Critical behavior of nonequilibrium models in short-time Monte Carlo simulations

Roberto da Silva*
Departamento de Informática Teórica, Instituto de Informática, Universidade Federal do Rio Grande do Sul, Av. Bento Gonçalves 9500, CEP 90570-051, Porto Alegre, RS, Brazil

Ronald Dickman†
Departamento de Física, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, Av. Antônio Carlos 6627, CEP 30123-970, Belo Horizonte, Minas Gerais, Brazil

J. R. Drugowich de Felício‡
Departamento de Física e Matemática, Faculdade de Filosofia, Ciências e Letras, Universidade de São Paulo, Av. Bandeirantes 3900, CEP 014040-901, Ribeirão Preto, SP, Brazil
(Received 8 July 2004; published 3 December 2004)

We analyze two alternative methods for determining the dynamic critical exponent z of the contact process and the Domany-Kinzel cellular automaton in Monte Carlo simulations. One method employs mixed initial conditions, as proposed for magnetic models [Phys. Lett. A **298**, 325 (2002)]; the other is based on the growth of the moment ratio $m(t)=\langle\rho^2(t)\rangle/\langle\rho(t)\rangle^2$ starting with all sites occupied. The methods provide reliable estimates for z using the short-time dynamics of the process. Estimates of $\nu_\parallel$ are obtained using a method suggested by Grassberger.

DOI: 10.1103/PhysRevE.70.067701 PACS number(s): 05.10.−a, 64.60.Ht, 02.50.−r

I. INTRODUCTION

The dynamics of spin models quenched from high temperature to the critical point is a subject of considerable current interest, because the initial phase of the relaxation (the so-called short-time dynamics) carries important information about static and dynamic critical behavior [1]. Using a phenomenological renormalization group analysis, Janssen, Schaub, and Schmittmann [2] demonstrated the following scaling law for the order parameter at the critical point:

$$\langle M\rangle(t) \sim m_0 t^{\theta}, \tag{1}$$

characterized by the new critical exponent θ. (Here $\langle\cdot\rangle$ denotes an average over initial configurations consistent with initial magnetization m_0, and over the noise in the stochastic dynamics.) Relation (1) holds for times $t<t_{\max}\sim m_0^{-z/x_0}$, where z is the dynamic exponent and x_0 its anomalous dimension. The "critical initial slip" described by Eq. (1) emerges from an initially disordered state, and is characteristic of a stochastic, far from equilibrium relaxation process. This approach also offers a way to determine the *static* critical exponents, since the scaling argument used to deduce Eq. (1) can also be applied to higher moments of the order parameter, yielding

$$\langle M^k\rangle(t,m_0) = L^{-k\beta/\nu}\langle M^k\rangle(L^{-z}t, L^{x_0}m_0). \tag{2}$$

Models with absorbing states exhibit scaling behavior at the critical point marking the transition between active and absorbing stationary states, even though the stationary state is not given by a Boltzmann distribution [3,4]. The order parameter is the activity density $\rho\geqslant 0$, given by $\rho(t)=L^{-d}\Sigma_{i=1}^{L^d}\sigma_i\geqslant 0$, where $\sigma_i=1(0)$ corresponds to the presence (absence) of activity at site i (d is the dimensionality of the system). (Activity at site is commonly associated with the presence of a "particle.") For such models the following scaling law [3] has been conjectured:

$$\rho(t) \sim t^{-\beta/\nu_\parallel} f((p-p_c)t^{1/\nu_\parallel}, t^{d/z}/N, \rho_0 t^{\beta/\nu_\parallel+\theta}), \tag{3}$$

where ρ_0 is the initial density, p is a temperaturelike control parameter, p_c is its critical value, and $N=L^d$ is the number of sites. The exponent β is associated with the dependence of the stationary value of ρ on the control parameter: $\rho\sim(p-p_c)^{\beta}$, while $\nu_\parallel$ and $\nu_\perp$ are the critical exponents associated with the correlation time ($\xi_\parallel\sim|p-p_c|^{-\nu_\parallel}$) and correlation length ($\xi_\perp\sim|p-p_c|^{-\nu_\perp}$). Given the defining relation $\xi_\parallel\sim\xi_\perp^z$, the dynamic exponent $z=\nu_\parallel/\nu_\perp$. Letting $p\to p_c$ and $N\to\infty$, we expect the scaling function f in Eq. (3) to have the property

$$f[0,0,u] = \begin{cases} u, & u\simeq 0 \\ C, & u\to\infty \end{cases}, \tag{4}$$

where C is a constant.

In a realization of the process at criticality ($p=p_c$) beginning with a completely filled lattice ($\rho_0=1$), the activity density decays via the power law $\rho(t)\sim t^{-\beta/\nu_\parallel}$ for $t\ll L^z$. On the other hand, in realizations starting with only a single particle or active site (spreading process), the average number of particles increases with time: $\rho(t)\sim t^{\eta}$, where $\eta=(d\nu_\perp-2\beta)/\nu_\parallel$.

An interesting crossover phenomenon in the evolution of $\rho(t)$, between the initial increase ($\sim t^{\eta}$) asymptotic decay ($\sim t^{-\beta/\nu_\parallel}$), emerges in a critical spreading process with low

*Corresponding author. Electronic address: rdasilva@inf.ufrgs.br
†Electronic address: dickman@fisica.ufmg.br
‡Electronic address: drugo@usp.br

initial particle density. The crossover time t_c is related to the initial density ρ_0 via

$$t_c \sim \rho_0^{-1/(\beta/\nu_\parallel+\eta)}. \tag{5}$$

A process starting with a single particle ($\rho_0=1/L$) corresponds to $\rho_0 \to 0$ for large lattices, so that t_c diverges and the spreading regime $\rho(t) \sim t^\eta$ extends over the entire evolution. For correlated initial conditions the evolution follows a power law intermediate between the extreme cases mentioned above [5].

A method for determining the critical exponent z proposed in the context of the short-time behavior of magnetic models [6], suggests that we consider the function

$$F_2(t) = \frac{\langle \rho \rangle_{\rho_0=1/L^d}}{\langle \rho \rangle^2_{\rho_0=1}} \tag{6}$$

which has the asymptotic behavior $F_2(t) \sim t^{d\nu_\perp/\nu_\parallel} = t^{d/z}$. Thus we can obtain z by analyzing short-time simulation results with mixed initial conditions.

In this paper we employ this approach to calculate z for the contact process (CP) and the Domany-Kinzel cellular automaton (DK), both known to belong to the universality class of directed percolation [4]. We note that in the literature on absorbing-state phase transitions z is commonly used to denote the exponent governing the growth of the mean-square distance of particles from the original seed, in spreading simulations. To avoid confusion we denote the latter exponent as Z, so that $R^2 \sim t^Z$. The dynamic exponent is then related to the spreading exponent via $z=2/Z$.

A method to estimate the exponent $\nu_\parallel$ was suggested by Grassberger [7], who used the relation

$$D(t) \equiv \left. \frac{\partial \ln \rho}{\partial p} \right|_{p=p_c} \sim t^{1/\nu z}, \tag{7}$$

where in a simulation the derivative is evaluated numerically via

$$D(t) = \frac{1}{2h} \ln\left(\frac{\rho(p_c+h)}{\rho(p_c-h)} \right), \tag{8}$$

which evidently requires data for values of p slightly off criticality. In this context a reweighting scheme that permits one to study various values of p in the same simulation is particularly convenient [8].

In the following section we present details on the models and our simulation technique. In Sec. III we report and analyze the simulation results, and in Sec. IV present our conclusions.

II. MODELS AND SIMULATION METHOD

The contact process was introduced by Harris as a toy model of epidemic propagation [9]. It evolves in continuous time. Denoting the number of occupied nearest neighbors of site i by $n_i = \Sigma_{j \in \langle i \rangle} \sigma_j$, where $\langle i \rangle$ denotes the set of nearest neighbors of site i, the transition rates are

$$w(0 \to 1; n) = \frac{\lambda n}{2d} \text{ (creation)},$$

$$w(1 \to 0; n) = 1 \text{ (annihilation)}. \tag{9}$$

The model suffers a continuous transition at a critical value λ_c; in one dimension $\lambda_c = 3.297\,85(8)$ [4].

As described in Refs. [4,8], our simulations employ a list of occupied sites and sample reweighting to improve efficiency. Since the choice of sites is restricted to the occupied set, the time increment Δt associated with each event (annihilation or creation) is $1/N_p$, where N_p is the number of occupied sites immediately prior to the event. A given realization of the process ends at a predetermined maximum time, or when all particles have been annihilated. Reweighting is used to study the effects of window size h in Eq. (8), in determining $\nu_\parallel$ for the CP, using $\rho_0=1/L$.

The Domany Kinzel (DK) cellular automaton is a discrete-time process exhibiting a phase transition between an active and an absorbing phase of the same kind as in the CP [10]. Each site of the lattice can be in one of two states, $\sigma_i=1$ (active) or $\sigma_i=0$ (inactive). The transition probabilities for $\sigma_i(t)$ given the values of its neighbors $\sigma_{\pm 1}(t-1)$ are: $P(1|0,0)=0$, $P(1|1,0)=P(1|0,1)=p$, and $P(1|1,1)=q$. This model has a line of continuous phase transitions separating the active and absorbing phases in the p-q plane. For $q=p(2-p)$ the DK model is equivalent to bond directed percolation (DP), with $p_c=0.644\,700$. The critical behavior along the transition line falls in the DP universality class, with the exception of the point $p=1/2$, $q=1$, corresponding to so-called compact DP [10,11].

III. RESULTS

We study the time-dependent order-parameter moments $\langle \rho^k(t) \rangle$ in Monte Carlo simulations of the one-dimensional DK and CP, obtaining time series $\langle \rho(t) \rangle_{\rho_0=1/L}$ and $\langle \rho(t) \rangle_{\rho_0=1}$, for the two initial conditions described above. Note that these quantities are evaluated over the sample of realizations surviving at time t. They then are combined to yield F_2 defined in Eq. (6).

In these simulations we used systems of size $L=4096$ sites in $N_s=50\,000$ independent realizations, extending to $t_{\max}=1000$. The evolution of F_2 for the two models is shown in Fig. 1.

To determine z we divide the evolution into subintervals equally spaced in $\ln t$. (This avoids placing an unduly large weight on longer times, as would occur if each integer time were treated as a separate data point.) Analyzing our results, we find $z=1.581(1)$ for both the CP and the DK cellular automaton. These results are in agreement with previous results on DP [$z=1.580\,745(10)$ [12]] obtained via a low-density expansion, and on the CP [$z=1.58077(2)$] from exact diagonalization of the master equation [13].

The local slope z_t can be estimated from a least-squares linear fit to the data shown in Fig. 1; it is plotted versus t_a^{-1}, t_a being the geometric mean of the t values over the subintervals. The exponents z_t and $\nu_\parallel$ are similarly obtained, and an extrapolation $t_a^{-1} \to 0$ is performed. In Fig. 2 we show this extrapolation for the CP and DK, showing convergence towards $z \approx 1.581$.

The ratio

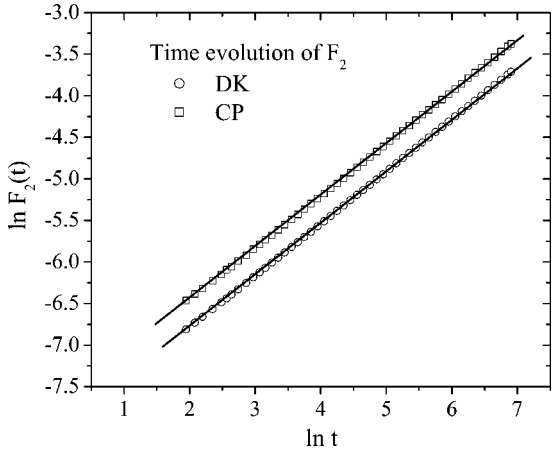

FIG. 1. Time evolution of the F_2 in the CP and the DK cellular automaton.

$$m(t) = \frac{\langle \rho^2(t) \rangle_{\rho_0=1}}{\langle \rho(t) \rangle^2_{\rho_0=1}} \tag{10}$$

converges to the expected value for models in the DP universality class, $m_\infty \simeq 1.174$ for DP in $(1+1)$ dimensions [14]. At short times, $m-1=\mathrm{var}(\rho)/\langle\rho\rangle^2$ increases as a power law. The associated exponent is found by noting that

$$\chi \equiv L^d \,\mathrm{var}(\rho) \sim t^{\phi} g[(p-p_c)^{\nu_\parallel} t] \overset{t\to\infty}{\to} (p-p_c)^{\gamma} \tag{11}$$

so that $g(x) \sim x^{-\gamma/\nu_\parallel}$ for large x. Observing that $\phi = \gamma/\nu_\parallel = (d\nu_\perp - 2\beta)/\nu_\parallel$, and that $\langle\rho\rangle \sim t^{-\beta/\nu_\parallel}$, we expect $m-1 \sim t^{d/z}$. Our simulations of the CP ($L=5000$, $N_s=10\,000$) confirm the anticipated power law, and yield $z=1.577(7)$.

In the determination of $\nu_\parallel$ via Eq. (8), we used $t_{\max}=2980$, and a total of the $N_s=10\,000$ realizations. Figure 3 shows the nuerical derivative $D(t)$. For the DK cellular automaton, using systems of $L=8192$ sites and $\Delta h=0.0002$, we obtain $\nu_\parallel=1.731(9)$, by extrapolating the effective exponent $\nu_\parallel(t)$ to $t\to\infty$, consistent with the expected value $\nu_\parallel = 1.733\,847(6)$ [4,12]. We find that the result is quite sensitive to the interval Δh used in the analysis. For example, using $\Delta h=0.002$ we obtain $\nu_\parallel=1.65$, far smaller than the accepted value.

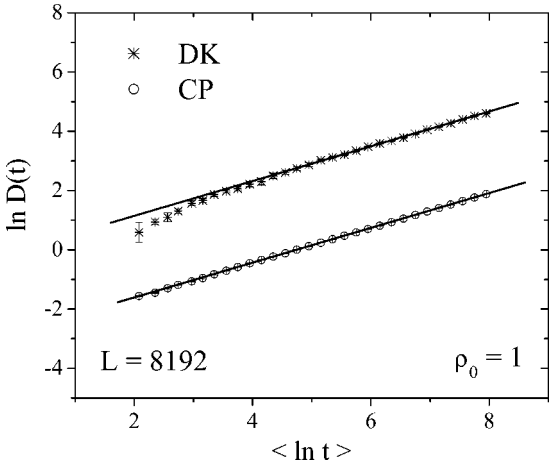

FIG. 3. Plot of time evolution of $D(t)$, Eq. (8), in the CP and the DK cellular automaton.

In the implementation of Eq. (8) to the CP, we used the reweighting method proposed in Ref. [8]. Systems of 8192 sites are again used. The sample of realizations generated at λ_c is reweighted for nearby values, $\lambda_c \pm n\delta$, where n is an integer, so that $\Delta h = 2n\delta$. As before, we analyze the local slope $\nu_\parallel(t)$ as a function of $1/t$. The last ten points of each curve are extrapolated to $1/t \to 0$ to estimate $\nu_\parallel$. For $\Delta h = 0.0002$ the value found via extrapolation is $\nu_\parallel = 1.734(8)$, in agreement with the accepted value. The influence of Δh on the estimate for $\nu_\parallel$ is shown in Fig. 4, showing convergence to the expected value of 1.734.

IV. SUMMARY AND CONCLUSIONS

We apply several simulation methods based on analysis of short-time behavior to determine the critical exponents z and $\nu_\parallel$ in models exhibiting a continuous phase transition to an

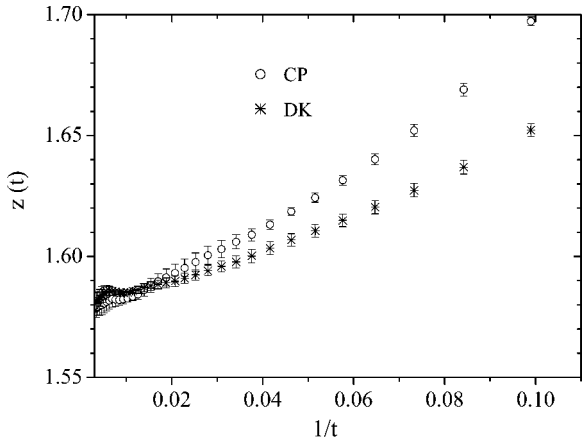

FIG. 2. Effective exponent $z(t)$ vs $1/t$ in the CP and the DK cellular automaton. Note the convergence to $z \approx 1.58$ in both cases.

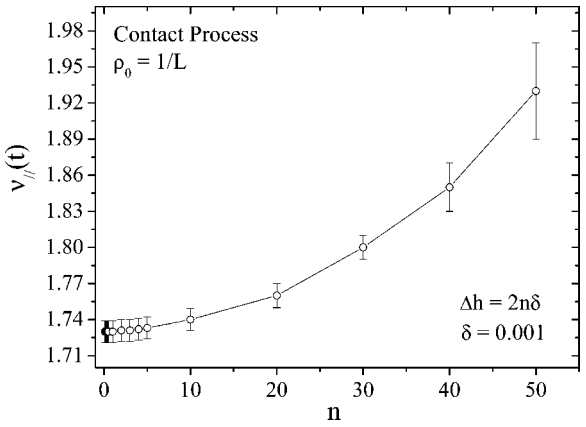

FIG. 4. Plot of $\nu_\parallel$ in the CP as a function of n, where $\Delta h = 2n\delta$.

absorbing state. The methods involve the ratios $F_2(t) = \langle \rho \rangle_{\rho_0=1/L^d} / \langle \rho \rangle^2_{\rho_0=1}$ and $m(t) = \langle \rho(t)^2 \rangle_{\rho_0=1} / \langle \rho(t) \rangle^2_{\rho_0=1}$, as well as the derivative $D(t)$ defined in Eq. (7). We find these methods to be quite useful determining critical exponents, since they yield estimates in good agreement with accepted values for the CP and the DK cellular automaton, using relatively short simulations. We note that in the implementation of Eq. (7) to determine $\nu_\parallel$, care must be taken to use an increment h that is sufficiently small. One should in fact study several values of h (which is quite feasible using sample reweighting), to identify the value below which the result no longer depends on increment size.

We believe that the methods investigated here will be useful in the analysis of other models with absorbing states, in particular, in establishing the universality class using short-time simulations, which are typically less computationally demanding than studies of the stationary process.

ACKNOWLEDGMENTS

R. da Silva thanks Ricardo D. da Silva (in memoriam), for all words of incentive in his career and life. The authors thank CNPq, Brazil, for financial support.

[1] T. Tomé, J. Phys. A **36**, 6683 (2003).
[2] H. K. Janssen, B. Shaub, and B. Schmitmann, Z. Phys. B: Condens. Matter **73**, 539 (1989).
[3] H. Hinrichsen, Adv. Phys. **49**, 815 (2000).
[4] J. Marro and R. Dickman, *Nonequilibrium Phase Transitions in Lattice Models* (Cambridge University Press, Cambridge, England, 1999).
[5] H. Hinrichsen and G. Ódor, Phys. Rev. E **58**, 311 (1998).
[6] R. da Silva, N. A. Alves, and J. R. Drugowich de Felício, Phys. Lett. A **298**, 325 (2002).
[7] P. Grassberger and Y. Zhang, Physica A **224**, 169 (1996).
[8] R. Dickman, Phys. Rev. E **60**, R2441 (1999).
[9] T. M. Liggett, *Interacting Particle Systems* (Springer-Verlag, New York, 1984).
[10] E. Domany and W. Kinzel, Phys. Rev. Lett. **53**, 311 (1984).
[11] J. W. Essam, J. Phys. A **22**, 4927 (1989).
[12] I. Jensen, J. Phys. A **32**, 5233 (1999).
[13] J. R. G. de Mendonça, J. Phys. A **32**, L467 (1999).
[14] R. Dickman and J. Kamphorst Leal da Silva, Phys. Rev. E **58**, 4266 (1998).