

How to simulate the quasistationary state

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For a large class of processes with an absorbing state, statistical properties of the surviving sample attain time-independent values in the quasistationary (QS) regime. We propose a practical simulation method for studying quasistationary properties, based on the equation of motion governing the QS distribution. In applications to the contact process, the method is shown to reproduce exact results (for the process on a complete graph) and known scaling behavior to high precision. At the critical point, our method is about an order of magnitude more efficient than conventional simulation.

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I. INTRODUCTION

Stochastic processes with an absorbing state arise frequently in statistical physics [1,2], epidemiology [3], and related fields. In autocatalytic processes (in lasers, chemical reactions, or surface catalysis, for example), and population models, a population of $n \geq 0$ individuals goes extinct when the absorbing state, $n=0$, is reached. Phase transitions to an absorbing state in spatially extended systems, exemplified by the contact process [4,5], are currently of great interest in connection with self-organized criticality [6], the transition to turbulence [7], and issues of universality in nonequilibrium critical phenomena [8–10]. Such models are frequently studied using deterministic mean-field equations, Monte Carlo simulation, and renormalization group analyses.

It is desirable to develop additional methods for studying processes with absorbing states. In this work we study models that admit an active (nonabsorbing) stationary state in the infinite-size limit, but which always, for a finite system size, end up in the absorbing state. The *quasistationary* (QS) distribution for such a system provides a wealth of information about its behavior. (In fact, simulations of “stationary” properties of lattice models with an absorbing state actually study the quasistationary regime, given that the only true stationary state for a finite system is the absorbing one.)

In particular, it would be valuable to have a simulation method that yields quasistationary properties directly. Currently available methods involve a somewhat complicated procedure for determining QS properties: a large sample of independent realizations are performed, and the mean $\phi(t)$ of some property (for example, the order parameter) is evaluated over the surviving realizations at time t . At short times $\phi(t)$ exhibits a transient as it relaxes toward the QS regime; at long times it fluctuates wildly as the surviving sample decays. Normally one is able to identify an intermediate regime free of transients and with limited fluctuations, which can be used to estimate the QS value of ϕ . This method requires careful scrutiny of the data and is not always free of ambiguity [11].

A number of strategies have been devised to circumvent the difficulties associated with simulating models exhibiting absorbing states. One involves replacing the absorbing state with a *reflecting* boundary in configuration space [12]. In another approach the activity is fixed at a nonzero value, in a “constant coverage” simulation [13] or a “conserved” version of the model [14]. If one includes a weak external source of activity, h , the zero-activity state is no longer absorbing, but it is possible to obtain information on critical behavior by analyzing scaling properties as $h \rightarrow 0$ [11]. A further possibility is to clone surviving realizations of the process, enriching the sample to compensate for attrition as the survival probability decays [15]. While all of these approaches are useful, none affords direct, unbiased sampling of the QS state of the original process.

For models without spatial structure, such as uniformly distributed populations or well stirred chemical reactors, the full QS distribution can be found from the master equation, via recurrence relations or an iterative scheme [16,17]. In models with spatial structure, typified by nearest-neighbor interactions on a lattice, mean-field-like approximations to the QS distribution have been derived, but descriptions in terms of one or a few random variables cannot capture critical fluctuations. The simulation method developed here does not suffer from this limitation. It provides a sampling of the QS probability distribution just as conventional Monte Carlo simulation does for the equilibrium distribution. In the following section we discuss the basis of our method. Then in Sec. III we show how it may be applied to the contact process on a complete graph, for which exact (numerical) results are available for QS properties. Results for the contact process on a ring are presented in Sec. IV. We summarize our findings in Sec. V.

II. BACKGROUND

We begin by reviewing the definition of the quasistationary distribution. Consider a continuous-time Markov process X_t taking values $n=0, 1, 2, \dots, S$, with the state $n=0$ absorbing. We use $p_n(t)$ to denote the probability that $X_t=n$, given some initial state X_0 . The survival probability $P_s(t) = \sum_{n \geq 1} p_n(t)$ is the probability that the process has not become trapped in the absorbing state up to time t . We suppose that

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as $t \rightarrow \infty$ the p_n , normalized by the survival probability $P_s(t)$, attain a time-independent form. The quasistationary distribution \bar{p}_n is then defined via

$$\bar{p}_n = \lim_{t \rightarrow \infty} \frac{p_n(t)}{P_s(t)} \quad (n \geq 1), \quad (1)$$

with $\bar{p}_0 \equiv 0$. The QS distribution is normalized so

$$\sum_{n \geq 1} \bar{p}_n = 1. \quad (2)$$

We now discuss the theoretical basis for our simulation method. The QS distribution is the stationary solution to the following equation of motion [16] (for $n > 0$):

$$\frac{dq_n}{dt} = -w_n q_n + r_n + r_0 q_n, \quad (3)$$

where $w_n = \sum_m w_{m,n}$ is the total rate of transitions out of state n , and $r_n = \sum_m w_{n,m} q_m$ is the flux of probability into this state. To see this, consider the master equation [Eq. (3) without the final term] in the QS regime. Substituting $q_n(t) = P_s(t) \bar{p}_n$, and noting that in the QS regime $dP_s/dt = -\bar{r}_0 = -P_s \sum_m w_{0,m} \bar{p}_m$, we see that the right-hand side of Eq. (3) is identically zero if $q_n = \bar{p}_n$ for $n \geq 1$. The final term in Eq. (3) represents a redistribution of the probability r_0 (transferred to the absorbing state in the original master equation), to the nonabsorbing subspace. Each nonabsorbing state receives a share equal to its probability.

Although Eq. (3) is not a master equation (it is nonlinear in the probabilities q_n), it does suggest a simulation scheme for sampling the QS distribution. In a Monte Carlo simulation one generates a set of realizations of a stochastic process. In what follows we call a simulation of the original process X_t (possessing an absorbing state) a *conventional* simulation. Our goal is to define a related process X_t^* , whose *stationary* probability distribution is the *quasistationary* distribution of X_t . (Note that in order to have a nontrivial stationary distribution, X_t^* cannot possess an absorbing state.) The probability distribution of X_t^* is governed by Eq. (3), which implies that for $n > 0$ (i.e., away from the absorbing state), the evolution of X_t^* is identical to that of X_t . [Since Eq. (3) holds for $n > 0$, the process X_t^* must begin in a nonabsorbing state.] When X_t enters the absorbing state, however, X_t^* instead jumps to a nonabsorbing one, and then resumes its “usual” evolution (with the same transition probabilities as X_t), until such time as another visit to the absorbing state is imminent.

A subtle aspect of Eq. (3) is that the distribution q_n is used to determine the value of X_t^* when X_t visits the absorbing state. Although one has no prior knowledge of q_n (or its long-time limit, the QS distribution \bar{p}_n), one can, in a simulation, use the history X_s^* ($0 < s \leq t$) up to time t , to estimate the q_n . This is done by saving (and periodically updating) a sample n_1, n_2, \dots, n_M of the states visited. [If the state space is characterized by a small set of variables, one may instead accumulate a histogram $H(n)$ giving the time spent in state n .] As the evolution progresses, X_s^* will visit states according to the QS distribution. We therefore update the sample $\{n_1, n_2, \dots, n_M\}$ by periodically replacing one of these con-

figurations with the current one. In this way the distribution for the process X_t^* (and the sample drawn from it), will converge to the QS distribution [i.e., the stationary solution of Eq. (3)] at long times. Summarizing, the simulation process X_t^* has the same dynamics as X_t , except that when a transition to the absorbing state is imminent, X_t^* is placed in a nonabsorbing state, selected at random from a sample over the history of the realization. In effect, the nonlinear term in Eq. (3) is represented as a *memory* in the simulation.

III. CONTACT PROCESS ON A COMPLETE GRAPH

To explain how our method works in practice, we detail its application to the *contact process* (CP) [4,5,8]. In the CP, each site i of a lattice is either occupied [$\sigma_i(t)=1$] or vacant [$\sigma_i(t)=0$]. Transitions from $\sigma_i=1$ to 0 occur at a rate of unity, independent of the neighboring sites. The reverse transition can only occur if at least one neighbor is occupied: the transition from $\sigma_i=0$ to 1 occurs at rate λr , where r is the fraction of nearest neighbors of site i that are occupied; thus the state $\sigma_i=0$ for all i is absorbing. (λ is a control parameter governing the rate of spread of activity.) The order parameter ρ is the fraction of occupied sites.

To begin we study the contact process on a *complete graph* (CPCG), in which the rate for a vacant site to turn occupied is λ times the fraction of all sites that are occupied, rather than the fraction of nearest neighbors. Since each site interacts equally with all others, all pairs of sites are neighbors, defining a complete graph. (The critical value in this case is $\lambda_c=1$; the stationary value of ρ is zero for $\lambda < \lambda_c$.) The state of the process is specified by a single variable n : the number of occupied sites. This is a one-step process with nonzero transition rates

$$W_{n-1,n} = n, \quad (4)$$

$$W_{n+1,n} = \lambda \frac{n}{L} (L-n) \quad (5)$$

on a graph of L sites. In Ref. [16] the exact QS distribution for the CPCG is obtained via a set of recurrence relations.

We simulate the quasistationary state of the CPCG by realizing the process corresponding to the transition rates of Eqs. (4) and (5) and maintaining a list of $M=10^4$ states. Each time a (nonabsorbing) state is visited, we update the list with probability $\gamma \Delta t$ where $\Delta t=1/w_n$ is the mean duration of this state. Whenever a transition to the absorbing state ($n=0$) is generated, we instead select a state from the list. The results for a system of 100 sites, using $\gamma=0.5$, are shown in Fig. 1, illustrating excellent agreement with the exact QS distribution obtained in Ref. [16]. The simulation result is in good agreement with the exact result even for $\lambda=0.1$, deep in the subcritical regime, in which the lifetime of the original process is very short.

IV. CONTACT PROCESS ON A RING

We turn to the one-dimensional contact process (i.e, the model defined in Sec. III on a ring of L sites). Although no

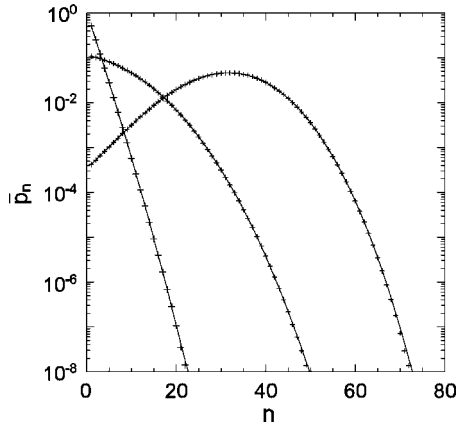


FIG. 1. QS distributions via recurrence relations (solid lines) and QS simulation (symbols) for the CP on a complete graph of 100 sites. $\lambda=0.5, 1.0$, and 1.5 (left to right).

exact results are available, the model has been studied intensively via series expansion and Monte Carlo simulation. The model has attracted much interest as a prototype of a non-equilibrium critical point, a simple representative of the directed percolation (DP) universality class. Since its scaling properties have been discussed extensively [8–10] we review them only briefly. The best estimate for the critical point in one dimension is $\lambda_c=3.297\ 848(20)$, as determined via series analysis [18]. As the critical point is approached, the correlation length ξ and correlation time τ diverge, following $\xi \propto |\Delta|^{-\nu_\perp}$ and $\tau \propto |\Delta|^{-\nu_\parallel}$, where $\Delta=\lambda-\lambda_c$ is the distance from the critical point. The order parameter (i.e., the fraction of active sites) scales as $\rho \propto \Delta^\beta$ for $\Delta > 0$. In simulations it is most convenient to study the size dependence of the lifetime and the order parameter at λ_c . The expected finite-size scaling behaviors are $\rho \propto L^{-\beta/\nu_\perp}$ and $\tau \propto L^{\nu_\parallel/\nu_\perp}$. In addition, the ratio $m = \langle \rho^2 \rangle / \langle \rho \rangle^2$ attains a universal value (characteristic of DP in 1+1 dimensions) at the critical point. This quantity is analogous to Binder's reduced fourth cumulant [19] at an equilibrium critical point: the curves $m(\lambda, L)$ for various L cross near λ_c . (Since the crossings approach λ_c as L increases, analysis of m represents an alternative method for determining λ_c , as discussed in [20]. Here however we simply use the series result for λ_c .)

In the QS simulations we use a list size $M=(2 \times 10^3) - 10^4$, depending on the lattice size. The process is simulated in runs of 10^8 or more time steps. As is usual, annihilation events are chosen with probability $1/(1+\lambda)$ and creation events with probability $\lambda/(1+\lambda)$. A site is chosen from a list of currently occupied sites, and, in the case of annihilation, is vacated, while, for creation events, a nearest-neighbor site is selected at random and, if it is currently vacant, it becomes occupied. The time increment associated with each event is $\Delta t = 1/N_{occ}$, where N_{occ} is the number of occupied sites just prior to the attempted transition [8].

In the initial phase of the evolution, the list of saved configurations is augmented whenever the time t increases by 1, until a list of M configurations is accumulated. From then on, we update the list (replacing a randomly selected entry with the current configuration), with a certain probability p_{rep} , whenever t advances by one unit. A given configuration

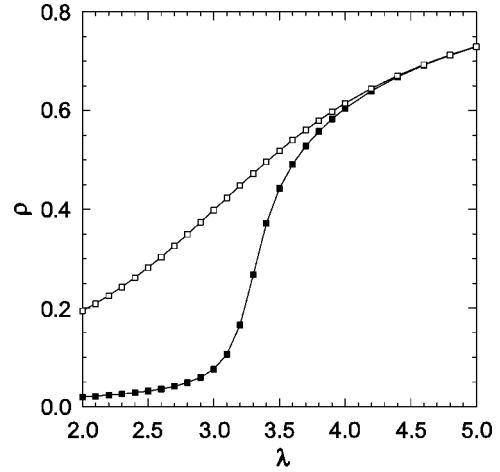


FIG. 2. Quasistationary density ρ in the one-dimensional CP. Open symbols, QS simulation, $L=20$; filled symbols, QS simulation, $L=200$. Solid lines represent results of conventional simulations.

therefore remains on the list for a mean time of M/p_{rep} . (Values of p_{rep} in the range $10^{-3}-10^{-2}$ are used; the results appear to be insensitive to the precise choice.)

Figure 2 shows that our method reproduces the order parameter ρ obtained via conventional simulations. In Fig. 3 the QS and conventional results for the moment ratio $m = \langle \rho^2 \rangle / \langle \rho \rangle^2$ are compared. As discussed in Ref. [16], the lifetime of the QS state is given by $\tau = 1/\bar{p}_1$. The lifetime obtained in QS simulations compares well with the lifetime obtained via conventional simulation [using $P_s \sim \exp(-t/\tau)$], as shown in Fig. 4. Detailed comparison shows that there is no significant difference between the QS and conventional simulation results. For $\lambda < 3$, conventional simulations are subject to relatively large uncertainties, since almost all realizations become trapped in the absorbing state before the quasistationary regime is attained. At the critical point, quasistationary simulations require about an order of magnitude less CPU time than conventional simulations, to achieve results of the same precision. (Below λ_c the savings are even

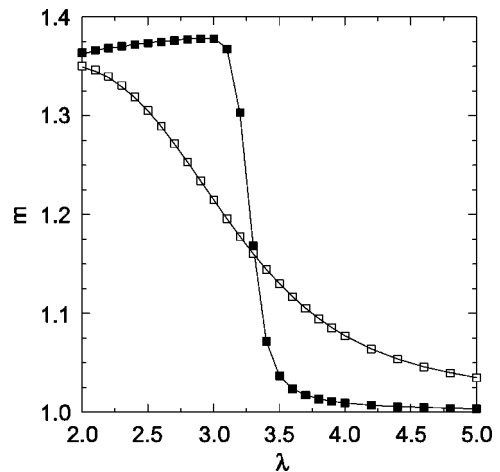


FIG. 3. Quasistationary moment ratio M in the one-dimensional CP. Symbols as in Fig. 2.

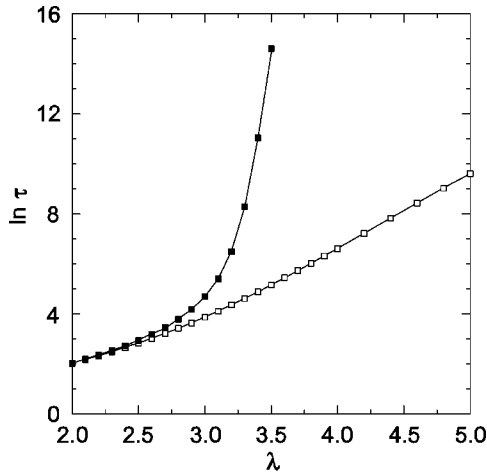


FIG. 4. Quasistationary lifetime τ in the one-dimensional CP. Symbols as in Fig. 2.

greater; well above λ_c the two methods are equally efficient, since visits to the absorbing state are extremely rare.)

As a further application of our method we study the critical CP ($\lambda_c=3.297\,848$) on rings of 20,40,80,...,1280 sites. We perform 50 realizations, each extending to 5×10^8 time steps. Results from the first 10^7 time steps (2×10^7 for $L=1280$) are discarded from the averages; convergence to the QS state occurs on a considerably shorter timescale. The studies reported here employed a list size $M=2000$ and replacement probability $p_{rep}=0.001$. In studies of the critical process on a lattice of 320 sites, we found no significant dependence of the results on varying p_{rep} between 0.01 and 0.001, or varying M between 100 and 2000. A small but significant decrease (0.2%) in the value for the order parameter appears when M is reduced to 20.

Our results confirm the estimate for the critical moment ratio $m_c=1.1736(2)$ obtained in Ref. [20] from simulations of systems of up to 320 sites. Based on our data for $L=80-1280$ we estimate $m_c=1.1736(1)$. Our estimates for the lifetime (Fig. 5) follow $\tau(\lambda_c, L) \sim L^{\nu_{\parallel}/\nu_{\perp}}$ to good precision; a fit to the data for $L=320, 640,$ and 1280 yields $\nu_{\parallel}/\nu_{\perp}=1.5815(10)$. For smaller sizes there are systematic corrections to this pure power law, as shown in the inset of Fig. 5. Observing that the magnitude of the correction decays proportional to $L^{-0.75}$, we fit (using a least-squares procedure), the following expression to the data for $L=20-1280$:

$$\ln \tau = \frac{\nu_{\parallel}}{\nu_{\perp}} \ln L + \frac{A}{L^{0.75}} + \text{const.} \quad (6)$$

The exponent ratio and the constant A are treated as adjustable parameters, yielding $A=0.20(4)$ and confirming the value quoted above for $\nu_{\parallel}/\nu_{\perp}$. The latter is consistent with the standard value of $1.5807(1)$ (from series analysis [21]), to within a statistical uncertainty of 0.06%.

Similarly, the QS simulation data for the order parameter $\rho(\lambda_c, L)$ follow the power-law $\rho \sim L^{-\beta/\nu_{\perp}}$ to good precision (Fig. 6); the data for the three largest sizes furnish $\beta/\nu_{\perp}=0.2528(3)$. Once again there are systematic corrections to

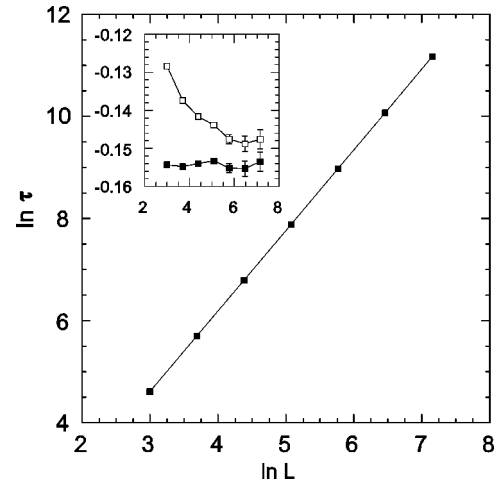


FIG. 5. Quasistationary lifetime τ vs system size L in the critical one-dimensional CP. The inset shows the deviation from the pure power law, $\tau \propto L^{1.5815}$ (open symbols), and from the power law with a correction to scaling term decaying as $L^{-0.75}$ (filled symbols, shifted vertically for visibility).

scaling for smaller system sizes. Allowing a correction to scaling term proportional to $L^{-0.75}$ as before, we obtain the best fit using

$$\ln \rho = -0.2528 \ln L + \frac{B}{L^{0.75}} + \text{const} \quad (7)$$

with $B=0.051(10)$. Compared with the standard value $\beta/\nu_{\perp}=0.252\,08(5)$ [21], our result overestimates the exponent ratio by 0.3(1)%. [A simple power-law fit to the data for $L=20-1280$ yields $\beta/\nu_{\perp}=0.2517(2)$.]

Summarizing, the QS simulation method yields results fully consistent with conventional simulation, and with established scaling properties, when applied to the contact pro-

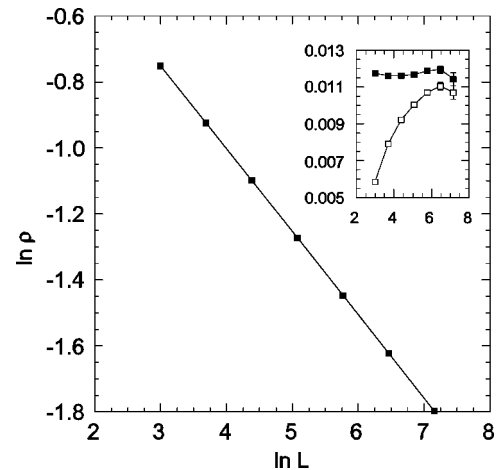


FIG. 6. Quasistationary order parameter ρ vs system size L in the critical one-dimensional CP. The inset shows the deviation from the pure power law, $\tau \propto L^{-0.2528}$ (open symbols), and from the power law with a correction to scaling term decaying as $L^{-0.75}$ (filled symbols, shifted vertically for visibility).

cess on a ring. Exponent and moment ratio values are reproduced to three significant figures or better.

It is interesting to compare the QS distribution with that obtained using a reflecting boundary at $n=0$, as was used in [12]. In the case of the CP on a complete graph the stationary distribution with a reflecting boundary (RB) is given in [16], where it is called the “pseudostationary” distribution. We find that for large systems, in the active phase (λ well above λ_c) the RB and QS distributions are essentially the same, but that nearer (and below) the transition the RB distribution yields a much higher probability for states near $n=1$ than does the QS. The reflecting boundary is equivalent to a modified process X_t^* which, when a visit to the absorbing state is imminent, is always reset to the previous configuration. Since the latter is but one step removed from the absorbing state, the buildup of probability in the vicinity is not surprising. In general, we expect the QS and RB distributions to be in good accord when the lifetime of the process is reasonably long, since this implies a small QS probability in the vicinity of the absorbing state.

V. SUMMARY

We have devised and tested a simulation method for quasistationary properties of models with an absorbing state. The method is easy to implement, and yields reliable results in a fraction of the time required for conventional simulations in the critical regime, of prime interest in the context of scaling and universality. It also opens the possibility of investigating QS properties in the subcritical regime, which is essentially inaccessible to conventional simulations. We expect the method to be applicable to many problems currently under investigation, such as branching-annihilating random walks, conserved sandpiles, and stochastic population models.

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