computed.

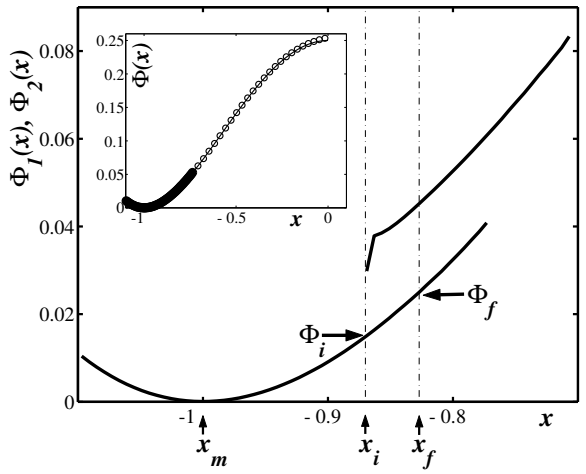

Fig. 1: *The first ($\Phi_1(x)$, lower curve) and second ($\Phi_2(x)$, upper curve) pieces of the inferred potential $\Phi(x)$ for the system (1) with $D = 0.005$. The discontinuity in the gradient of $\Phi_2(x)$ near x_i is an artefact due to a boundary effect in the calculation of the discrete probability distribution. To avoid this problem $\Phi_1(x)$ and $\Phi_2(x)$ are merged at the point x_f and the initial part of $\Phi_2(x)$ is discarded. We normalize $\Phi_1(x)$ choosing $\Phi_1(x_m) = 0$, and each successive piece of $\Phi(x)$ is normalized in order to match with the previous one at the point where they join.* Inset: *The inferred potential $\Phi(x)$ for the system (1) with $D = 0.005$. The new technique (circles) is compared with standard Monte Carlo simulations (bold line) and with the Duffing potential $U(x)$ (thin line).*

The merging of the two pieces of the inferred potential (the original $\Phi_1(x)$ and the new $\Phi_2(x)$) at x_f can be effected in a unique way. Continuing this procedure, the probability distribution and the corresponding potential can be built, step by step, for the whole region of interest. The inset in Fig. 1 shows the resultant potential, built from 13 such pieces between the minimum at $x_m = -1$ and the maximum at $x = 0$. It coincides closely with the Duffing potential $U(x)$ itself. The potential $\Phi(x)$ is thus inferred within a region of coordinate space that is inaccessible in a conventional simulation (shown as bold curve for comparison). The advantage of our new technique is immediately evident. We stress that, in the simulations, no *a priori* knowledge of the dynamics was required.

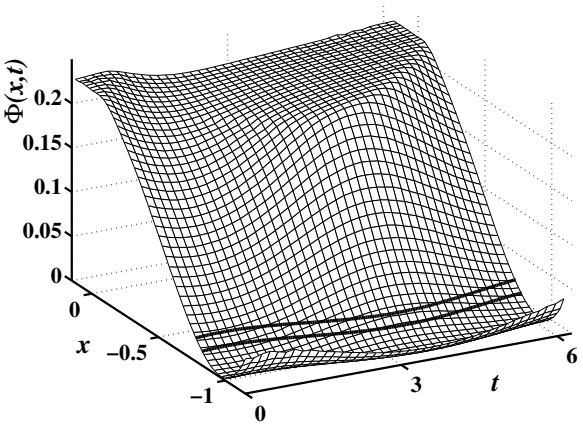

Fig. 2: *The whole inferred $\Phi(x,t)$ for the system (2) for $A = 0.1$, $\Omega = 1$, $D = 0.005$. Two lines are the lines of constant probability found after the first step of simulations. The corresponding levels of probability were chosen as $\Phi_i = 3D$ and $\Phi_f = 5D$.*

Essentially the same procedure can be applied to a two dimensional system. The main difference is that, instead of identifying two boundary points x_i and x_f, we need to identify two boundary lines of constant probability. One line is for staring simulations from, and another one is a reference line for matching together different pieces of the probability distribution (see Fig.2 for clarification). In turn, this implies that we should consider the reinjection location probability (RLP) along the "lower" boundary line corresponding to ρ_i. Starting from the second step of the simulations, the system should be reinjected back according to the RLP after it relaxes across the boundary. We emphasize that the RLP is not the same as the probability distribution $\rho(\mathbf{x})$, which is constant on the boundary line. The RLP is an additional important measure which describes local discrete dynamics in the neighborhood of the boundary line. It is a distribution along the boundary of how often the system crosses the boundary.

The principle of detailed balance that applies in equilibrium systems provides a symmetry that can be used to reinject the system back at the boundary level, without any need to compute the RLP. For non-equilibrium systems, however, detailed balance does not apply and so the procedure cannot be used. The RLP must be considered separately (and calculated explicitly) for the particular system being investigated. It can be obtained from an analysis of the finite difference equation corresponding to the model. In the limit of small integration time

step the probability to cross the boundary is proportional to the diffusion-related term in the finite difference equation. Then the RLP is simply proportional to the projection of the vector orthogonal to the boundary onto the coordinate affected by the noise ξ. It can also be computed numerically.

3. APPLICATION TO NON-EQUILIBRIUM SYSTEMS

As a first example of a non-equilibrium system, consider the periodically-driven overdamped Duffing oscillator

$$\dot{x} = -U'(x) + A\cos\Omega t + \xi(t). \qquad (2)$$

We infer $\Phi(x,t)$ as $-D\ln\rho(x,t)$. This quantity corresponds to the theoretical "global minimum of the modified action" in the Hamiltonian theory of large fluctuations [Bandrivskyy et al., 2003] and, in the limit $D \to 0$, it becomes the non-equilibrium potential.

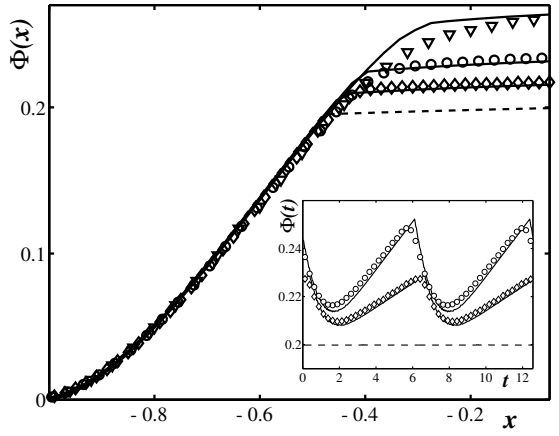

Fig. 3: *A time section of the inferred $\Phi(x, t = 4.1)$ for the system (2) with $A = 0.1$, $\Omega = 1$, and different noise intensities: $D = 0.005$ (diamonds); $D = 0.01$ (circles); and $D = 0.02$ (triangles). The theoretical predictions are shown by full lines for finite noise intensities, and by dashed line for $D = 0$. Inset: oscillations of $\Phi(x,t)$ at the boundary of attraction for different noise intensities.*

The limit of small noise intensity is of particular interest and importance in the case of non-equilibrium systems. A sufficiently small D gives rise to the possibility of revealing the non-equilibrium potential

$$\Phi(\mathbf{x}) = \lim_{D\to 0} -D\ln\rho(\mathbf{x}),$$

directly through a numerical experiment. Observations of the predicted singular shape of $\ln\rho(\mathbf{x})$, and of its dependence on D, are thus of considerable interest.

Fig. 2 shows the complete $\Phi(x,t)$, constructed from 12 such pieces, and a time section of $\Phi(x,t)$ calculated for different noise intensities together with the results of theoretical calculations (Hamiltonian theory including the prefactor) [Bandrivskyy et al., 2003] is shown in Fig. 3. The RLP in the simulations can be taken as constant if a small enough integration time step is used in the scheme. A small difference between the theory and the simulations results appears for the larger noise intensities, and then the asymptotic theory starts to break down and becomes inapplicable.

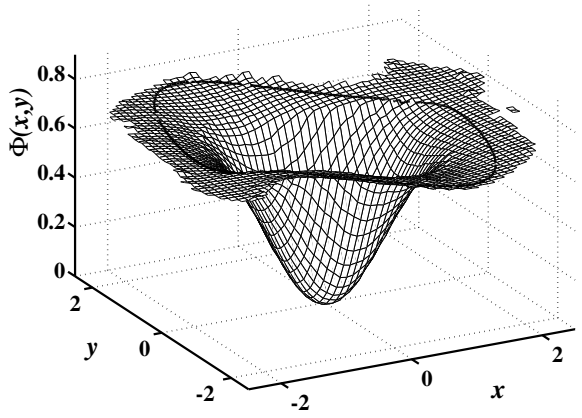

Fig. 4: *Inferred $\Phi(x,y)$ for the system (3) with $\omega_0 = 1$, noise intensity $D = 0.01$, and $\eta = 0.5$. The boundary of attraction (unstable limit cycle) is shown by a bold curve.*

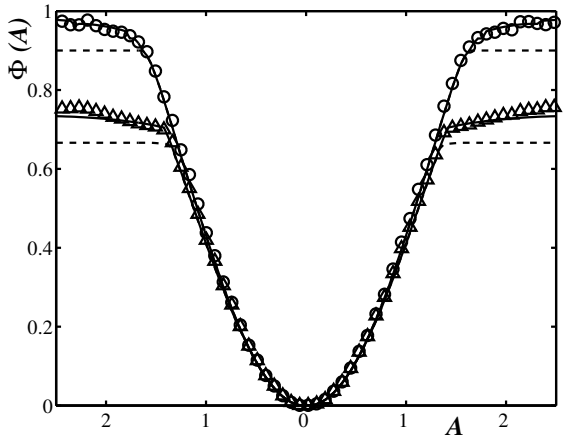

Fig. 5: *A section ($x = y$) of the inferred $\Phi(A)$ for the system (3) with $\omega_0 = 1$, noise intensity $D = 0.01$ and $\eta = 0.25$ (circles); and $\eta = 0.5$ (diamonds). Theoretical predictions are shown in each case for $D = 0$ (dashed curves) and $D = 0.01$ (full curves).*

We now consider, as a second more complicated non-equilibrium example, the inverted Van-der-Pol oscillator

$$\ddot{x} + 2\eta(1 - x^2)\dot{x} + \omega_0^2 x = \xi(t) \qquad (3)$$

In order to be able to merge more easily the different pieces of $\Phi(x, y)$, we apply a coordinate transformation from x and $y = \dot{x}$ to amplitude A and phase ϕ

$$x = A\cos(\phi), \quad y = -A\omega_0 \sin(\phi).$$

It is then possible to analyse the probability $\rho(x, y)$ in the (A, ϕ) coordinate space. This makes the problem very similar to the periodically driven Duffing oscillator: the only difference is the RLP which, in the case of the Van der Pol oscillator, turns out to be strongly modulated. It is essential for this modulation to be taken into account when reinjecting the system back to the boundary of constant probability. The complete $\Phi(x, y)$ built by the Fast Monte Carlo simulations is shown in Fig.4. Two sections of $\Phi(x, y)$, obtained from the simulations for two different parameters η, are compared with the theory in Fig. 5. Here again, excellent agreement is obtained between numerics and theory.

4. CONCLUSIONS

The same structure of singularities is found in both of the non-equilibrium systems considered in this paper. Using the fast Monte Carlo simulations we reveal plateaus, the essentially flat regions in the probability distribution, which can be observed close to boundaries of attraction. They result from a purely dynamical effect that is not associated with the flatness of any potential. We have shown that its origin is related to switching between different types of optimal fluctuational path, and it is a general feature of non-equilibrium systems with metastable states [Bandrivskyy et al., 2003, 2002]. The switching lines [Smelyanskiy et al., 1997] are revealed as lines along which the "global minimum of the modified action" $\Phi(\mathbf{x})$ exhibits sharp bends – corresponding to the predicted line at which the non-equilibrium potential is non-differentiable. In the boundary region we found the oscillations of the probability distribution and their dependence on noise intensity (see the inset in Fig.3) discussed in the recent publications [Smelyanskiy et al., 1999a; Lehmann et al., 2000; Maier and Stein, 2001]. The noise-induced shift of the singularities and the optimal escape path revealed by the simulations has stimulated a new step in the development of the theory [Bandrivskyy et al., 2003].

It is only in the limit of extremely small noise intensity that the singularities can be confidently observed, so that the use of our new fast technique is crucial to their investigation. In addition to being fast, it preserves dynamical information. It can be further extended to encompass higher dimensional systems and maps, and it can readily be modified to analyse optimal fluctuational paths, including those that arise in the energy-optimal control problem [Khovanov et al., 2000].

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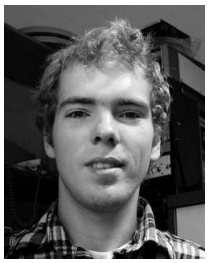

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