A Monte Carlo from Belén

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The Event-Driven Monte Carlo algorithm is introduced. It applies to problems with discrete degrees of freedom, accurately finding the temporal evolution at all time scales.

Back in 2010, when now Prof. Alejandro Mendoza-Coto was a master student in Cuba, we stumbled on the fact that, to the best of our knowledge, there were no numerical methods to study the dynamics of an Ising-like spin system in real, physical time. Not very aware of the current literature on Kinetic Monte Carlo (KMC) techniques, we started to consider the possibility of simulating single realizations of the master equation in one of the many discussions we had at my place, at the rooftop of an old building of the Belén neigborhood in Old Havana.

After many sessions, the general idea seemed to be very simple: the full system can be decomposed in a set of two-level subsystems containing all possible changes. Indeed, all the transitions the full system could immediately undergo from a state X, can be mapped as a set of N two-level "new systems" with energies corresponding to that of states X and Y_i, where Y_i is the final configuration for each possible change $i \in [1, 2, ..., N]$. Thus, the immediate evolution of the full system in a state X can be studied by preparing N two-level subsystems in an initial state of energy $E(X)$, and letting them race for transition to the corresponding level $E(Y_i)$. The winner $i = w$ will reset the whole configuration, so that we can make $X = Y_w$ and start all over again. The project, nevertheless, got not too far from coffee talks and a bunch of useless formulas and code lines.

Five years later, we met in Strasbourg under the hosting of Prof. Guido Pupillo, who became interested in the potential of the original idea, particularly when addressing the very early stages of the dynamics. By that time we were quite familiar with KMC and time-quantified Monte Carlo methods, and could see more clearly the advantages of the Belén's scheme. We realized that, despite several decades of improvement, no reliable numerical technique was capable of reproducing the master equation kinetics at very short times. So we finally designed and implemented what was eventually published with the name of Event-Driven Monte Carlo algorithm [1], applicable to all systems of discrete variables (like Ising spins), whose summarized flowchart is shown in Fig. 1.

For systems of discrete variables following stochastic evolution, the probability distribution $\mathcal{P}(X,t)$ of being at a given state X at time t is given by the master equation

$$\frac{\partial \mathcal{P}(X,t)}{\partial t} = \sum_Y W(X|Y)\mathcal{P}(Y,t) - \sum_Y W(Y|X)\mathcal{P}(Y,t) \quad (1)$$

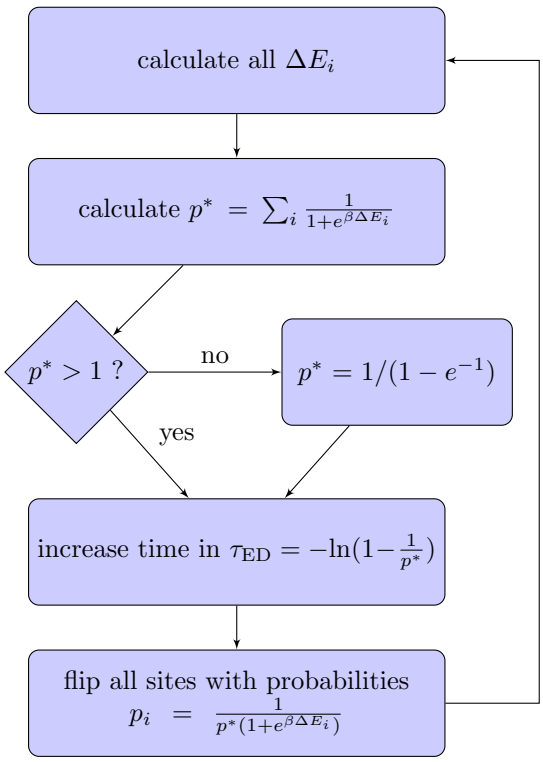

Figure 1: Flowchart for the elementary step of the Even-Driven algorithm. The energy difference ΔE_i is associated to the flipping of spin i while all the rest are fixed, i.e. the energy differences between the two levels of the subsystems.

where $W(Y|X)$ is the transition rate from state X to state Y. Let's now consider the subsystems corresponding to state X. For single-spin-flip dynamics, each spin i defines a subsystem occupying the level o, while level f, corresponding to the spin flip, is initially free. So that if $P_k^l(t)$ is the probability of subsystem k to be at the level l at a time t, then $P_i^o(0) = 1$ and $P_i^f(0) = 0$. While no transition has occurred, the race can be described by N independent systems of two equations

$$\frac{dP_i^o(t)}{dt} = \Gamma_i^{fo} P_i^f(t) - \Gamma_i^{of} P_i^o(t) \quad (2)$$

$$\frac{dP_i^f(t)}{dt} = \Gamma_i^{of} P_i^o(t) - \Gamma_i^{fo} P_i^f(t) \quad (3)$$

where Γ_i^{of} and Γ_i^{fo} are the transition rates of the two-level subsystem associated to the flip of spin i. Imposing the Boltzmann occupation probabilities for the

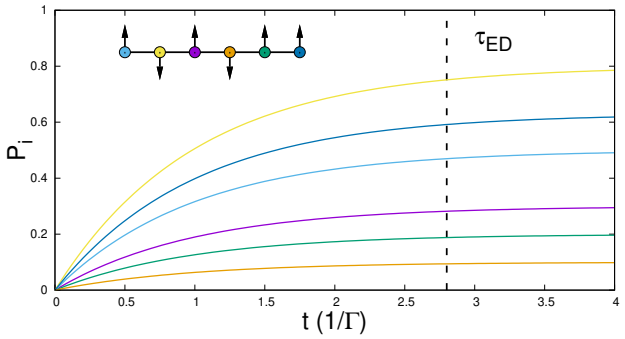

Figure 2: Schematic representation of P_i for a system of six spins marked with different colors. The interacting Hamiltonian (not shown) sets the prefactors $P_i^f(\infty)$.

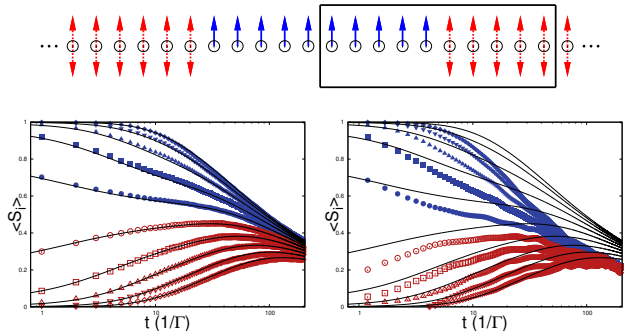

Figure 3: Top: Initial condition of a long Ising chain prepared with ten central spins in a ferromagnetic configuration; the black rectangle highlights the spins whose average magnetization is plotted below. Left: Average magnetization obtained with Event-Driven MC simulations. Right: Average magnetization obtained with KMC simulations. The solid black curves are the exact solution by R. J. Glauber [3].

infinite-time limit, and using the simple form of the partition function of the two-level subsystem, transition probabilities $P_i(t)$ can be solved analytically to give

$$P_i(t) = P_i^f(t) = P_i^f(\infty)\left[1 - e^{-(\Gamma_i^{of}+\Gamma_i^{fo})\ t}\right], \qquad (4)$$

where $P_i^f(\infty) = 1/[1 + e^{\beta(E_i^f - E^o)}]$, and the unit of time can be taken to be the inverse of the characteristic frequency $\Gamma = \Gamma_i^{of} + \Gamma_i^{fo}$ assumed as constant.

The probabilities of Eq. (4) are schematically shown in Fig. 2 for a finite chain of Ising-like spins interacting via some Hamiltonian. The goal then is to propose spin flips with these probabilities evaluated in some time $\tau_{\rm ED}$, large enough to be useful but small enough to ensure that Eqs. (2) and (3) are still valid. This is naturally guaranteed by imposing the normalization condition $\sum_i P_i(\tau_{\rm ED}) = 1$ and solving for $\tau_{\rm ED}$, which leads to

$$\Gamma\tau_{\rm ED} = -\ln\left[1 - P_*^{-1}\right], \qquad (5)$$

where $P_* = \sum_i P_i^f(\infty)$. Thus defined, the time $\tau_{\rm ED}$ is such that, in average, only one spin has made the transition, and hence the full system is in a new state.

We compared the outcome of our algorithm with state-of-the-art implementations of he KMC schemes [2] by recording the local magnetization of a spin chain prepared in a known initial state. This is perhaps the most complex problem of discrete-variables in statistical physics for which an exact solution of the dynamics is known at all timescales [3].

In the top panel of Fig. 3 the initial condition of the ensemble of chains is represented with blue arrows for spins that start with $\langle S_i\rangle = 1$ and red double arrows for spins starting with $\langle S_i\rangle = 0$. As can be seen from the lower panels, and unlike the KMC scheme, the results from the Event-Driven algorithm are in a pretty nice agreement with the exact solution for the local magnetization.

In summary, we found that the heuristic assumptions and phase-space constructions lying at the basis of KMC techniques are not good for studying times of the order of consecutive elementary events. In the context of ultrafast dynamics, the algorithm first discussed in Belén became perhaps the first one to reproduce the exact master equation along the time axis. The formulation of this Event-Driven MC can be made very general to attack any discrete variable problem. The only requirements are that i) the system can be decomposed into a set of N two-level subsystems, and ii) any dynamical evolution can be described by sequential transitions of these individual subsystems.

Notes

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References

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