

Critical exponents of the pair contact process with diffusion

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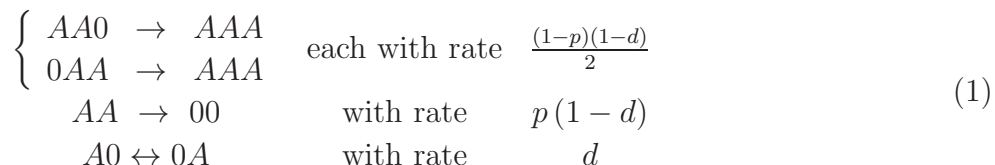
Abstract. We study the pair contact process with diffusion (PCPD) using Monte Carlo simulations, and concentrate on the decay of the particle density ρ with time, near its critical point, which is assumed to follow $\rho(t) \approx ct^{-\delta} + c_2t^{-\delta_2} + \dots$. This model is known for its slow convergence to the asymptotic critical behavior; we therefore pay particular attention to finite-time corrections. We find that at the critical point, the ratio of ρ and the pair density ρ_p converges to a constant, indicating that both densities decay with the same powerlaw. We show that under the assumption $\delta_2 \approx 2\delta$, two of the critical exponents of the PCPD model are $\delta = 0.165(10)$ and $\beta = 0.31(4)$, consistent with those of the directed percolation (DP) model.

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1. Introduction

The pair contact process with diffusion (PCPD) is a one-dimensional model of fermionic particles on a lattice. In this context, *fermionic* means that a site cannot be occupied by more than one particle. When two particles are adjacent, they can interact in two ways: they can annihilate each other, or alternatively, they can create another particle on an adjacent lattice site. Particles can also diffuse by hopping from one site to the next. The reactions of the PCPD model and their rates are given by:



Given a value for the diffusion coefficient d , we can discern three different regimes depending on the annihilation rate p . If p is very large, then annihilation dominates the process, and the particles on the lattice will die out quickly. This is the inactive phase. On the other hand, if p is very small, the particle creation reaction will ensure that (with extremely high probability) the system will maintain a high density. This is called the active phase. Well into the active or the inactive phase, long-ranged interactions are absent, and both these regimes can therefore be described well by mean-field theory. However, if the boundary between the active and inactive phase is approached from either side, length and time scales diverge in a power-law fashion. In analogy with equilibrium phase transitions, one expects that the system then exhibits critical behaviour in the transition between these regimes, at the critical value p_c . From equilibrium statistical physics it is well established that phase transitions can be classified in universality classes, each of which characterized by a unique set of critical exponents. Moreover, these exponents are typically insensitive to small changes in the model, such as details of short-ranged interactions. A central question in non-equilibrium statistical physics is whether also dynamical phase transitions can be classified into universality classes, which also are insensitive to such small changes.

In this paper we will concentrate on the scaling relations concerning the particle density ρ , which are given by:

$$\begin{aligned} \rho_{p=p_c} &\sim t^{-\delta} \quad (\epsilon = 0) \\ \rho_{t \rightarrow \infty} &\sim \epsilon^\beta \quad (\epsilon > 0) \end{aligned} \quad (2)$$

where $\epsilon \equiv |p - p_c|$ is the distance from criticality, and δ and β are two of the critical exponents of the PCPD system. A conjecture by Grassberger [1] and Janssen [2] states that all systems with a single order parameter and a single absorbing state will belong to the universality class of the Directed Percolation (DP) model. The critical exponents of the one-dimensional DP model are known to very high accuracy ($\delta = 0.159464(6)$ and $\beta = 0.276486(8)$) [3]. The values for δ and β of the PCPD model have been disputed extensively, with estimates of δ ranging from 0.16(1) to 0.27(4) and estimates of β

varying from $\beta < 0.34$ to $\beta = 0.58(1)$ [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]. For a more extensive overview, see [4]. The main interest in the PCPD model is whether it shares its critical exponents with DP, or not; the latter would disprove the Grassberger-Jansen conjecture.

The difficulties with the determination of the exponent δ of the PCPD model is that there are large finite-time corrections [4, 16], and the effective exponent thus shows a drift with simulation time. In this paper we generate high-quality data, exploiting the computational power of graphics processing units (GPUs); a description of the implementation will be published elsewhere. We then analyze these data in a way that suppresses the leading finite-time corrections.

2. Simulation results

At criticality, the asymptotic decay of the density is described by a power-law of the form $\rho(t) \sim t^{-\delta}$. For the DP model the corrections to this power-law decay very rapidly, and therefore δ_{DP} is known with very high accuracy. However, as the history of the PCPD model shows, the density decay in the PCPD model does not show such a clean power-law in the time range accessible to computer simulations. Consequently, one must account for finite-time corrections, in order to obtain an accurate estimate of δ . Different finite-time corrections have been proposed in the past, including logarithmic corrections [11] and power-law corrections [13]. Our data suggest power-law corrections, so that the density decay at the critical point is given by

$$\rho(t) = c_1 t^{-\delta} + c_2 t^{-\delta_2} + \dots, \quad (3)$$

with $\delta < \delta_2 < \dots$. By differentiating the logarithm of the density vs. the logarithm of the time, one can define an effective decay exponent as

$$\delta_{\text{eff}}(t) \equiv -\frac{\partial \log(\rho)}{\partial \log(t)} \approx \delta + \frac{c_2}{c_1}(\delta_2 - \delta)t^{-(\delta_2 - \delta)} + \dots \quad (4)$$

Note that in the limit of infinite time, the effective exponent δ_{eff} approaches the true asymptotic value δ . Moreover, the direction from which it approaches the asymptotic value is governed by the sign of c_2/c_1 , and the speed of convergence by the gap $\delta_2 - \delta$.

At this point, we want to make some practical remarks:

i) In practice with simulation data, the differentiation is carried out numerically, and one makes the approximation $\delta_{\text{eff}} \approx \frac{-\log(\rho(2t)/\rho(t))}{\log 2}$.

ii) When simulation measurements of δ_{eff} are presented, it is usually more convenient for the eye if the presentation is such that the infinite-time behavior is inside the plot, rather than at infinite distance. A common approach to achieve this, is to plot δ_{eff} as a function of $1/t$; this is not a good idea! If the gap is less than 1, the approach to the vertical axis will eventually become infinitely steep, and it is hard to predict how far an infinitely steep curve will shoot up (or down). Ideally, one should therefore plot δ_{eff} as a function of $t^{-(\delta_2 - \delta)}$, as then the approach to the vertical axis will follow a straight

line (and indirectly provide information on $\delta_2 - \delta$). Alternatively, one can plot δ_{eff} as a function of $\rho^{(\delta_2/\delta-1)}$.

iii) Besides the particle density ρ , another numerically accessible quantity is the pair density ρ_p , defined as the fraction of neighboring sites, both of which are being occupied by a particle. For the pair density at the critical point, relations equivalent to eqs.(3) and (4) can be defined. Barkema and Carlon [13] provided numerical evidence that the ratio of the densities of single particles and pairs tends to a constant; further on in this paper we will confirm this. This has as a consequence that the asymptotic density decay of singles and pairs is governed by a unique exponent δ . Also, this means that as long as the effective exponents δ_{eff} and $\delta_{p,\text{eff}}$ do not coincide, finite-time corrections are still significant.

The first results, presented in figure 1, are measurements of δ_{eff} as a function of ρ , for values of p close to the critical point, on either side. The figure shows that δ_{eff} approaches its asymptotic value from above. Assuming that at the end of our simulations, corrections are dominated by δ_2 , this indicates that c_2 is positive. Furthermore, under this assumption, the maximal value of δ_{eff} with a p value lying in the inactive phase provides an upper bound for the asymptotic exponent: $\delta < 0.19$ at $p = 0.15247$. This bound is less tight than the bound reported by Hinrichsen[16], because it depends strongly on the maximal simulation time of the dataset, which was higher in Hinrichsen's simulation, and less on the accuracy of the dataset, which is higher in our simulations. We do however confirm the conclusion of Hinrichsen that most of the values reported for the exponent δ in PCPD are ruled out by this upper bound.

Interestingly, the data in figure 1 are consistent with a linear convergence to an asymptotic value of $\delta = \delta_{DP}$. The most important conclusion drawn from this observation is that our data do not provide evidence of a violation of the Grassberger-Janssen conjecture; and since the product of system size, length of the simulations, and the number of these is higher in our simulations than in earlier studies which claim to provide evidence for violation of the conjecture, our conclusion is that earlier claims of such violation based on numerical measurements of δ_{eff} are ill-founded. A second observation is that the observed linear convergence indicates that $\delta_2/\delta - 1 \approx 1$ and thus that $\delta_2 \approx 2\delta$. Although our simulations are more extensive than those of earlier reports, the data is still not accurate enough to unambiguously rule out combinations of (δ, δ_2) which are slightly different from $(\delta_{DP}, 2\delta_{DP})$; in particular there is quite some ambiguity in δ_2 .

We now turn to an accurate estimation of the critical point p_c . For this, we want to capitalize on our numerical knowledge on the value for the correction exponent δ_2 , to suppress finite-time corrections. We do so by defining an adjusted density:

$$\rho^*(t) = 2\rho(t) - \rho(2^{-1/\delta_2}t), \quad (5)$$

for some assumed value of δ_2 . Asymptotically, the densities $\rho(t)$ and $\rho^*(t)$ at the critical point will coincide, but at long but not infinite times, the corrected density

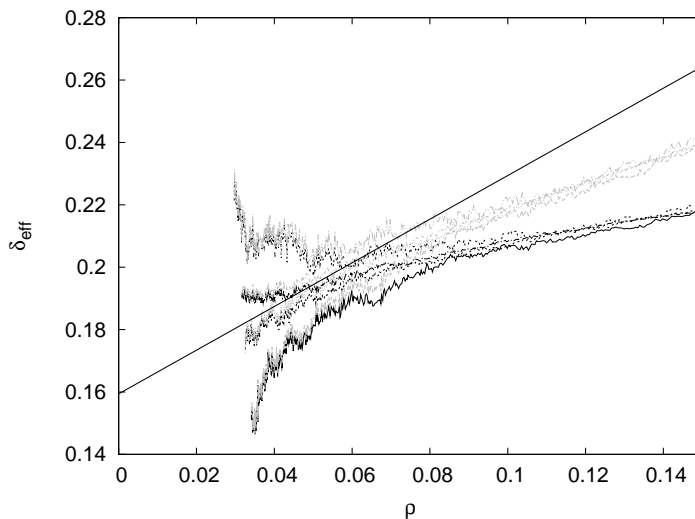


Figure 1. The effective exponent δ_{eff} as obtained for both the particle density ρ (colored black) and the pair density ρ_p (gray), as a function of the particle density, with a diffusion factor $d = 0.5$. For $d = 0.25$ and $d = 0.75$, we found similar results. Starting from low to high in the picture, the simulations are performed with $p = 0.15246$ (1600 runs), 0.15247 (3300 runs), 0.152475 (7400 runs) and 0.152485 (1000 runs). The lattice contained $L = 2^{18} = 262144$ sites. Each simulation reached a time of approximately $t = 1.6 \cdot 10^7$. The curve for $p = 0.152475$ is closest to the critical value, which we estimate to be $p_c = 0.152473(2)$. The straight line signifies a possible extrapolation to $\delta = \delta_{\text{DP}}$.

suppresses correction terms with exponents δ_i close to δ_2 ; with the correct numerical choice for δ_2 the first correction term will even be completely removed, and for a reasonable approximation of δ_2 , the power-law decay of $\rho^*(t)$ should be much cleaner than that of $\rho(t)$.

Figure 2 shows the corrected density and corrected pair density as a function of time in a log-log plot, with the choice $\delta_2 = 2\delta_{\text{DP}} = 0.319$. This gives us the estimate $\delta = 0.165(10)$. We conclude that the choice of δ_2 tightly defines our estimates of both δ and p_c .

An accurate method to determine the critical point p_c is to use a data collapse method on the corrected density ρ^* . The data collapse method maps the dataset with off-critical p values onto a single curve for $p > p_c$ and a second curve for $p < p_c$, if we select the correct values for δ , β and p_c . To achieve this, the (pair) density and the time are rescaled as follows:

$$t' = e^{\beta/\delta} t, \quad \rho' = \epsilon^{-\beta} \rho^*. \quad (6)$$

Using the diffusion factor $d = 0.5$, we obtain a very good data collapse, shown in figure 3. We find that the critical value is $p_c = 0.152473(2)$. Our estimate of the exponent β is less precise than our estimate of δ : $\beta = 0.31(4)$, which is consistent with the value known for DP: $\beta = 0.2765$. The fact that the curve for $p = 0.15240$ shows a statistically significant increase, after reaching a (pseudo-)equilibrium, indicates that the

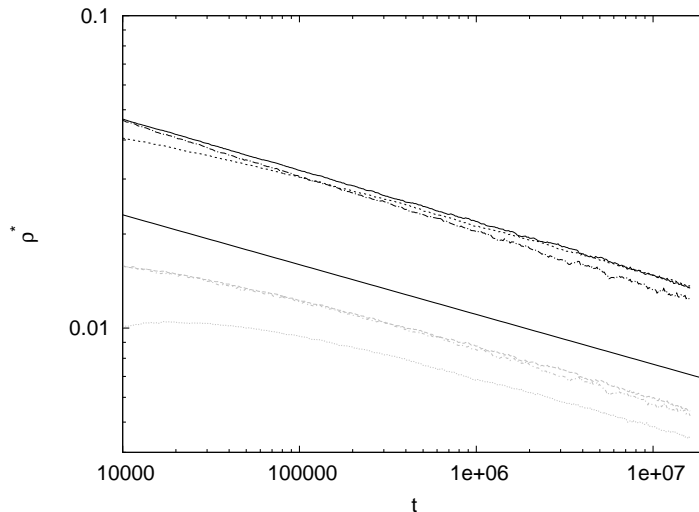


Figure 2. Corrected particle density ρ^* (black) and corrected pair density ρ_p^* (gray) as a function of time, for $d = 0.25$, $p = 0.125142$ (dashed); $d = 0.5$, $p = 0.152475$ (solid); and $d = 0.75$, $p = 0.191790$ (dotted-dashed). In the correction procedure, we used $\delta_2 = 0.319$ and a lattice size of $L = 2^{18} = 262144$. The thick black line shows a possible line with $\delta = \delta_{\text{DP}}$.

corrections due to finite time and due to off-critical values for p are not simply additive: our procedure to suppress the leading finite-time corrections at p_c is not working equally well for the off-critical curves. The ‘best’ value we find for β is therefore still experiencing significant corrections to scaling.

The question that remains is how these parameters depend on our choice for δ_2 . We used the same methods described above to obtain estimates with δ_2 ranging from 0.319 to 0.5. The results are presented in Table 1. Note that for our choice $\delta_2 = 0.319$, the leading exponent δ shows little dependence on the diffusion coefficient d .

In Ref. [4] the leading correction term $\sim t^{-\delta_2}$ was removed by using a linear combination of the density ρ and the pair density ρ^* . This is a valid strategy as long as the dominant correction term ($c_2 t^{-\delta_2}$) does not cancel in the ratio ρ/ρ_p . In that case this ratio will asymptotically go to a constant with a power law (at criticality):

$$\rho/\rho_p = k_1 + k_2 t^{\delta - \delta_2} + \dots \quad (7)$$

Thus, if the density ratio ρ/ρ_p is plotted against $t^{\delta - \delta_2}$, one should find a straight line (with finite-time corrections from higher-order correction terms). Since we found previously that $\delta_2 \approx 2\delta$, we have plotted the ratio versus the density ρ in figure 4. The density ratios for the three values of d are clearly not approaching the vertical axis under a fixed angle in this plot, but seem to arrive horizontally at $\rho = 0$. Thus, we find that the leading correction disappears in the ratio and the method described in [4] fails.

We plotted the ratio against $t^{\delta - \Delta}$ and we found that the most straight line has a value of $\Delta \approx 0.51$. The large discrepancy between δ_2 and Δ increases our confidence in the fact that the correction term $\sim t^{-\delta_2}$ vanishes in the ratio ρ/ρ_p .

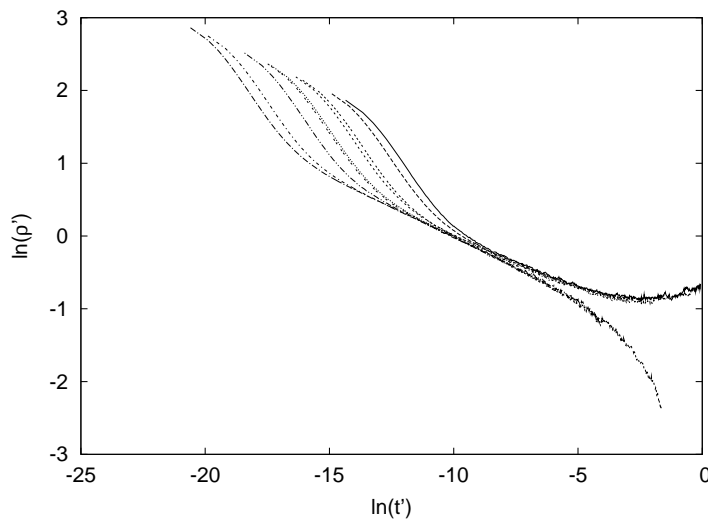


Figure 3. Data collapse of curves obtained with various values for p at $d = 0.5$. The rescaled corrected density is plotted as a function of rescaled time (see Eqs. (6)). The data are obtained from the same simulations as in Fig. 1; added to these data are simulations with $p = 0.1524$ (500 runs on a smaller lattice with $L = 65536$), $p = 0.15242$ (1000 runs), $p = 0.15245$ (1000 runs), $p = 0.15248$ (500 runs) and $p = 0.1525$ (1000 runs). In the correction procedure, we used $\delta_2 = 0.319$. In the rescaling, we used $\delta = 0.159$ and $\beta = 0.2765$ as in the DP model, combined with $p_c = 0.152473$.

Table 1. Values for the exponents δ and β and critical point p_c , obtained by our analysis approach, for three values of the diffusion coefficient d and for our estimated value $\delta_2 = 0.319$, as well as for some other values for δ_2 .

d	δ_2	δ	β	p_c
0.25	0.319	0.176(8)	-	0.125141(2)
0.5	0.319	0.164(4)	0.31(4)	0.152473(2)
0.75	0.319	0.159(4)	-	0.191789(2)
0.25	0.37	0.187(8)	-	-
0.5	0.37	0.175(4)	0.32(4)	0.152476(2)
0.75	0.37	0.165(4)	-	-
0.25	0.43	0.190(8)	-	-
0.5	0.43	0.181(4)	0.32(4)	0.152476(2)
0.75	0.43	0.172(4)	-	-
0.25	0.5	0.195(8)	-	-
0.5	0.5	0.185(4)	0.33(4)	0.152477(2)
0.75	0.5	0.177(4)	-	-

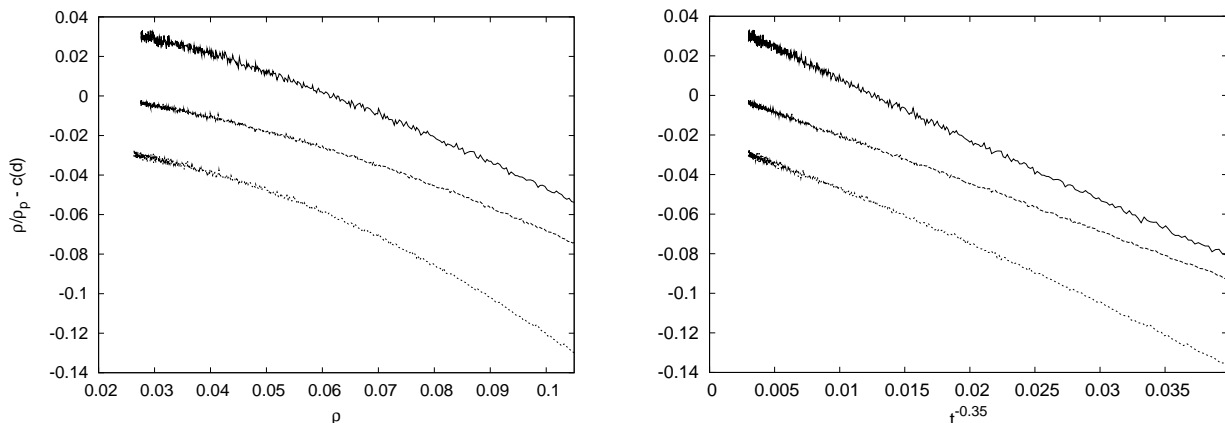


Figure 4. Left panel: ratio ρ/ρ_p of the particle and pair densities, as a function of the particle density. Right panel: same data, plotted as a function of $t^{\delta-\Delta}$ with $\Delta = 0.51$. The different curves correspond to $d = 0.25$ (solid line), $d = 0.5$ (larger dashes) and $d = 0.75$ (smaller dashes). Curves are shifted vertically by some arbitrary, d -dependent constant $c(d)$, to let them fit nicely into a single figure; lower curves correspond to higher values of d .

Thus, the ratio between the particle density and the pair density goes to a constant even faster than expected. This still means that the exponent δ is equal for the particle and the pair density.

3. Summary and conclusion

We have performed extensive simulations of the one-dimensional PCPD model, using a highly efficient GPU-based simulation approach. The analysis of the simulation results was performed in a way that takes account of finite-time effects. Our main goal was to verify the Grassberger-Janssen conjecture, which predicts that the exponents for PCPD coincide with those of directed percolation.

We find that our data are consistent with DP values for the exponents δ which describes the decay of the particle density at the critical point, and β which describes the asymptotic particle density for simulations close to the critical point, but slightly in the active phase.

Additionally, we find that the the leading correction exponent δ_2 is numerically found to be close to 2δ , which would suggest corrections to scaling of order ρ^2 . We also find that these leading corrections do not seem to manifest themselves in the ratio of the particle and pair densities.

Under the assumption that the Grassberger-Janssen conjecture is correct, we find strong indications that $\delta_2 \approx 2\delta$, by using the corrected density. There is a small dependence of δ on the diffusion factor d . We attribute this to the differences in the amplitudes of the second- and higher-order corrections. This induces a (small) systematic error in the values for δ given in Table 1.

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