Quasi-stationary simulations of the directed percolation universality class in $d = 3$ dimensions

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Abstract. We present quasi-stationary simulations of three-dimensional models with a single absorbing configuration, namely the contact process (CP), the susceptible–infected–susceptible (SIS) model and the contact replication process (CRP). The moment ratios of the order parameters for the DP class in three dimensions were set up using the well established SIS and CP models. We also show that the mean-field exponent for $d = 3$ reported previously for the CRP (Ferreira 2005 Phys. Rev. E 71 017104) is a transient observed in the spreading analysis.

Keywords: finite-size scaling, phase transitions into absorbing states (theory), stationary states
1. Introduction

Phase transitions to a single absorbing configuration, a state which the system cannot escape from, are nowadays a topic at the frontier of non-equilibrium statistical physics [1,2]. Concomitantly with the increasing interest in absorbing/active phase transitions in complex topologies [3]–[7], there are still a lot of open problems being intensively investigated for regular lattices such as the effects of quenched disorder [8]–[10], diffusion [11], as well the modelling of predator–prey systems [12], and clonal replication [13,14].

Under the renormalization group point of view, it is expected [1,15,16] that the absorbing phase transitions in models with a positive one-component order parameter, with short-range interactions and without additional symmetries or quenched disorder will belong generally to the universality class of directed percolation (DP). This conjecture is known as the Janssen–Grassberger criterion [1]. It is worthwhile to mention that interest in such phase transitions was raised by the recent experimental observation of the DP class in absorbing-state phase transitions [18,19]. On the other hand, while DP is considered the most robust universality class of the absorbing-state phase transitions, the precise numerical determination of the critical exponents of a specific model can be masked by factors like diffusion [11] and weak quenched disorder [10].

The contact process (CP), the standard example of the DP universality class, is a toy model of epidemics [20]. More recently, a novel variation of the CP was introduced for the modelling of clonal (copies of themselves) replication, the contact replication process (CRP) [13,14]. Since neither additional symmetries nor long-range interactions were included, the CRP fulfils the requirements of the Janssen–Grassberger criterion. However, the first dynamic spreading analysis of CRP in $d = 1$–3 dimensions, reported in [13,14], intriguingly classified the model in the DP universality class in one and two, but not in

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3 A CP variation called the susceptible–infected–susceptible (SIS) model is more widely applied in epidemiological studies [3].

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three dimensions. Surprisingly, for $d = 3$ the reported spreading exponents were those predicted by the mean-field approach [14].

In the present work we applied spreading analysis and the method of quasi-stationary simulations [22,23] in three-dimensional models that fulfil the Janssen–Grassberger criterion. In particular, we turned back to the CRP model and showed that the mean-field behaviour observed previously for $d = 3$ [14] is a transient associated with the closeness between critical creation and annihilation events. Additionally, we have analysed several moment ratios for $d = 3$ and have determined the universal values for the DP class on the basis of the results obtained from CP and SIS models. The paper is outlined as follows. In section 2, the models and simulation procedures are described. Simulation results are presented and discussed in section 3. Conclusions are drawn in section 4.

2. Models and methods

2.1. Models

The contact process (CP) is defined in a hypercubic lattice $\mathbb{Z}^d$ in which the sites represent individuals in two states: healthy ($Z_i = 0$) and infected ($Z_i = 1$). Infected sites become healthy (empty) at unitary rate 1 while healthy sites are infected at a rate $n_i \lambda/q$, where $q$ is the lattice coordination number and $n_i$ the number of infected sites surrounding (first neighbours in the distance) the healthy site $i$. These rules imply, for values of the infection rate above a certain $\lambda_c$, an infection flowing in an equally distributed manner among all nearest neighbours (NN) of infected sites.

The susceptible–infected–susceptible model is a variation of the CP dynamics in which any empty site with one or more infected nearest neighbours becomes infected at rate $\lambda$. Again, a unitary cure rate is assumed. In the literature, the SIS model is also known as the A model [17].

Contact replication process rules are very similar to those of CP. Instead of individuals, the sites represent places where cells lie. Analogously to the spontaneous cure in CP, cells die at unitary rate. However, a cell replicates at a rate $\lambda$ and the offspring occupies one of its empty NN chosen at random. So, an empty site $i$ is occupied at rate $\lambda \sum_j Z_j/n_j$. The sum is taken over all neighbours of the site $i$ and $n_j$ is defined as before. Notice that the creation process is facilitated in the CRP in relation to CP since the occupation flows uniformly among only empty neighbours, implying lower critical rates. Indeed, the estimates reported for CRP were $\lambda_c = 2.02634(4), 1.08320(7)$, and $1.0000(1)$ for $d = 1, 2$, and 3 [13,14], in comparison with those for the CP, $\lambda_c = 3.29785(2), 1.64877(3)$, and $1.31686(1)$ [21], respectively. Notice that the three models share the same symmetries and, consequently, they are expected to belong to the same universality class.

For all these models, Monte Carlo simulations were performed using the usual procedure [1]: an event, creation or annihilation, is selected with probabilities $p = \lambda/(1+\lambda)$ and $1 - p$, respectively, and an occupied site $i$ is chosen at random. In the annihilation process, the occupied sites become empty in all models while the creation depends on the model. In CP, one nearest neighbour (NN) of $i$ is chosen at random and infected if empty; otherwise nothing occurs. In SIS, all empty sites neighbouring the site $i$ are occupied. Finally, in CRP one of the empty neighbours, if there are any, is chosen at random and occupied. In all cases, the time is incremented by $\Delta t = 1/N$, where $N$ is total number of infected sites.
2.2. Quasi-stationary simulations

Stationary analyses of systems with transitions to absorbing configurations in the proximity of the critical point are ruled by strong finite size effects. Indeed, the unique actual stationary state of finite systems is the absorbing one. A common alternative for avoiding this difficulty is restricting the averages to the survival samples and applying a finite size analysis. However, such a procedure is not free of ambiguities or misinterpretations [23]. An alternative approach is the quasi-stationary QS simulation method [22,23]. This method consists of storing a list with $M$ configurations visited in the history of the system and periodically replacing one of them by the current state. Whenever the system tries to visit the absorbing state, the configuration is replaced by an active one selected at random from the list containing the sample of configurations and the simulation continues as usual.

The QS simulations were performed as follows. Firstly, the list of configurations is incremented whenever the time increases by a unity up to a list with $M$ configurations being achieved. Secondly, a configuration of the list randomly chosen is replaced by the current one with a given probability $p_{\text{rep}}$. We used a large value of $p_{\text{rep}} = 0.05$ for an initial relaxation period, more precisely for $t < 5 \times 10^7$, aiming to speed up the erasing of the memory of the initial conditions. In turn, $p_{\text{rep}} = 2 \times 10^{-5}$ was adopted for the remainder of the simulation. Runs with $t_{\text{rel}} = 2 \times 10^8$ steps and averages after a relaxation time $t_r = 1 \times 10^8$ were used. Finally, the averages and uncertainties were obtained with at least 15 (for the largest system) independent runs with a full lattice as the initial condition. Periodic boundary conditions were always used.

2.3. Spreading analysis

The critical point $\lambda_c$ can be efficiently determined by the spreading analysis, which consists of evolving the system from a perturbation to the absorbing state (a single occupied site at the origin of the lattice) and computing the survival probability $P$ and mean number of occupied sites $N$ as time functions. In this analysis, the averages are done over all samples, surviving or not. Asymptotic power law dependences,

$$P(t) \sim t^{-\delta} \quad \text{and} \quad N(t) \sim t^\eta,$$

are expected at criticality. Since $N \sim t^d$ for the upper critical case and exponentially decays in the sub-critical regimes, deviations from power laws are expected around the critical point and a null curvature criterion of the double-logarithm plots of $N$ against $t$ can be used to determine the critical point [13]. Analogous analysis can be done with the survival probability.

The spreading is defined by

$$R^2(t) = \frac{1}{N(t)} \left\langle \sum_{j \in \mathbb{Z}^d} r_j^2 Z_j \right\rangle,$$

in which $r_j$ is the distance from the original seed where the perturbation was introduced. At criticality, one expects an asymptotic power law

$$R^2(t) \sim t^z.$$

The spreading exponents obey a hyperscaling relation $4\delta + 2\eta = dz$ [1, 2].

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In order to illustrate the method, we present results from quasi-stationary simulations of the two-dimensional CRP model. The QS density vanishes as usual at $\lambda = \lambda_c = 1.08322(2)$ when $L \to \infty$ (the critical rates were determined using the spreading analysis). Figure 1 shows the critical densities and lifetimes of the QS state versus system size. Lifetime was calculated as

$$\tau = 1/p_1,$$

(4)

where $p_1$ is the probability of attempting the absorbing configuration in QS simulations.

The power laws

$$\rho_s \sim L^{-\beta/\nu_\perp},$$

(5)

and

$$\tau \sim L^{\nu_\parallel/\nu_\perp},$$

(6)

were verified and the slopes for $L > 20$ provide $\beta/\nu_\perp = 0.800(7)$ and $\nu_\parallel/\nu_\perp = 1.764(14)$. As expected, these exponents are in very good accordance with those reported for the DP universality class [21] (table 1). Also, the critical variance of the order parameter, defined by $\chi = L^d((\rho^2) - \langle \rho \rangle^2)$ [1], scales as

$$\chi \sim L^{\gamma/\nu_\perp},$$

(7)

with an exponent $\gamma/\nu_\perp = 0.412(8)$, again agreeing with the DP value.

\textsuperscript{4} In [14] only results from spreading simulations were reported.
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![Figure 2.](image)

**Figure 2.** Left: critical QS quantities against system size for three-dimensional CP. Lines are least squares fits by (8). Right: critical QS quantities for SIS rescaled using pure (filled symbols) and corrected (open symbols) power laws. Curves were shifted for the sake of visibility.

**Table 1.** Critical exponents for the DP class calculated from spreading exponents given in [21]. Scaling relations $\beta = \delta \nu_\parallel$, $z = 2\nu_\perp/\nu_\parallel$, and $\gamma = d\nu_\perp - 2\beta$ [1] were used whenever necessary.

| Exponent | Quasi-stationary $d = 2$ | Quasi-stationary $d = 3$ | Spreading $d = 2$ | Spreading $d = 3$ |
|----------|--------------------------|--------------------------|-------------------|-------------------|
| $\nu_\parallel/\nu_\perp$ | 1.765(3) | 1.919(4) | 0.452(1) | 0.756(1) |
| $\beta/\nu_\perp$ | 0.799(2) | 1.394(5) | 0.229(3) | 0.110(1) |
| $\gamma/\nu_\perp$ | 0.401(4) | 0.212(96) | 1.133(2) | 1.042(2) |

The ratio between moments of the order parameter is in widespread use as a useful tool for the determination of the critical point of equilibrium systems [24]. This concept has been extended to non-equilibrium systems, particularly to models belonging to the DP universality class for which the moment and cumulant ratios have proven to be universal quantities [17]. The inset of figure 1(b) shows the ratio $m = \langle \rho^2 \rangle/\langle \rho \rangle^2$ for the two-dimensional CRP model at criticality for varying system sizes. It was shown that this ratio assumes the critical value $m_c = 1.3257(5)$ for CP in two dimensions [17]. Using data for $L \geq 80$ we found $m_c = 1.3274(9)$ for two-dimensional CRP, again in accordance with DP universality class. Additionally, we also verified the agreement of higher moment ratios with the predictions for DP classes for $d = 1$ and 2.

3. Results for $d = 3$

Quasi-stationary simulations of the CP and SIS for $d = 3$ dimensions are shown in figure 2. The CP critical rate $\lambda_c = 1.31686(1)$ was taken from [21] whereas $\lambda_c = 0.24805(2)$ for the SIS model was estimated in the present work using spreading analysis. Least squares fits for $L \geq 20$ provide the exponents $\beta/\nu_\perp = 1.400(8)$, $\gamma/\nu_\perp = 0.233(5)$, and $\nu_\parallel/\nu_\perp = 1.919(9)$ for CP while $\beta/\nu_\perp = 1.395(5)$, $\gamma/\nu_\perp = 0.252(14)$, and $\nu_\parallel/\nu_\perp = 1.944(6)$ were obtained.
Figure 3. Spreading analysis for the three-dimensional CRP around the critical point. Bottom and top groups of curves correspond to survival probability $P$ and mean number of occupied sites $N$. In each group are shown curves for $\lambda = 1.00362, 1.00363, \text{ and } 1.00364$ from bottom to top. Dashed lines represent slopes 0 and $-1$ corresponding to the DP mean-field exponents $\eta$ and $\delta$, respectively. Inset: mean critical density (not the QS one) rescaled using the power law $t^{-\delta}$ for an initial condition with all sites occupied.

for the SIS model. Notice that all of them are consistent with DP class, although data are deviated from pure power laws for small sizes. This effect can be taken into account with a suitable correction to the amplitude of the scale law for lifetime given by [23]

$$\ln \tau = \frac{\nu_\parallel}{\nu_\perp} \ln L + \frac{A}{L^{d\vartheta}} + \text{const.}, \quad (8)$$

and so on for the other QS quantities. Actually, our results are not significantly affected by the particular choice of the correction. The value $\vartheta = 0.75$ was established for CP for $d = 1$ [23] and also adopted here for $d = 3$. Using this correction, the exponents are $\beta/\nu_\perp = 1.395(4), \gamma/\nu_\perp = 0.216(3),$ and $\nu_\parallel/\nu_\perp = 1.916(5)$ for contact processes representing a significant reduction of the error estimates and an improvement of the closeness with DP class. For the SIS model, the correction to the scaling provides $\beta/\nu_\perp = 1.403(4), \gamma/\nu_\perp = 0.209(2),$ and $\nu_\parallel/\nu_\perp = 1.922(2)$, an even better improvement of the estimates as well as their proximities with the DP class. In the left panel of figure 2, the rescalings through pure power laws, $\tau/L^{\nu_\parallel/\nu_\perp}$ and so on, are compared with those given by (8). The superposition fit between the data and the ansatz (8) is neat.

A central point of the present work is the QS analysis of CRP in three dimensions for which the universality class was left as an open question. Firstly, we recalculated the critical point determination using spreading analysis and found a value approximately 0.3% larger than the originally reported one [14]. Using the criterion of downward and upward curvatures of the plots $N$ versus $t$, our best estimate is $\lambda_c = 1.00363(1)$. This

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small discrepancy is central since this certainly excludes the equality between creation and annihilation critical rates. The curves $N(t)$ and $P(t)$ have transients consistent with the DP mean-field exponents (figure 3), in agreement with the previously reported CRP simulations [14]. Even though a large power interval was not obtained for the largest time simulated, the exponents fitted in the interval $t = 10^4 - 10^5$, namely, $\eta = 0.09(2)$, $\delta = 0.78(3)$ and $z = 1.04(1)$, do not exclude the DP class (table 1). Additionally, the critical density for a fully occupied initial configuration decays as $\rho \sim t^{-0.76(1)}$ for $t > 10^3$, in excellent agreement with the DP class (inset of figure 3).

Results of QS simulations for the CRP model at the critical point are shown in figure 4. The QS exponents obtained from fits in the range $L > 20$ are $\beta/\nu_\perp = 1.325(5)$, $\gamma/\nu_\perp = 0.29(5)$, and $\nu_\parallel/\nu_\perp = 1.79(1)$ which are not conclusive as regards the agreement with the DP universality class. However, with the exception of the lifetime, the exponents seem convergent to the DP value. Applying a correction to the scaling (8), the corrected exponents for $\rho_s$ and $\chi$, $\beta/\nu_\perp = 1.374(3)$ and $\gamma/\nu_\perp = 0.19(4)$, are closer to the DP class. The lifetime analysis deserves some comments. The QS method used in the present work involves the transition to the absorbing configuration passing by the state with a single occupied site. In the critical CRP, the creation event occurs with a frequency slightly larger than the annihilation, which can be easily verified from the model critical rate together with its rules. Consequently, large clusters of occupied sites are much more seldom in CRP than in CP and, mainly, in SIS models, implying a too small frequency of visiting the pre-absorbing state (figure 5). Moreover, the average time for which a sample is kept in the list containing the system history, given by $M/p_{\text{rep}}$, must be much larger than the sample lifetime, $\tau = 1/p_1$, to avoid the same run anomalously contributing many times to the list of configurations [23]. Obviously, this effect is enhanced as the system size increases. Thus, a computationally prohibitively small $p_{\text{rep}}$ and/or large $M$ together
with too large relaxation and averaging times are demanded. Instead of the lifetime, we can determine the characteristic time $\tau_\rho$ for the density reaching the QS state in conventional QS simulations [1, 13]. The scale relations $\rho \sim L^{1.41(2)}$ and $\tau_\rho \sim L^{1.88(2)}$ were found for CRP, in agreement with the DP class as predicted from the Janssen–Grassberger conjecture.

Moments and cumulants for the DP class for $d = 1–5$ with a homogeneous constant external source were recently reported by Janssen et al [25]. So, let us introduce the notation $\mu_n = \langle \rho^n \rangle$ and $\kappa_n$ for the $n$th moment and cumulant of the order parameter, respectively. In particular, we have

$$\kappa_2 = \mu_2 - \mu_1^2$$  \hspace{1cm} (9)$$

and

$$\kappa_4 = \mu_4 - 4\mu_3\mu_1 - 3\mu_2^2 + 12\mu_2\mu_1^2 - 6\mu_1^4.$$  \hspace{1cm} (10)$$

Dickman and da Silva [17] showed that the ratios $\kappa_2/\mu_1^2$, $\kappa_4/\mu_2^2$, $\mu_3/\mu_1^2$, $\mu_3/\mu_1\mu_2$, and $\mu_4/\mu_2^2$ assume universal values for the DP class for $d = 1$ and 2 dimensions. It is important to
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Figure 6. Moment rations for SIS, CP and CRP models for $d = 3$ dimensions. Solid lines are nonlinear fits with the function $m(L) = m(\infty) + aL^{-\psi}$ with a correlation coefficient $r > 0.999$.

Table 2. Asymptotic moment ratios for SIS and CP for $d = 3$.

| Model | $\kappa_2/\mu_1^2$ | $\kappa_4/\mu_2^2$ | $\mu_3/\mu_1^3$ | $\mu_3/\mu_1\mu_2$ | $\mu_4/\mu_2^2$ |
|-------|-----------------|-----------------|----------------|-----------------|----------------|
| SIS   | 0.469(3)        | 0.490(6)        | 2.678(12)      | 1.822(3)        | 2.629(12)      |
| CP    | 0.470(2)        | 0.454(10)       | 2.697(6)       | 1.833(3)        | 2.649(18)      |

notice that both even and odd moments can be studied, since the order parameter is non-negative. Several moment and/or cumulant ratios as functions of the system size for $d = 3$ models are shown in figure 6. The moment ratios for SIS and CP models exhibit finite size effects, but seem to converge monotonically to a constant value when $L \to \infty$. Assuming a correction given by $m(L) = m(\infty) + aL^{-\psi}$, where $\psi$ and $a$ are fit parameters, the asymptotic moment ratios can be estimated. Since some data for the fourth moment were ruled by very large error bars, these data were excluded from the fits. Extrapolated moment ratios for CP and SIS are listed in table 2 and are consistent with the hypothesis of universality. It is worth stressing that the ratios shown in table 2 differ from those reported by Janssen et al [25] since, in our studies, there is no external source. The same occurs for $d = 1$ and 2 when the results of Janssen et al [25] are compared with those from [17].

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CRP seems to be different from CP and SIS. Indeed, instead of the monotonic convergence to a constant value, the moment ratios decrease after a maximum. This difference can again be associated with the proximity between critical creation and annihilation events and the resultant high diffusivity. Actually, the ratio $\mu_2/\mu_1^2 = \kappa_2/\mu_1^2 + 1$ first grows towards the value 1.550. This value is near to the established value of 1.660 for CP on a complete graph [22]. Again, we have a mean-field behaviour for small systems that must converge to the usual DP for asymptotic large systems.

4. Conclusions

We performed large-scale simulations of the contact process, the susceptible–infected–susceptible model and the contact replication process in three dimensions. Applying the quasi-stationary simulation method, we were able to determine the moment ratios of the order parameters for the DP class in three dimensions in the absence of an external field. We also show that the mean-field exponents for $d = 3$ for the CRP reported in [14] are a transient observed in the spreading analysis.

Quasi-stationary simulations and suitable corrections to the scaling revealed that the CRP model belongs to the directed percolation universality class, as expected from the Janssen–Grassberger criterion. However, the moment ratios for CRP agree with the universal DP values for $d = 1$ and 2 dimensions but do not do this for $d = 3$. The discrepancy lies in the closeness between critical creation and annihilation events, which gives rise to a diffusive transient behaviour in the CRP model, also responsible for the transient mean-field exponents obtained for $d = 3$.

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