Dynamical Monte Carlo method for stochastic epidemic models

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(Dated: August 19, 2002; Received textdate; Revised textdate; Accepted textdate; Published textdate)

Abstract

In this work we introduce a new approach to Dynamical Monte Carlo methods to simulate markovian processes. We apply this approach to formulate and study an epidemic generalized SIRS model. The results are in excellent agreement with the fourth order Runge-Kutta method in a region of deterministic solution. Introducing local stochastic interactions, the Runge-Kutta method is no longer applicable. Thus, we solve the system described by a set of stochastic differential equations by a Dynamical Monte Carlo technique and check the solutions self-consistently with a stochastic version of the Euler method. We also analyzed the results under the herd-immunity concept.
I. INTRODUCTION

Epidemic systems have been systematically and mathematically formulated in a continuous-deterministic approach, taking immediate advantages of many numerical methods and techniques developed to solve differential equations. The stochastic framework is more complex to analyze because of the required detail; therefore it could be traditionally less preferable than the deterministic ones, even being more realistic in principle [1, 2, 3]. However, improved machine technology has spread the use of computationally intensive methods to solve a great diversity of epidemic models, and simulation techniques, as Monte Carlo (MC) [4, 5], are becoming more popular in this matter. Some MC studies hide the effective role of the time, on time-dependent phenomena, reporting its results as function of integral Monte Carlo steps (MCS) [6]. Ambiguities of the relationship between MC time and real time preclude rigorous comparison of simulated results between theory and experiment. However, in the past few years, the idea of use MC methods to simulate dynamical processes has advanced in many publications [7, 8, 9, 10].

The aim of the present work is to present a Dynamical Monte Carlo (DMC) method for simulation of markovian processes. Another purpose is to incorporate explicit spatial components into epidemic models and analyze the dynamics of infections spread based on this method. We will apply the method to the compartmental Susceptible-Infected-Recovered (SIR) model. By the inclusion of a reflux of susceptible into the system we obtained a variant model: SIRS; i.e., once recovered the individual can turns back again to the class of susceptibles. Mean field and local interactions will be considered. We compare the results obtained by DMC, for mean field models, with Runge-Kutta method. In cases where Runge-Kutta method is not applicable, the MC space-dependent results are checked self-consistently using a stochastic version of the Euler method [11] and analyzed under the herd-immunity concept [12].

We subdivided the work in the following way: method description (section II), Monte Carlo Simulation technique (section III), epidemic models (section IV), and finally we apply the methodology for the solution of the SIRS model (section V).
II. THE METHOD

Stochastic process approaches could simulate non-equilibrium systems, even the deterministic ones, introducing random variables to describe them in a microscopic scale. The macroscopic behavior of some system is resulting from averages of its microscopic properties. Here, we will simulate systems only with markovian processes. Thus, we describe the evolution of the distribution of probabilities with the Master Equation:

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

where \( P_i(t) \) is the probability to find the system in the state \( i \) in the time \( t \), and \( w_{i\rightarrow j} \) is the probability of transition per unit of time. The first term on the right side describes the rate of all transitions to reach the considered state (increasing its probability), and the second term describes the rate of all transitions leaving the considered state (decreasing its probability). Considering \( T_{ij} \) as the probability of transition from the state \( i \) to \( j \), we can write \( w_{ij} = \frac{T_{ij}}{\tau_i} \), where \( \tau_i \) is the characteristic time constant (lifetime) of the state \( i \). The probabilities, \( P_i(t) \) and \( T_{ij} \), obey the normalization conditions: \( \sum_i P_i(t) = 1 \) and \( \sum_j T_{ij} = 1 \).

We now start by choosing a convenient physical extensive microscopic quantity \( A_i \), which depends only of the system’s state \( i \). Since the time must change for every successful event, for our purposes here, from now on we will consider only counting events related quantities. The mean value for a given quantity at the time \( t \) is

\[
A(t) = \langle A \rangle = \sum_i P_i(t) A_i .
\]

This equation represents the macroscopic physical quantity \( A(t) \). Differentiating both sides of the equation above with respect to \( t \), we obtain

\[
\frac{dA(t)}{dt} = \sum_i \frac{dP_i(t)}{dt} A_i ,
\]

and by substituting (1) in (3) follows:

\[
\frac{dA(t)}{dt} = \sum_i \sum_j w_{j\rightarrow i} P_j A_i - \sum_i \sum_j w_{i\rightarrow j} P_i A_i .
\]

Defining \( \Delta A_{ij} = A_i - A_j \), and as \( i \) and \( j \) sweep all possible states of the system, we may rewrite (1) as

\[
\frac{dA(t)}{dt} = \sum_i \sum_j w_{j\rightarrow i} P_j \Delta A_{ij} .
\]
Consider now a discretized system with \( N \) interacting elements. Each element has \( g \) degrees of freedom given by the set \( \{ \gamma_i \} \) with \( g \) dynamic variables \( \gamma_i, \ i = 1, 2, ..., g \). By doing an element move, i.e., changing some \( \gamma_i \) value of a chosen element, the system will reach a next-neighbor microscopic state. Suppose that we are in a time scale where only one event occurs, and each event produces only one element move. In another words, we are neglecting transitions between states that need more than one element move to take place. Thus, let us measure “distances” among the states, say with the amount \( |\Delta A_{ij}| \), with non null minimum value \( |\Delta A_{ij}| = q \) that defines the distance between first neighbor states.

With the above considerations, an approach to the equation (5) can be done as

\[
\frac{dA(t)}{dt} = \sum_{(ij)} w_{j\rightarrow i} P_j q \delta_{ij},
\]

in which the symbol \((ij)\) denotes a pair of first neighbor states, and \( \delta_{ij} = \Delta A_{ij}/|\Delta A_{ij}| \).

Now consider other physical quantity \( A^\dagger \) as the source for the quantity \( A \). The use of the term source here is in the following sense: increasing \( A \) by the quantity \( q \), \( A^\dagger \) decreases by the same quantity and vice-versa. Thus, we can rewrite (6) as:

\[
\frac{dA(t)}{dt} = \sum_j r^+_j P_j A^\dagger_j - \sum_j r^-_j P_j A_j,
\]

where the rate \( r_j = \langle w_{j\rightarrow i} \rangle \) results from the average of the transition probabilities per unit of time, over the ensemble of first neighbor states \( i \) of \( j \) in the time \( t \), i.e., the mesoscopic rates. The word ensemble here means a group of accessible configurations in a small time interval around the time \( t \). We are using the time dependent ergodicity idea\[14\], and in this sense, usually, the systems are non ergodic in non equilibrium states. The superscripts “+” and “−” label the contributions to increase and to decrease the quantity \( A(t) \), respectively.

In the particular cases where \( r^+_j = r^+ \) and \( r^-_j = r^- \) are constant (or only function of the time) we have:

\[
\frac{dA}{dt} = r^+ A^\dagger - r^- A,
\]

which is similar to the kinetic equation for chemical reactions of first order \( \mathcal{A}^\dagger \rightleftharpoons \mathcal{A} \), being \( A^\dagger \) and \( A \) the respective concentrations of the chemical elements \( \mathcal{A}^\dagger \) and \( \mathcal{A} \). The system is in equilibrium when the balance at macroscopic level: \( r^+ A^\dagger = r^- A \), is satisfied. We can reach the equilibrium imposing the detailed balance, although this assumption is not necessary\[5\]; as we will see, the equilibrium is consequence from the chosen hierarchy, that solves the Master Equation in any instant.
To solve the equation (6) we write it in the integral form:

\[ A(t) - A(t_0) = \int_{t_0}^{t} \sum_{(ij)} w_{j \rightarrow i} P_j(t) q \delta_{ij} dt. \] (9)

Discretizing the equation (9), we can write:

\[ A(t) - A(t_0) \simeq \sum_{k=0}^{n} \sum_{(ij)} w_{j \rightarrow i} P_j(t_k) q \delta_{ij} \Delta t_k. \] (10)

Let the group of possible probabilities of transition per unit of time \( w_{j \rightarrow i} \) represented by the set \( P_t = \{ w_{j \rightarrow i} \} \), being the \( i \) and \( j \) states occurring around an instant \( t \), with \( w_{i}^{\text{max}} = \sup P_t \), that is, the largest probability in \( P_t \). Each element of the time in the equation (10) could be

\[ \Delta t_k = \frac{1}{w_{i}^{\text{max}} N}. \] (11)

Starting from some initial condition, we can do the following iterative process:

\[ A(t_{k+1}) = A(t_k) + \sum_{(ij)} w_{j \rightarrow i} P_j(t_k) q \delta_{ij} \Delta t_k. \] (12)

At each step \( k \) a time interval \( \Delta t_k \) is calculated using (11). The probabilities per unit of time \( w_{j \rightarrow i} \in P_{t_k} \) are randomly drawn using the hierarchy described in the next section of this work. Repeating the procedure, in a sufficient number, to get a good sample of \( A(t_k) \), we estimate the averages of \( A(t_k) \) for every \( t_k \). This procedure is a stochastic version of the Euler method.

### III. MONTE CARLO SIMULATION

In a dynamical interpretation, the MC method provides a numerical solution to the Master Equation. In order to do this, a sequence of events is generated based on the transition probabilities. The task of the MC algorithm is to create a chronological sequence of the distinct events separated by certain interevent times. In according to the hypothesis that leads to the equation (6), these interevent times are on a scale at which no two events occur simultaneously.

To find a hierarchy to the MC algorithm, we consider \( n = lN \), with \( l \) sweepings on the discretized system phase space, in which we are measuring a physical quantity represented in the equation (10); in the limit of \( N \to \infty \) we have the exact solution of the integral (9).
for a given initial condition. With this consideration, and using the expression (11), the equation (10) goes to the form:

\[ A(t) - A(t_0) = \sum_{k=0}^{\ell N} \sum_{(ij)} \left( \frac{w_{j \rightarrow i}}{w_{\text{max}}^{t_k}} \right) \left( \frac{1}{N} \right) P_j(t_k) q_{ij}. \]  

(13)

We can, thus, create a hierarchical process choosing the transition probabilities as:

\[ T_{j \rightarrow i}^* = \frac{w_{j \rightarrow i}}{w_{\text{max}}^{t_k}}, \]  

(14)

which reproduces the correct frequencies of events in every time \( t_k \) to solve (13).

To execute the MC procedure, an element is randomly selected with probability \( 1/N \), and thus an attempted move, with probability given by (14), is done to change the state from \( j \) to \( i \). Therefore, an event that changes a dynamic variable \( \gamma_i \), of the chosen element, controls the microscopic transition \( j \rightarrow i \). When the system has “degeneracy” as for the events occurrence, we need to decide what event will have chance (given by (14)) to take place; thus, we chose one of them with equal a priori probability [15], supposing a local equilibrium over the time. The local equilibrium hypothesis means that we can measure the properties of the system at any instant \( t \). Repeating the procedure, the space is swept \( l \) times, with the increment of time in each MCS given by (11), up to the system reach some desired final time. We denoted 1 MCS as a single trial to change the state of the system. Beginning with the same initial condition for the physical quantities, repeating the whole process described above, we obtain the average quantity \( A(t) \) over each instant \( t \). As a given state is chosen with its correct probability in a given time, an ideal MC procedure leads to

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

(15)

where the averages are done over the ensemble of the \( j_k \) states in each instant \( t_k \).

Observing some points is necessary: first, generally different runs give different time results \( t_k \) at the same MCS \( k \), and we obtain the sample average with either linear interpolation or extrapolation data group, in each MC realization of the system [16], as we will describe below. Second, in a complete sweep around a time \( t_k \), the value \( w_{\text{max}}^{t_k} \) should be approximately constant in order not to change the hierarchy and consequently the result. Third, as the configurations do not vary drastically in few steps, the microscopic transitions reproduce the mesoscopic results.
Another approach to calculate the real time consists in estimating the interevent times with the following rule:

\[ \Delta t^e_k = \frac{f^e_k q}{r^e_{jk} A^e_{jk}}, \]

where \( r^e_{jk} = r^+_{jk} \) and \( A^e_{jk} = A^+_{jk} \), or \( r^e_{jk} = r^-_{jk} \) and \( A^e_{jk} = A^-_{jk} \) depending, whether the result of the experiment increases or decreases the quantity \( A \). The quantity \( f^k_e \) is an \( e \)-event factor dependent and it obeys the relationship \( \sum_e f^k_e = 1 \) (normalization condition), for each time \( t_k \). We note that the time given by (16) represents the mean waiting time for transitions from a given state \( j_k \) to any neighbor state \( i \); if the microscopic state stays unchanged, the time also does not change. We can show that this procedure leads to the same result found using (11) in each MCS, observing that

\[ \Delta t_k = \sum_e \sum_i \left( \frac{w_{jk-i}}{w_{\text{max}}^-} \right) \left( \frac{1}{N} \right) \Delta t^e_k, \]

using the equation (16), the normalization condition for \( f^k_e \) and the definition \( r^e_{jk} A^e_{jk} = q \sum_i w_{jk-i} \) in (17), we obtain the expression (11). In particular, if we choose \( f^k_e = 0 \), for every event, except \( e = s \), we have \( f^k_s = 1 \). Under this condition, the time between \( s \)-events is the waiting time. Based on this, to estimate the waiting time in a coarse-grained way, we may define \( f^k_s \equiv n^k_s / N_k \); where \( n^k_s \) is the number of \( s \)-events, and \( N_k = \sum_e n^k_e \) is the total number of events, in a time interval (arbitrary) near to some time \( t_k \).

Note that at each MCS, the minimum quantity \( q \) is either added or subtracted from the resulting quantity \( A \) following the prescribed hierarchy. This procedure, in according to (15) reproduces statistically the average quantity \( A(t) \). Therefore, since we have the rates, or the probabilities of transition per unit of time, defining the time intervals between events in some scale, we construct a \( MC \) algorithm to solve the \textit{Master Equation}; consequently, we obtain the time evolution of physical quantities of the system.

In order to define the errors on macroscopic quantities, we will do a direct approach to calculate average quantities. We start supposing a \textit{local equilibrium} of the system over some instant \( t_0 \). With use of appropriated transition rates, we can reach any state \( i \) with probability \( P_i(t_0) \); so constructing several independent markov chains generates the distribution, which produces an \textit{ensemble} of configurations over the time \( t_0 \). Thus, we can use directly the equation (2) to calculate \( A(t) \) at the time \( t_0 \). If we chose a given state \( i \) of the system
with probability $P_i^*(t_0)$, we may rewrite the equation (2) by

$$A(t_0) = \frac{\sum_i P_i(t_0) A_i}{\sum_i P_i(t_0) / P_i^*(t_0)}.$$  \hfill (18)

A natural choice of $P_i^*(t_0)$, under equilibrium, is $P_i^*(t_0) = P_i(t_0)$, obtaining

$$A(t_0) = \frac{\sum_{i=1}^{L^*} A_i}{L^*},$$  \hfill (19)

where $L^*$ is the number of all possible states of the system at the time $t_0$. This result extends readily to any time $t$. The states labeled by $i$ may be considered as virtual states corresponding to possible data interpolation or extrapolation. The practical procedure is the following: at a given $MC$ realization of the system (experiment), in the construction of a trajectory, labeled by $\ell$, we may get the measurements of any appropriated physical quantity $A_\ell(t)$ obtained by either linear extrapolation or interpolation using two consecutive data points. After perform $L$ Monte Carlo experiments, at some time $t$, the mean value of $A$ is $A(t) \approx \frac{\sum_{\ell=1}^{L} A_\ell}{L}$. Note that if we idealize this procedure doing $L \rightarrow \infty$, we obtain the complete ensemble that give-us the correct mean values of physical quantities for each time $t$. Ensuring that different experiments are independent, the error for the involved quantities in the process for each time $t$ could be:

$$\frac{\sigma_A}{\sqrt{L}} = \sqrt{\frac{<A^2> - <A>^2}{L}},$$  \hfill (20)

where $A$ can be, for example, in this work context, the number of infected individuals.

IV. EPIDEMIC MODELS

The conventional treatment of epidemic systems is formulated based on a group of compartments that represents each of the possible statuses, of its elements, for which we may assign dynamic variable values, with rates of transfer among pairs of compartments. Mathematically this subject turns into a set of differential equations. Considering a generic system (population, epidemic agents, etc.) and its space distributions, the temporal and space evolution characterizes any epidemic, and in each region, the density of the elements can vary with the time. Under this optics we considered the epidemic phenomenon as a stochastic process in which one random variable is the time. This focus seeks to propitiate the incorporation of more details in the study of epidemic process and to allow the analysis of more complex models and therefore more realistic.
The SIRS model considers a population with $N$ individuals divided in three classes: $S$ (susceptible individuals), $I$ (infected) and $R$ (recovered). The evolution of the disease occurs according to the outline $S \rightarrow I \rightarrow R \rightarrow S$. Based on the equation (7), we formalize the SIRS model in a quite generic way through the following group of differential equations:

$$\frac{dS}{dt} = \sum_j r_{RS}^j P_j R_j - \sum_j r_{SI}^j P_j S_j, \quad (21)$$

$$\frac{dI}{dt} = \sum_j r_{SI}^j P_j S_j - \sum_j r_{IR}^j P_j I_j, \quad (22)$$

$$\frac{dR}{dt} = \sum_j r_{IR}^j P_j I_j - \sum_j r_{RS}^j P_j R_j, \quad (23)$$

where $S$, $I$ and $R$ are the (average) number of susceptible, infected and recovered individuals, respectively, over each instant $t$. The mesoscopic rates are $r_{SI}^j$, $r_{IR}^j$ and $r_{RS}^j$, for each state $j$, from $S \rightarrow I$, $I \rightarrow R$ and $R \rightarrow S$, respectively.

In order to reproduce the deterministic model in the reference [17] we did the following restrictions:

1) the effective increase rate of those susceptible (individuals) is directly proportional to the number of recovered, $\sum_j r_{RS}^j P_j R_j = mR$; and consequently the recovered decrease in the same proportion;

2) the effective increase rate of those infected is directly proportional to the number of infected and a power $\mu$ of susceptible, $\sum_j r_{SI}^j P_j S_j = bS^\mu I/N^\mu$; and consequently the susceptible decrease in the same proportion;

3) the effective removal rate of those infected is directly proportional to the number of infected, $\sum_j r_{IR}^j P_j I_j = aI$; and consequently the recovered increase in the same proportion.

Taken these restrictions to the set of differential equations (21−23) give:

$$\frac{dS}{dt} = mR - \frac{bS^\mu I}{N^\mu} \quad (24)$$

$$\frac{dI}{dt} = \frac{bS^\mu I}{N^\mu} - aI \quad (25)$$

$$\frac{dR}{dt} = aI - mR, \quad (26)$$

in which $\mu$ relates to the safety-in-numbers power [18]. The conditions: $dS/dt = 0$, $dI/dt = 0$, $dR/dt = 0$, determines the steady-state solutions; the nontrivial solution occurs for finite values of $S_\sigma$, $I_\sigma$, and $R_\sigma$, viz.,

$$S_\sigma = (a/b)^{1/\mu} N, \quad (27)$$
\[ I_\sigma = \frac{1 - (a/b)^{1/\mu}}{1 + a/m} N, \quad (28) \]
\[ R_\sigma = \frac{1 - (a/b)^{1/\mu}}{1 + m/a} N. \quad (29) \]

Depending on the removal rate \( a \) of the infectives, infection parameter \( b \), and renewal \( m \), there exist stable solutions around the steady state that correspond to recurrent epidemics, or damped (fading) recurrent waves. These variant supplies oscillatory solutions that vanish with the time, reaching a stationary state, in which, the number of elements in each class stays constant. This model is a generalization of the classical SIR system \[2, 19, 20\], readily recovered from \((24-26)\) by setting \( \mu = 1, m = 0 \), that gives \[21\]:

\[ \frac{dS}{dt} = -bSI, \quad (30) \]
\[ \frac{dI}{dt} = bSI - aI, \quad (31) \]
\[ \frac{dR}{dt} = aI. \quad (32) \]

The SIR class of compartmental models has several deterministic and stochastic versions, as the SIS and the SEIR model \[20, 22, 23\]. With no inclusion of spatial variables, they are often considered as deterministic mean field models, based on the chemical “mass action” principle.

In this work, we considered epidemic processes as a result from the action of a mean field and the interaction among the closest individuals (local interaction). To promote the infection by the contact between infected individuals and susceptibles, a stochastic term is added to the deterministic SIRS model. Therefore, the transition probabilities per unit of time became

\[ w_{R \rightarrow S} = m, \quad (33) \]
\[ w_{S \rightarrow I} = \Gamma \frac{b}{N^\mu} S^{\mu - 1} I + \Lambda [1 - (1 - p_0)^n], \quad (34) \]
\[ w_{I \rightarrow R} = a. \quad (35) \]

The \( \Gamma \) and \( \Lambda \) parameters balance, the global (mean field) and the local (nearest neighbors) variables, respectively; the relation \( \Gamma + \Lambda = 1 \) is satisfied. The parameter \( p_0 \) is the probability for a susceptible to become infected due to a unique infected neighbor. Therefore, \( (1 - p_0)^n \) is the probability of no infection of a susceptible if it has \( n \) infected neighbors, thus \( 1 - (1 - p_0)^n \) is the probability of infection of a susceptible if it has \( n \) infected neighbors.
The standard infection rate \( b \), recovery rate \( a \), exponent \( \mu \) and the renewal rate \( m \) are positive \( O(1) \) parameters, and \( S(t) + I(t) + R(t) = N \), with \( dN/dt = 0 \). When the renewal parameter is non zero \( (m \neq 0) \), a continuous influx of susceptible rises up into the system, producing oscillations in the number of elements of the populational class \( C = \{S, I, R\} \). Therefore, fading recurrent epidemics may occur before it reaches the steady (endemic) state. The power \( \mu \) introduces a modification in the original SIR model that takes in account nonhomogeneous mixing of susceptible and infective.

When only the mean field interaction is considered, the Runge-Kutta method is enough to solve the SIRS model. However, the DMC method, besides to solve systems with local interactions, also supplies the stochastic dynamic one.

V. APPLICATION OF THE DMC TO THE SIRS MODEL

In this work we consider a square lattice of \( N = M \times M \) sites with \( M = 200 \). The initial condition for the system is set up by randomly distributing \( I_0 \) infectives on the lattice \( (N >> I_0) \) and the remaining sites occupied by \( S_0 = N - I_0 \) susceptibles; therefore, \( R_0 = 0 \). The simulation develops systematically by choosing one site of the lattice at a random at a time. Depending on its status (susceptible, infected or recovered), a trial to go to another status is done through a set of transition probabilities given by \[33-35\], properly updating the populational class \( C \). If the transition is successful, the system is now in a new state, and so we assign a time delay to this transition. We repeat the process until the system reaches the steady state.

In order to construct a hierarchical process, we set the probability of transition \( T^*_{k,\alpha} \), at the MCS \( k \), for a particular event \( \alpha \) (\( S\rightarrow I \), \( I\rightarrow R \), or \( R\rightarrow S \), in our case), in accord with \[14\], as follows:

\[
T^*_{k,\alpha} = \frac{w_{\alpha}}{w_{\text{max}}},
\]

where \( w_{\alpha} \in \mathcal{P} = \{w_{S\rightarrow I}, w_{I\rightarrow R}, w_{R\rightarrow S}\} \) is the transition probability per unit of time for the event \( \alpha \), and \( w_{\text{max}} = \sup \mathcal{P} \). Thus, each particular trial is gauged according to a balance of rates, producing a hierarchical sequence of events. Operationally, we compare \( T^*_{k,\alpha} \) against a random number, \( 0 \leq R_1 \leq 1 \), taken from a uniform distribution. When \( R_1 > T^*_{k,\alpha} \), we reject the new state; otherwise accept it and calculate an incremental random time \( \Delta t^g_k \) from \[10\], with \( q = 1 \), as follows: \( \Delta t^{RS}_k = \frac{f^k_{S\rightarrow I}}{r^k_{S\rightarrow R}} \), or, \( \Delta t^{SI}_k = \frac{f^k_{I\rightarrow R}}{r^k_{I\rightarrow S}} \), or, \( \Delta t^{IR}_k = \frac{f^k_{R\rightarrow S}}{r^k_{R\rightarrow I}} \), where
\[ f^k_+ = \frac{n^k_+}{N_k}, \quad f^k_- = \frac{n^k_-}{N_k}, \quad f^k_{S^+} = \frac{n^k_{S^+}}{N_k}, \quad I^\dagger = S, \quad \text{and} \quad S^\dagger = R. \]

The numbers: \( n^k_+, n^k_-, \) and \( n^k_{S^+}, \) are numbers of events that increase \( I, \) decrease \( I \) and increase \( S, \) respectively, at the time \( t_k. \)

The number \( N_k = \sum_e n^k_e \) is the total number of events, and the rates are:

\[ r^R_S k = w_{R \rightarrow S} = m, \]
\[ r^S_I k = \Gamma b N \mu S \mu - 1 I + \Lambda < [1 - (1 - p_0)^n] > j_k, \]
\[ r^R_I k = w_{I \rightarrow R} = a. \]

The average \(<> j_k \) was estimated doing the sum of all local interaction terms over the system configuration \( j_k, \) sweeping only the susceptible individuals. Overall sum and search of \( w_{\text{max}} \), was in fact done only once, at the beginning of the simulation, after that we updated tables. We accumulated the number of events to obtain the factors, \( f^k_\alpha, \) in two ways: first, over each 100 MCS; thus, each new time interval was determined using the former calculated factor, except in the first 100 MCS, in which we progressively calculated the factors. Second way, we let the number of events progressively increase, and thus, calculated the factors at each step. As the results agreed for both approaches, we adopted the second one because the averages converged faster.

The figures, 1 and 2, show the temporal evolution of \( S(t), I(t) \) and \( R(t) \) for SIR and SIRS models respectively. Continuous lines represent numerical (fourth-order Runge-Kutta) checking solutions, and open circles correspond to the DMC simulation. Accuracies of the numerical solutions were checked using the steady state exact solution and the estimate of the errors were less than 0.1\%. The results, shown in these figures, with respect to the DMC simulation correspond to an average of 20 independent trajectories, a number sufficient to produce soft curves and illustrate the agreement with the checking solutions.

We introduce now the local term, with the weight \( \Lambda, \) and the variable \( n \) as an integer in the interval from \( n = 0 \) up to 8, since first and second nearest infected neighbors are indistinguishably considered for each susceptible. From a computational point of view, the main consequence of introducing space-dependent variables is that the Runge-Kutta method is no longer applicable to the resulting model. To check the self-consistency of the approach we integrate numerically (21-23), using the Stochastic Euler method described in Section II; we calculated the \( S, I \) and \( R \) quantities with iterations and chose the rates randomly as in the MC procedure. MC solutions were checked with this method, showing excellent agreement [11], less then 1\% of difference, results not shown. The time evolution (number of infective) shown in Figure 3 correspond to \( \Lambda = 0.1, 0.5 \) and 0.9, and \( p_0 = 0.1. \) Note that increasing \( \Lambda \) the epidemic severity reduces. Therefore, those epidemic outbreak mechanisms
involving only local contacts are less efficient than those whose propagation is due to some wider-range mechanisms. Note also, that for larger $\Lambda$ the second peak of the curve displaces significantly to the right. The establishment of a protecting shield (herd immunity effect) may explain this effect. Depending on local contact probability, $(1 - (1 - p_0)^n)$, the size of the removal class interferes essentially in the infection mechanism because the number of infectives of the neighborhood (shield effect) determines the infective character of the neighborhood of one susceptible. Figure 4 illustrates graphically the shield effect.

VI. CONCLUSIONS

In this work we examined and applied the Dynamical Monte Carlo method to the epidemic $SIRS$ model. We showed that, once established the hierarchy and the relationship between Monte Carlo step and real time, we simulate the dynamic aspects of the system, including properties out of the equilibrium. Therefore, we can use the power and the generality of the Monte Carlo simulation to obtain the temporal evolution of deterministic or stochastic systems.

We emphasize that, here, are not required uncorrelated events as they were in the reference [17]. The results for independent runs need to be uncorrelated, so we can properly use the averages obtained for each time $t$ to represent the physical quantities of the process. In order to do this we use a local equilibrium hypothesis, what may be at first glance restrictive. However we may even reduce the time observation enough, for the system does not have time to leave some metastable states, say order of the lifetime $\tau_i$; we can so obtain the averaged quantities. We can obtain a good convergence to the ideal averages, in the practice of the simulation, by increasing the number of observations, i.e., the number of time experiments.

The system studied is sufficiently general to illustrate several aspects of the real-time evolution determined by Dynamical Monte Carlo simulation.

The authors gratefully acknowledge funding support from FAPESP Grant n. 00/11635-7 and 97/03575-0. The authors would also like to thank Drs. A. Caliri and M. C. Nonato for many stimulating discussions and suggestions.
Figure Captions

FIG. 1. *SIR* model. The figure shows the evolution of the number of susceptible *S*, infective *I* and recovered *R* with time *t*. The numerical values for the model parameters are \( r = 0.2, b = 0.8 \). There is a good agreement between the *MC* results (open circles) and solutions provided by Runge-Kutta method (line).

FIG. 2. *SIRS* model. The figure shows the time evolution of the *S*, *I*, *R*. The parameter values are \( r = 0.2, b = 0.8, m = 0.01 \) and \( \mu = 2 \). The error between the *MC* results (open circles) and Runge-Kutta calculations are less than 0.1%.

FIG. 3. In this figure, it is shown the effect of spatial variables for the *SIRS* model: the \( \Lambda \) and \( \Gamma \) parameters balance the local and global variables (\( \Lambda + \Gamma = 1 \)); the herd immunity effect increases with \( \Lambda \) and it is responsible for the displacement of the curve second peak to the right.

FIG. 4. The shield effect: a snapshot of the system evolution at \( t \approx 40 \), when \( S = 19400 \) (yellow surface), \( R = 19200 \) (black) and \( I = 1400 \) (red spots) for \( \Lambda = 0.9 \).
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FIGURE 1

Time (days)

I(t) x 10^3

S(t)

I(t)

R(t)

Runge-Kutta

MC
FIGURE 2

![Graphs showing S(t)×10^3, R(t)×10^3, and I(t)×10^3 over time (days). The graphs compare Runge-Kutta and MC methods.](image-url)
FIGURE 3

$I(t) \times 10^{-3}$ vs. Time (days)

- $\Lambda = 0.1$
- $\Lambda = 0.5$
- $\Lambda = 0.9$
