New approach to Dynamical Monte Carlo Methods: application to an Epidemic Model

O.E. Aiello and Marco A.A. da Silva
Departamento de Física e Química da FCFRP,
Universidade de São Paulo, 14040-903 Ribeirão Preto, SP, Brazil

(Dated: October 29, 2001; Received text; Revised text; Accepted text; Published text)

Abstract

A new approach to Dynamical Monte Carlo Methods is introduced to simulate markovian pro-
cesses. We apply this approach to formulate and study an epidemic Generalized SIRS model. The
results are in excellent agreement with the forth order Runge-Kutta Method in a region of deter-
ministic solution. We also demonstrate that purely local interactions reproduce a poissonian-like
process at mesoscopic level. The simulations for this case are checked self-consistently using a
stochastic version of the Euler Method.
I-Introduction - Monte Carlo (MC) methods have been used mainly to equilibrium systems\[1\], and they have broad applications, since simple systems like hard spheres\[2\] up to complex systems like proteins[3, 4]. Good reviews in applications of MC methods to statistical physics can be seen in the references[1, 5]. In the last decades the development of techniques dealing with non-equilibrium systems has been increased[6], specially those that concern with stochastic processes. Several attempts were done[7]-[11] to simulate real time processes with this method. Some success was achieved within the scope of poissonian processes[8] that has been only recently properly formalized by Fichtorn and Weinberg[9]. Another important approach from a theoretical point of view is the waiting (or residence) time distribution used by Prados et al.[7], whose application is limited to simple systems, like Ising models. Some improvement in the real time calculation was presented by Cao[10], but in a particular and non rigorous way. In this letter we surmount this problem using directly the Master Equation, ignoring thus what type of distribution we are dealing. In this way, we also avoid the direct waiting (fine-grained) time distribution calculation; this is substituted by the calculation of interevent (coarse-grained) times. In our approach, the time is a dependent stochastic variable whose distribution is constructed from the Master Equation with appropriate transition probabilities. This gives the hierarchy of the process. The approach is developed for a class of markovian processes with no simultaneous events in the smallest scale considered. Thus, it is for a restricted markovian, but more general than poissonian processes. This method has already been applied[14] to an extensive study of the epidemic Susceptible-Infected-Recovered-Susceptible (SIRS) systems (to details of these epidemic systems see[11] and references therein). Here, we apply this new approach to formulate an epidemic Generalized SIRS (GSIRS) model, and study two particular cases of it.

II-The Method - For discrete systems, the markovian Master Equation is given by:

\[
\frac{dP_i(t)}{dt} = \sum_j \ w_{j\to i}P_j - \sum_j \ w_{i\to j}P_i ,
\]

(1)

where \( P_i \) is the probability to find the system at the state \( i \) at the time \( t \), and \( w_{i\to j} \) is the transition probability per unity of time. Considering \( T_{ij} \) the probability of transition from \( i \) to \( j \), we may write \( w_{i\to j} = \frac{T_{ij}}{\tau_i} \)[12], where \( \tau_i \) is a time constant (lifetime) characteristic of the state \( i \).

We now start by choosing a convenient physical extensive microscopic quantity \( A_i \) that
is time independent for each state $i$. The mean value for this quantity at the time $t$ is given by:

$$A(t) = \langle A \rangle = \sum_i P_i(t) A_i.$$ (2)

This equation represents a continuous physical macroscopic quantity $A(t)$. We can differentiate both sides of the equation above, with respect to $t$. After that, using (1), and by defining $\Delta A_{ij} = A_i - A_j$, we get

$$\frac{dA(t)}{dt} = \sum_i \sum_j w_{j \rightarrow i} P_j \Delta A_{ij}.$$ (3)

Consider now the nearest-neighbor states $j$ of a given state $i$; if we measure the “distance” between the states, say by the quantity $|\Delta A_{ij}|$, such that the non-null minimum value is $|\Delta A_{ij}| = a$, we may approach the equation (3) by:

$$\frac{dA(t)}{dt} = \sum_{<ij>} w_{j \rightarrow i} P_j a \delta_{ij},$$ (4)

where the symbol $<ij>$ denotes a nearest-neighbour pair of states, and $\delta_{ij} = \Delta A_{ij} / |\Delta A_{ij}|$. Now we consider another physical quantity $A^\dagger$ that is a source for the quantity $A$. Thus, we can rewrite (4) as:

$$\frac{dA(t)}{dt} = \sum_j r_j^+ P_j A_j^\dagger - \sum_j r_j^- P_j A_j,$$ (5)

where $r_j = <w_{j \rightarrow i}>_i$ are the transition probabilities per unity of time averaged over the ensemble of the nearest-neighbour states $i$ of $j$ at some time $t$, i.e., the mesoscopic rates. Here, ensemble means a set of configurations accessible at a some finite (small) time around a time $t$; in this sense we are using a time dependent ergodicity idea[5], and so generally the systems are non ergodic in non equilibrium states. The superscripts “+” and “−” mean respectively the contributions to increasing and to decreasing the quantity $A(t)$. In the particular case that $r_j^+ = r^+$ and $r_j^- = r^−$ are constants (or only function of the time) we have:

$$\frac{dA}{dt} = r^+ A^\dagger - r^- A,$$ (6)

what is the analogous to the kinetic equation for the first order chemical reaction $A^\dagger \rightleftharpoons A$, being $A^\dagger$ and $A$ the respective concentrations of the chemical elements $A^\dagger$ and $A$. The equilibrium can be reached by imposing the balance at macroscopic (or mesoscopic) level.
\[ r^+ A^\dagger = r^- A. \] This follows immediately if we require the detailed balance, but it is not necessary at all[13].

We can write the equation (4) in an approximated form of a discrete integral

\[ A(t) - A(t_0) \simeq \sum_{k=0}^{n} \sum_{\langle ij \rangle} w_{j\to i} P_j(t_k) a \delta_{ij} \Delta t_k. \quad (7) \]

Let now be the set of possible \( w_{j\to i} \) represented by \( \mathcal{P}_t = \{ w_{j\to i} \} \), being the states \( i \) and \( j \) occurring around a given instant \( t \), and \( w_{t}^{\text{max}} = \sup \mathcal{P}_t \). The phase space may be divided into \( N \) parts, in such way that each part may contain only one element of the system. Thus, each element of time in the equation (7) may be represented by

\[ \Delta t_k = \frac{1}{w_{t_k}^{\text{max}} N}. \quad (8) \]

We can do the approach to the equation \( A(t) \) considering \( n = \ell N \), with \( \ell \) sweeps over the discretized space; in the limit of \( N \to \infty \) we have the exact solution of the equation (4) for a given initial condition.

**Monte Carlo Approach** - With the considerations above the equation (7) may be written in the form:

\[ A(t) - A(t_0) = \ell N \sum_{k=0}^{n} \sum_{\langle ij \rangle} \left( \frac{w_{j\to i}}{w_{t_k}^{\text{max}}} \right) \left( \frac{1}{N} \right) P_j(t_k) a \delta_{ij}. \quad (9) \]

We can create a hierarchical process choosing the probabilities of transition

\[ T^*_{j\to i} = \frac{w_{j\to i}}{w_{t_k}^{\text{max}}}, \quad (10) \]

that reproduce the correct frequencies of events at each time \( t_k \) to solve (9). This hierarchy have subtle differences with an earlier hierarchy introduced by Fichtorn et al[9]: first in that work (mesoscopic) rates were required, while here we primarily use transition probability per unity of time. Second, they used a global maximum to the rates, while here we use a more local maximum; in recent work[11] this was done without a rigorous proof, based only in the detailed balance principle applied to a specific case. To carry out the MC procedure, an element is selected randomly with a probability \( \frac{1}{N} \), and thus a transition is tried with probability given by (10). The space is swept \( \ell \) times, with the increment of time in each MC step (one MC step here, means a single try to change the state of one element of the
system) given by (8) up to reach a time $t$. Starting from the same initial conditions for the physical quantities, the process may be repeated, and we can get the average quantity $A(t)$ at each instant $t$. We must emphasize that the probabilities $P_j$ are generated by this process. As a given state is chosen with its correct probability in a given time, an ideal MC procedure leads to

$$A(t) - A(t_0) = \sum_{k=0}^{\ell N} \left( \langle r^+ A^\dagger \rangle_{jk} - \langle r^- A \rangle_{jk} \right) \left( \frac{1}{w_{t_k}^{\text{max}}} \right), \quad (11)$$

where the averages are taken over the ensemble of the states $j_k$ at each instant $t_k$. This is just an approach to the integration result of the equation (5).

We need to observe some important points: first, generally different runs give different time $t_k$ results at the same MC step $k$, and the sample averages may be done by linear interpolating or extrapolating the data set, in each MC realization, to do them at the same point of the time. Second, in one complete sweep around a time $t_k$, the value $w_{t_k}^{\text{max}}$ must be approximately constant in order do not change the hierarchy and so the result. Third, as the configurations do not change drastically in few steps, the microscopic transitions reproduce the mesoscopic result.

Another approach consists in estimating the interevent times by the following rule

$$\Delta t_k^e = \frac{f_k^e a}{r_{jk}^e A_{jk}^e}, \quad (12)$$

where $r_{jk}^e = r_{jk}^+$ and $A_{jk}^e = A_{jk}^+$, or, $r_{jk}^e = r_{jk}^-$ and $A_{jk}^e = A_{jk}$ depending on, respectively, if the outcome of the experiment increase or decrease the quantity $A$. The quantity $f_k^e$ is an arbitrary $e$-event dependent factor that must obey the relationship $\sum_e f_k^e = 1$, for each time $t_k$. We emphasize that the time given by (12) represents the average waiting time to transitions from a given state $j_k$ to any neighbor state $i$; if the microscopic state remains unchanged, the time does not evolve. It can be shown that this procedure leads to the same result as using (8) at each MC step observing that

$$\Delta t_k = \sum_e \sum_i \left( \frac{w_{jk-i}}{w_{t_k}^{\text{max}}} \right) \left( \frac{1}{N} \right) \Delta t_k^e. \quad (13)$$

As $r_{jk}^e A_{jk} = a \sum_i w_{jk-i}$, using the equation (12) and the normalization condition to $f_k^e$ in (13), we obtain the expression (8). In particular, if we choose $f_k^e = 0$, for most events $e$,
except some \( e = s \), we have \( f_s^k = 1 \), so, with this condition, the interevent time has the meaning of the waiting time between type-\( s \) events. Based on this and in the fact that at the equilibrium the relative frequencies of occurrence of events are all equal, we may define
\[
f_e^k \equiv \frac{n_e^k}{N_k},
\]
where \( n_e^k \) is the number of \( e \)-events, and \( N_k = \sum_e n_e^k \) is the total number of events, in a time interval (arbitrary) near to some time \( t_k \).

**III-GSIRS model** - Based on (5), we formulated the GSIRS model through the following set of differential equations and inter-classes rates:

\[
\frac{dS}{dt} = \sum_j r^j_{R \rightarrow S} P_j R_j - \sum_j r^j_{S \rightarrow I} P_j S_j,
\]

\[
\frac{dI}{dt} = \sum_j r^j_{S \rightarrow I} P_j S_j - \sum_j r^j_{I \rightarrow R} P_j I_j,
\]

\[
\frac{dR}{dt} = \sum_j r^j_{I \rightarrow R} P_j I_j - \sum_j r^j_{R \rightarrow S} P_j R_j,
\]

where \( S, I, \) and \( R \) are the populational classes, respectively, of the number of individuals in the susceptible, infective and recovered classes. Being the mesoscopic rates \( r^j_{S \rightarrow I} \), \( r^j_{I \rightarrow R} \) and \( r^j_{R \rightarrow S} \), for each state \( j \), respectively, from \( S \rightarrow I, I \rightarrow R \) and \( R \rightarrow S \). Note that we meant that, for example, if \( A = I \), then \( A^\dagger = S \) in the equation (5). The conservation law with the total number of individuals \( N = S(t) + I(t) + R(t) \) is satisfied. In particular, a model commonly used\[11, 15\] gives \( w_{R \rightarrow S} = m, w_{S \rightarrow I} = \Gamma \mu S^\mu - I + \Lambda [1 - (1 - p_0)^n] \), and \( w_{I \rightarrow R} = q \) to the transition probabilities per unity of time. We must observe that the mesoscopic rates are resulting from local ("instantaneous") averages of the respective transition probabilities per unity of time. For practical purposes the individuals are distributed on a square lattice of \( N = M \times M \) sites. All the individuals at the lattice boundary have their states fixed at susceptible state.

**IV-Results and Conclusions** - We set the lattice size to \( M = 200 \). This size was sufficient to get good results compared with the continuum limit when only global interactions (\( \Lambda = 0 \)) are considered. The initial condition for the system is set up by \( I_0 = 2000 \) infectives being randomly distributed on the lattice and the remaining sites being occupied by \( S_0 = N - I_0 \) susceptibles, so \( R_0 = 0 \).

We consider here two particular cases of the system defined by (14–16). First, we set \( \Lambda = 0 \), and the other model parameters as \( q = 0.2, b = 0.8, m = 0.01 \) and
\( \mu = 2 \). The non-minimum value, to the differences \( \Delta S \), \( \Delta I \) and \( \Delta R \), used in (12) is \( a = |\Delta I| = |\Delta S| = |\Delta R| = 1 \). Figure 1 shows the temporal evolution of \( I(t) \). Continuous lines represent numerical (fourth-order Runge-Kutta) checking solutions for the set of differential equations (14–16), and open circles correspond to the MC simulations. The accuracy of the deterministic solution (Runge-Kutta) was estimated as less than 0.1% (see ref.[11]). Results to the system far from equilibrium showed that the interevent times given by (12) have poissonian-like distribution (see inset in figure 1) as expected[11]. At the equilibrium, the present method leads to converge the distributions of interevent times to delta distributions, because the values to the rates and other physical quantities converge to constant values. A total of \( 4 \times 10^6 \) steps, corresponding to \( 3.5 \times 10^6 \) configurations, was generated by the MC procedure, leading to a total real time of approximately 500 days. The total number of configurations used to get the interevent times distribution was about \( 8 \times 10^4 \), what corresponds to approximately 60 days. Second, we set \( \Gamma = 0 \) and \( m = 0 \), i.e., a SIR system with purely local variables. The variable \( n \) is an integer ranging from \( n = 0 \) up to 8, since the first and second nearest infected neighbors are indistinguishably considered for each susceptible. To this case we use again the expression (12), but the rates \( r_{S \rightarrow I} \) are obtained by averaging the individual probabilities to the configurations in every successful event. This may coast some simulation time. A good optimization for an approximation to the exact average is done by drawing randomly susceptibles (1000 here was sufficient) for each configuration reached and doing a sample mean with the site transition probabilities per unit of time \( w_{S \rightarrow I} \). It must be observed that this type of average is equivalent to let the system advance some small time and take an average over the sample. As the system configurations do not change much around some time \( t_k \), the small time average corresponds to an average in an instantaneous time. To see the self-consistency of the approach, we integrate numerically (14–16) given constant (or piecewise constant) time step as in (7) by choosing the maximum local transition probability per unit of time. This maximum is in fact actualized at each MC step, when necessary, using a table. When a transition changes a state of an individual that changes the maximum, the table is updated. The quantities \( S, I \) and \( R \) are calculated with iterations; the rates are chosen randomly by the MC procedure, and thus we use the Euler Method procedure to solve first order differential equations. Experiments using poissonian distributions[9] to obtain the interevent times showed that the processes are poissonian-like to all ranges of \( p_0 \), being so, unnecessary the hypothesis of low
$p_0$ (“weak interaction”) as done by Aiello et al. To illustrate, we show in the Figure 2 the results to $p_0 = 0.8$. We compare, also, in figure 2 the iterative method with the MC technique described above (restricted markovian method), estimating the interevent time by (12). The total number of configurations used in the MC procedure was about $4 \times 10^4$ what gives approximately 10 days. The results are in excellent agreement among them. For both cases (Figures 1 and 2), results with respect to the MC simulations correspond to an average of 20 independent trajectories. The typical MC data errors are in the interval 0.1-1.0%, so most of the error bars are smaller than the symbols in the figures.

We believe that the class of epidemic SIRS models studied here are poissonian-like in the mesoscopic scale because of two factors. First, the approach itself implies that no two or more events occur in a short scale of time. Second, the mesoscopic rates are slowly varying with the time, resembling the independence between events. So, the two conditions for a poissonian process were met. We emphasize that low correlations between events are not required. It is necessary that the results for independent runs be uncorrelated, so we can use the averages obtained for each time $t$ to represent properly the physical quantities of the process. To do this we need a local equilibrium hypothesis, what may be at first glance restrictive, however we may even reduce the time observation sufficiently such that the system does not have time to leave some metastable states. So, we can average it there. In the practice of the simulation this is done by increasing the number of observations, i.e., the number of time experiments. In forthcoming works we expect to generalize still more the method, including up to non-markovian processes.

The authors gratefully acknowledges funding support from FAPESP Grant n. 00/11635-7 and 97/03575-0. The authors would also like to thank Drs. F.L.B. da Silva and A. Caliri for many stimulating discussions and suggestions.
Figure Captions

FIG. 1. Infected numbers I(t) vs Time. Continuous line: numerical forth-order Runge-Kutta solution. Open circles: restricted markovian DMC simulation. Inset: shows the behavior of the interevent time $\Delta t$ distribution.

FIG. 2. Infected numbers I(t) vs Time. Continuous line: iterative stochastic Euler Method solution. Squares: restricted markovian DMC simulation. Open circles: poissonian DMC simulation.
[1] K. Binder, *Monte Carlo Method in Statistical Physics* (Springer-Verlag, Berlin, 1986).

[2] A. Caliri, M. A. A. da Silva, and B. J. Mokross, J. Chem. Phys. 91, 6328 (1989).

[3] D. Bouzida, S. Kumar, and R. H. Swendsen, Phys. Rev. A 45, 8894 (1992).

[4] M. Cieplak, M. Henkel, J. Karbowski, and J.R. Banavar, Phys. Rev. Lett. 80, 3654 (1998).

[5] K. Binder, Rep. Prog. Phys. 60, 487 (1997).

[6] F.J. Alexander, A. L. Garcia, and B. J. Alder, in *25 Years of Non-Equilibrium Statistical Mechanics*, edited by J. J. Brey et al (Springer-Verlag, Barcelona, Spain, 1994).

[7] A. Prados, J.J. Brey, and B. Sánchez-Rey, Journal of Statistical Physics 89, 709 (1997).

[8] D. T. Gillespie, J. Comp. Phys. 22, 403 (1976).

[9] K. A. Fichtorn and W. H. Weinberg, J. Chem. Phys. 95, 1090 (1991).

[10] Pei-Lin Cao, Phys. Rev. Lett. 73, 2595 (1994).

[11] O.E. Aiello, V.J. Haas, A. Caliri, and M. A. A. Silva, Physica A. 282, 546 (2000).

[12] P.G. Hoel, S.C. Port, and C.J. Stone, *Introduction to Stochastic Processes* (Waveland Press, Inc., Prospect Heights, Illinois, 1987).

[13] L. D. Fosdick, in *Methods Comp. Phys.*, edited by B. Alder, S. Fernback and M. Rotenberg, Vol. 1 (Academic Press, 1963), p. 245.

[14] O.E. Aiello and M. A. A. Silva (to be published).

[15] V.J. Haas, A. Caliri, and M.A.A. da Silva, J. of Biol. Phys., 25, 309 (1999).
Figure 1

Restricted markovian DMC

Runge-Kutta
Figure 2

Iterative
Restricted markovian DMC
Poissonian DMC

$I(t) \times 10^{-3}$

Time (days)