Direct evaluation of large-deviation functions

Cristian Giardinà,[1] Jorge Kurchan,[2] and Luca Peliti[3, *]

[1]*Eurandom, P.O. Box 513 - 5600 MB Eindhoven, The Netherlands*
[2]*PMMH-ESPCI, CNRS UMR 7636, 10 rue Vauquelin, 75005 Paris, France*
[3]*Dipartimento di Scienze Fisiche and Unit INFM, Universit "Federico II", 80126 Napoli, Italy*
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We introduce a numerical procedure to evaluate directly the probabilities of large deviations of physical quantities, such as current or density, that are local in time. The large-deviation functions are given in terms of the typical properties of a modified dynamics, and since they no longer involve rare events, can be evaluated efficiently and over a wider ranges of values. We illustrate the method with the current fluctuations of the Totally Asymmetric Exclusion Process and with the entropy production distribution of a driven Lorentz gas.

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In the last few years there has been a renewed interest in the theory of large deviations of nonequilibrium systems, with the development of general results concerning the fluctuations of soft modes [1], of non-trivial and rich analytic solutions of concrete models [2, 3, 4, 5, 6, 7, 8, 9, 10], and by the discovery of strikingly simple and general nonequilibrium relations (the Fluctuation Theorem, Jarzynski's relation) obeyed by work fluctuations [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21]. We are having, perhaps for the first time, a few glimpses of truly general features of macroscopic systems well out of equilibrium.

Several issues cannot at present be completely resolved analytically, so one turns to simulations for inspiration. Unfortunately, direct numerical simulation of large deviations is hard, since, by definition, the events are rare, so that the ranges of fluctuations and the system sizes studied have been very limited. In this work we propose a method allowing to directly evaluate large deviations of quantities that are local in time, although not necessarily in space. It consists in biasing the dynamics with the appropriate weight, and it involves clones of the system that reproduce or die, a technique inspired by the Diffusion Monte Carlo methods [22] of quantum mechanics.

Let $\mathcal{C}, \mathcal{C}'$ denote two configurations in phase space and let $U_{\mathcal{C}\mathcal{C}'}$ be the transition matrix of the discrete (eventually continuous) time dynamics:

$$P_{\mathcal{C}}^{t+1} = U_{\mathcal{C}\mathcal{C}'} P_{\mathcal{C}'}^{t} \qquad (1)$$

A path $\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_T$ in the configuration space will have the probability

$$\text{Prob}[\mathcal{C}_1, \mathcal{C}_2, \ldots, \mathcal{C}_T] = U_{\mathcal{C}_T \mathcal{C}_{T-1}} \cdots U_{\mathcal{C}_2 \mathcal{C}_1} \qquad (2)$$

We shall consider physical quantities that are functions of the configuration, such as the density $\rho = \rho(\mathcal{C})$, and also quantities that depend on the transition $\mathcal{C}' \to C$, such as the current $J_{\mathcal{C}\mathcal{C}'}$. For example, in a lattice system:

$$J_{\mathcal{C}\mathcal{C}'} = \begin{cases} 1, & \text{if a particle jumps to the right;} \\ 0, & \text{if nothing happens;} \\ -1, & \text{if a particle jumps to the left.} \end{cases} \qquad (3)$$

We are interested for example in calculating the probability of having a total current $Q = Tq$, starting from a configuration $\mathcal{C}_1$:

$$\begin{aligned} P(Q) &= \left\langle \delta(J_{\mathcal{C}_1 \mathcal{C}_2} + \cdots + J_{\mathcal{C}_{T-1} \mathcal{C}_T} - Q) \right\rangle \\ &= \int d\lambda e^{-\lambda Q + T\mu(\lambda)}, \end{aligned} \qquad (4)$$

where the braces denote average over trajectories, and we have defined:

$$\begin{aligned} e^{T\mu(\lambda)} &= \left\langle e^{\lambda(J_{\mathcal{C}_1 \mathcal{C}_2} + \cdots + J_{\mathcal{C}_{T-1} \mathcal{C}_T})} \right\rangle \\ &= \sum_{\mathcal{C}_2, \ldots, \mathcal{C}_T} U_{\mathcal{C}_T \mathcal{C}_{T-1}} \cdots U_{\mathcal{C}_2 \mathcal{C}_1} e^{\lambda(J_{\mathcal{C}_1 \mathcal{C}_2} + \cdots + J_{\mathcal{C}_{T-1} \mathcal{C}_T})}. \end{aligned} \qquad (5)$$

One has, in the limit $T \to \infty$, $q = \mu'(\lambda)$, so that $\ln P(Q)/T$ and $\mu(\lambda)$ are Legendre transforms of each other.

Let $P_{\mathcal{C}}^{t+1} = \tilde{U}_{\mathcal{C}\mathcal{C}'}^{\lambda} P_{\mathcal{C}'}^{t}$, with

$$\tilde{U}_{\mathcal{C}\mathcal{C}'} \equiv e^{\lambda J_{\mathcal{C}\mathcal{C}'}} U_{\mathcal{C}\mathcal{C}'}, \qquad (6)$$

so that

$$e^{T\mu(\lambda)} = \sum_{\mathcal{C}_2, \ldots, \mathcal{C}_T} \tilde{U}_{\mathcal{C}_T \mathcal{C}_{T-1}} \cdots \tilde{U}_{\mathcal{C}_2 \mathcal{C}_1} = \sum_{\mathcal{C}_T} \left[\tilde{U}^T \right]_{\mathcal{C}_T \mathcal{C}_1}. \qquad (7)$$

Clearly, denoting by e^{Λ} the eigenvector of $\tilde{U}$ with the largest real part, and by $|\Lambda^R\rangle$, $|\Lambda^L\rangle$ the corresponding right and left eigenvectors, we have, for large times T,

$$e^{T\mu(\lambda)} = \sum_{\mathcal{C}_T} \langle \mathcal{C}_T | \Lambda^R \rangle \langle \Lambda^L | \mathcal{C}_1 \rangle \, e^{T\Lambda}, \qquad (8)$$

so that $\Lambda = \mu(\lambda)$.

In order to compute $\mu(\lambda)$, one possibility is to perform path-sampling over the trajectories with weight (6). Such a procedure has been proposed in the context of the work distributions [23] on nonequilibrium trajectories. In this paper we propose a different strategy: the idea is to to define a new effective dynamics whose expectation values directly give the large deviations. As we

shall see, the new dynamics involve the parallel evolution of clones which die and reproduce, a procedure inspired by the "Diffusion Monte Carlo" method of simulation of the Schroedinger equation [22]. In order to write Eq. (7) as a dynamics, let us put $K'_{\mathcal{C}} \equiv \sum_{\mathcal{C}} \tilde{U}_{\mathcal{C}\mathcal{C}'}$, and define the stochastic matrix:

$$U'_{\mathcal{C}\mathcal{C}'} \equiv \tilde{U}_{\mathcal{C}\mathcal{C}'} K_{\mathcal{C}'}^{-1}. \tag{9}$$

We now have, instead of eq. (8),

$$e^{T\mu(\lambda)} = \sum_{\mathcal{C}_2,\ldots,\mathcal{C}_T} U'_{\mathcal{C}_T\mathcal{C}_{T-1}} K_{\mathcal{C}_{T-1}} \cdots U'_{\mathcal{C}_2\mathcal{C}_1} K_1. \tag{10}$$

This can be realized by considering an ensemble of L copies ("clones") of the system, and by successively going, for all of them, through a process defined by the following three steps:

- A cloning step:

$$P_{\mathcal{C}'}^{t+\frac{1}{2}} = K_{\mathcal{C}'} P_{\mathcal{C}'}^t, \tag{11}$$

where the configuration $\mathcal{C}'$ gives rise to G identical clones, $G = [K_{\mathcal{C}'}] + 1$ with probability $K_{\mathcal{C}'} - [K_{\mathcal{C}'}]$, and $G = [K_{\mathcal{C}'}]$ otherwise ($[x]$ denotes the integer part of x). If $[K_{\mathcal{C}'}] = 0$, the copy may be killed and leave no offspring.

- A shift step without cloning of all the offspring of $\mathcal{C}'$ with the modified dynamics

$$P_{\mathcal{C}}^{t+1} = U'_{\mathcal{C}\mathcal{C}'} P_{\mathcal{C}'}^{t+\frac{1}{2}}. \tag{12}$$

- An overall cloning step with an adjustable rate K^t (at each time the same for all configurations), so as to keep the total number of clones constant. This amounts to multiplying $\tilde{U}$ by K^t times an identity, at each time.

It is easy to see that, in the long-time limit, the compensatory factor gives us $\mu(\lambda)$ through:

$$\ln[K_T \cdot K_{T-1} \cdots K_1] = T\mu(\lambda). \tag{13}$$

To conclude the evaluation of large deviations, let us note that if the quantity $\rho_{\mathcal{C}}$, whose average deviations we wish to compute depends on a single rather than on a pair of successive times, the same derivation goes through with the substitution $J_{\mathcal{C}\mathcal{C}'} \to \rho_{\mathcal{C}'}$.

The probability that a configuration $\mathcal{C}$ is visited after T steps of the dynamics described above is $\sim \sum_{\mathcal{C}'} \langle \mathcal{C}'|\mathcal{C}\rangle\langle\mathcal{C}|\Lambda^R\rangle$: this corresponds to the typical configurations *at the end* of the time-interval in which we are conditioning the large deviation, in general different from the typical configurations *well inside* this interval (which are visited with probability $\sim \langle\Lambda^L|\mathcal{C}\rangle\langle\mathcal{C}|\Lambda^R\rangle$). As we shall see, they contain however interesting information.

We now turn to two examples: the totaly Asymmetric Exclusion Process, and the Lorenz gas.

Totally Asymmetric Exclusion Process (TASEP)

The TASEP consists of particles on a ring with discrete sites with occupancy zero or one. A given particle chosen at random does no attempt to move with probability $(1-\alpha)$, and with probability α attempts to move to the right and succeeds if the corresponding site is empty. The parameter α can be made small to approach the continuous time limit. Here we shall set it to unity. Let us denote by $X_{\mathcal{C}'}$ the number of different configurations that can be reached by making a one-particle move (1PM) from $\mathcal{C}'$. Then the non-zero entries of $U_{\mathcal{C}\mathcal{C}'}$ are given by

$$U_{\mathcal{C}\mathcal{C}'} = \begin{cases} \alpha/N, & \text{if } \mathcal{C} \to \mathcal{C}' \text{ is a 1PM}; \\ 1 - (X_{\mathcal{C}'}\alpha/N), & \text{if } \mathcal{C} = \mathcal{C}'. \end{cases} \tag{14}$$

This implies for $\tilde{U}$

$$\tilde{U}_{\mathcal{C}\mathcal{C}'} = \begin{cases} \alpha e^{\lambda}/N, & \text{if } \mathcal{C} \to \mathcal{C}' \text{ is a 1PM}; \\ 1 - (X_{\mathcal{C}'}\alpha/N) & \text{if } \mathcal{C} = \mathcal{C}'. \end{cases} \tag{15}$$

Thus, for a configuration $\mathcal{C}'$ with $X_{\mathcal{C}'}$ mobile particles, we have

$$K_{\mathcal{C}'} = 1 + \frac{X_{\mathcal{C}'}\alpha}{N}(e^{\lambda} - 1), \tag{16}$$

and finally

$$U'_{\mathcal{C}\mathcal{C}'} = \begin{cases} (\alpha e^{\lambda}/N)/K_{\mathcal{C}'}, & \text{if } \mathcal{C} \to \mathcal{C}' \text{ is a 1PM}, \\ (1 - X_{\mathcal{C}'}\alpha/N)/K_{\mathcal{C}'}, & \text{if } \mathcal{C} = \mathcal{C}'. \end{cases} \tag{17}$$

Thus, with probability $(1 - X_{\mathcal{C}'}\alpha/N)/K_{\mathcal{C}'}$ no move is made; otherwise we move a particle randomly chosen with uniform probability among the $X_{\mathcal{C}'}$ mobile particles.

In figure 1 we show a space-time diagram of the system with $N = 100$ particles at density one-half and $\lambda = -50$. What we see is not quite the evolution of a shock, but rather the configuration at the end of the time-interval for time intervals ending at progressively longer times. As predicted by the theory, the shock does not drift, although different initial conditions lead to different shock positions. Figure 2 shows the case $\lambda = -30$, and density 0.3: we see that the shock has a net drift to the right, again as predicted. Finally, in figure 3 we show the numerical results obtained for $\mu(\lambda)$, and compare them to the analytic ones of Ref. [3]. The agreement is excellent, and the numerical effort corresponds to tens of minutes of a personal computer time.

A deterministic system: The Lorentz Gas and the Gallavotti-Cohen theorem

This system consists of of a number of particles (in our case only one) moving inside a billiard as in figure 4, with periodic boundary conditions. The particle is
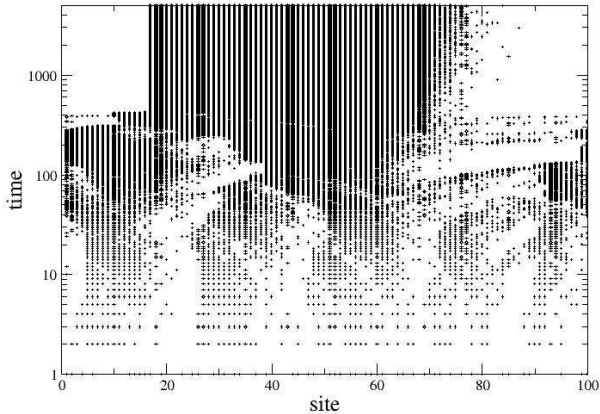
FIG. 1: Space-time diagram for a ring of $N = 100$ sites, $\lambda = -50$ and density 0.5. The shock is dense and does not advance. Note the logarithmic scale on the y-axis.
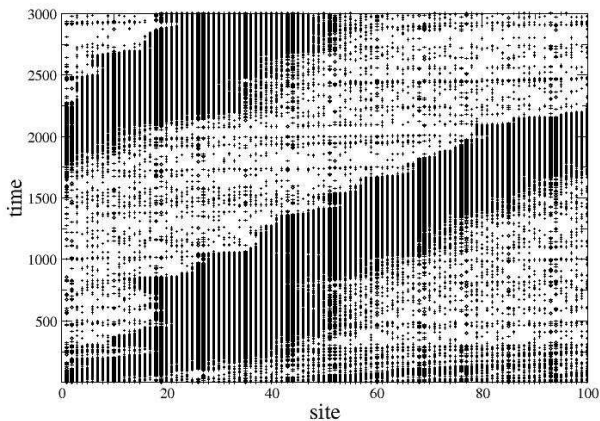

FIG. 2: Space-time diagram for a ring of $N = 100$ sites, $\lambda = -30$ and density 0.3. The shock drifts to the right.

under the action of a force field $\vec{E}$, and is subject to a deterministic thermostat that keeps the velocity modulus constant $|\vec{v}| = 1$. Between bounces, the equations of motion are:

$$\ddot{x}_i = -E_i + \gamma(t)\dot{x}_i, \qquad i = 1, 2;$$
$$\gamma(t) = \sum_i E_i \dot{x}_i. \qquad (18)$$

We wish to compute the probability of entropy production $\int_0^T dt\, \gamma(t)$, and check the Gallavotti-Cohen theorem, which states that $\mu(\lambda)$ is symmetric around $\lambda = -\frac{1}{2}$.
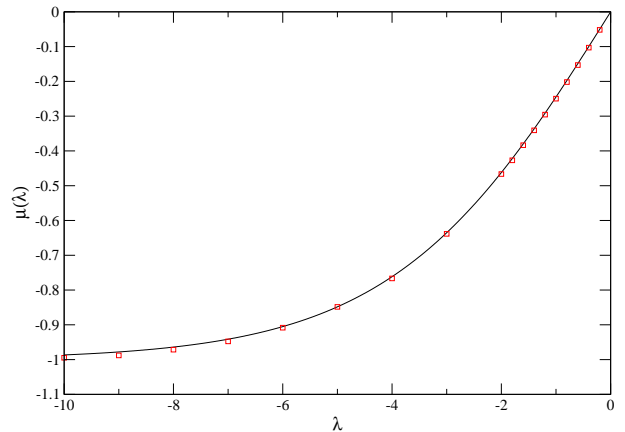

FIG. 3: Plot of $\mu(\lambda)$ vs. λ for the TASEP at density one-half. Numerical results and analytic results of ref. [3], with points and full line, respectively.
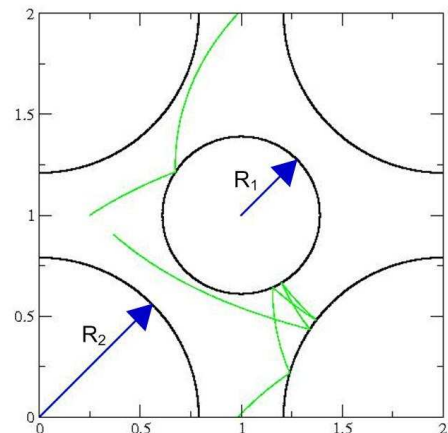

FIG. 4: The billiard. The radii are $R_1 = 0.39, R_2 = 0.79$. An example of trajectory is also shown for the external field $\vec{E} = (1, 0)$.

The dynamics are deterministic, and hence cloned systems will evolve together and perform a poor sampling. To get around this problem, we introduce a small stochastic noise, and check the stability of results in the limit of small noise. We evolve the system for *macroscopic* intervals $\mathcal{T}$, and clone with a factors $K_i = e^{\lambda \Gamma_{\mathcal{T}}}$, where $\Gamma_{\mathcal{T}}$ is the total entropy production over the interval. Before each deterministic step of time $\mathcal{T}$, clones are given random kicks of variance Δ in position and/or velocity direction. *The time-interval $\mathcal{T}$ and the noise intensity Δ are chosen so that twin clones have a chance to separate during time $\mathcal{T}$, and this depends on the chaotic properties of the system.* In the present case, we checked that $0.1 \leq \mathcal{T} \leq 1$ allows for a few collisions, which guarantees clone diversity for $10^{-3} \leq \Delta \leq 10^{-4}$.

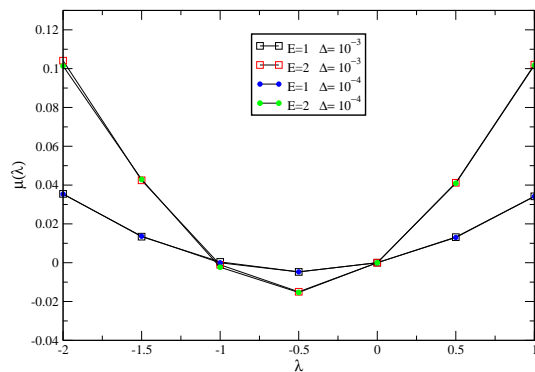In Fig. 5 we show the results of $\mu(\lambda)$ for $-2 \leq \lambda \leq 1$,

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FIG. 5: Plot of $\mu(\lambda)$ vs. λ for very large values of devia-
tions, ranging from minus three times to twice the typical
current. Data for $\vec{E} = (E, 0)$, $E = 1, 2$ and noise intensity
$\Delta = 10^{-3}, 10^{-4}$. The Gallavotti-Cohen theorem implies the
symmetry around $\lambda = -\frac{1}{2}$.

and for $\vec{E} = (E, 0)$ with $E = 1, 2$, corresponding to very
large current deviations.

The methods involving cloning have their own prob-
lems and dangers, for which a variety of solutions and
tests have been proposed over the years (see [22]). In
our case, we have found that for very small values of
the noise the clones have all nearby trajectories, a phe-
nomenon typical of systems of reproducing units with
fixed total size (the loss in diversity of family names in
a closed society). Our results in the billiard case were
noisy and unreliable when this diversity-loss set in. In
the case of the TASEP, the same phenomenon explains
the fact that all clones have the shock in essentially the
same position (which depends on the run), but in this
case this posed no problem for the sampling.

In conclusion, we have shown that sampling methods
based on a modified dynamics can be used to efficiently
compute large deviations, in times and within ranges of
values that would be unthinkable in a direct simulation.

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* Affiliato INFN, Sezione di Napoli.

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