Universality of the triplet contact process with diffusion

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Abstract. The one-dimensional triplet contact process with diffusion (TCPD) model has been studied using fast multispin GPU Monte Carlo simulations. In particular, the particle density $\rho$ and the density of pairs of neighboring particles $\rho_p$ have been monitored as a function of time. Mean field predictions for the time evolution of these observables at the critical point are $\rho \sim t^{-\delta}$ and $\rho_p \sim t^{-\delta_p}$ with $\delta = 1/3$ and $\delta_p = 2/3$. We observe that in the vicinity of the critical point of the model, the ratio $\rho_p/\rho$ tends to a constant, which shows that the one-dimensional TCPD model is not described by mean field behavior. Furthermore, our long simulations allow us to conclude that the mean field prediction of the exponent $\delta$ is almost certainly not correct either. Since the crossover to the critical regime is extremely slow for the TCPD model, we are unable to pinpoint a precise value for $\delta$, although we find as an upper bound $\delta < 0.32$.

Keywords: classical Monte Carlo simulations, critical exponents and amplitudes (theory), phase transitions into absorbing states (theory)
1. Introduction

The triplet contact process with diffusion (TCPD) model belongs to a set of closely related models of ‘fermionic’ particles on a lattice that follow very simple dynamical rules. By fermionic we mean in this context that only one particle can be present at each site. These models have been studied extensively, because they were conjectured by Grassberger [1] and Janssen [2] to belong to a relatively small number of dynamical universality classes, determined by coarse features such as the dimensionality, symmetries in the model, and conservation laws, in close analogy to universality classes in equilibrium statistical physics.

Historically, the first of these models to be studied extensively was the directed percolation (DP) model. This model lends itself extremely well to computer simulations, and its exponents are therefore known with high accuracy. For example, using exact enumeration techniques, the exponent $\delta$ was found to be 0.159 464(6) [3], where $\delta$ is defined through the time dependence of the particle density $\rho$ of the system, starting from a state with a uniform high density,

$$\rho \sim t^{-\delta}.$$ (1)

Even though this model is very easy from a numerical point of view, there are no theoretical predictions for these exponents, not even in one dimension. Since the Grassberger–Janssen conjecture states that the DP model belongs to a larger class of models with the same critical exponents, much effort has been undertaken to verify the exponents numerically in models that are also expected to be in the same universality class.

In one interpretation of the DP model, particles are placed on a lattice, and follow two reactions: with a statistical rate $p$, each particle annihilates, and with a statistical rate $1 - p$, each particle creates a new particle on an adjacent site, provided that it is vacant. Sometimes, the particles can also hop to neighboring lattice sites with a diffusion rate $d$. An extension of the DP model that has been studied thoroughly in the literature is the pair contact process with diffusion (PCPD) model, in which the annihilation and procreation reactions can only take place if two particles are placed next to each other (and with $d > 0$). There has been a lot of discussion about the critical exponents, mainly $\delta$, with estimates ranging from the DP value of $\delta = 0.159$ [4, 5] to 0.35 [6]. In [7], we...
performed simulations of the PCPD model in which the triple product $V = N \times L \times T$, where $N$ independent simulations were performed with a lattice of size $L$ over a time range $T$, was much larger than in previous studies. The resulting data showed that in the case of the PCPD model, finite-time corrections are particularly severe, and with careful analysis we found more evidence suggesting a value close to the DP value than the contrary.

Here, we simulate the TCPD model, which makes annihilation and procreation conditional on triplets of particles. Currently, the claim in the literature is that the TCPD model is fundamentally different from both the PCPD and DP models, as evidenced by different values for the exponents, e.g. $\delta = 0.27(1)$ [8] and $\delta = 1/3$ [9, 10]. We use the same efficient algorithm, described in [11], to reach a triple product $(N \times L \times T)$ that is almost three orders of magnitude larger than in these previous studies. We find that for shorter times, the exponent $\delta$ is very close to its mean field prediction of $1/3$, but for very long times, this exponent starts to drift. We attribute this to finite-time effects that are even stronger than in the case of the PCPD model. Even with our fast algorithm and long simulations, we were not able to reach time scales that make it possible to retrieve an accurate estimate for $\delta$. Importantly, however, we find that the DP value cannot be excluded, meaning that it is not yet proven that the TCPD model falls outside the DP universality class.

2. Method

Several slightly different versions of the TCPD model have been studied. We use a version with the reactions $3A \rightarrow 4A$ and $3A \rightarrow \emptyset$, which is described by the following reactions and rates:

\[
\begin{align*}
AAA0 & \rightarrow AAAA & \text{each with rate } (1-p)(1-d)/2 \\
0AAA & \rightarrow AAAA \\
AAA & \rightarrow 000 & \text{with rate } p(1-d) \\
A0 & \leftrightarrow 0A & \text{with rate } d.
\end{align*}
\]

In a straightforward implementation of this model, first the type of reaction is selected, based on a random number $r \in [0,1]$, and, depending on its value, one of the reactions is proposed (but not always carried out).

- If $r < d$, a random pair of neighboring sites $\{i, i + 1\}$ is selected; in the case where one site is occupied and the other is empty, the particle hops from the occupied site to the empty one.
- Else if $r - d < p(1-d)$, a random triplet of sites $\{i, i + 1, i + 2\}$ is selected; if all three sites are occupied, they are all made vacant.
- Else if $r - d - p(1-d) < (1-p)(1-d)/2$, a random triplet of sites $\{i, i + 1, i + 2\}$ is selected; if all three sites are occupied and site $i + 3$ is vacant, a particle is placed on this last site.
- Else, a random triplet of sites $\{i, i + 1, i + 2\}$ is selected; if all three sites are occupied and site $i - 1$ is vacant, a particle is placed on this last site.

Irrespective of the type of reaction and its success, the time scale is incremented by $\Delta t = 1/N$. These steps are then iterated many times. As noted in section 1, for the
results presented here, we used as a basis an algorithm that leverages the power of graphics processing units (GPUs), which is described in detail in [11].

Before one can actually measure the exponent \( \delta \), a prerequisite is to determine the critical annihilation rate \( p_c \). For low annihilation rates \( (p < p_c) \), the system will, given enough time, settle with extremely high probability for a more or less constant particle density. This regime is called the active regime. On the other hand, in the inactive regime with high annihilation rates \( (p > p_c) \), the particles will quickly die out. In between, exactly at \( p = p_c \), there is the critical regime, where the density decreases more slowly than in the inactive regime, following a power-law decay with a critical exponent \( \delta \).

Thus, it is necessary to first identify an estimate for the critical point \( p_c \), before we can estimate the critical exponent \( \delta \). To this effect we use as our main tool the effective exponent \( \delta_{\text{eff}} \) as a function of time, defined as

\[
\delta_{\text{eff}}(t = \sqrt{t_1t_2}) = -\frac{\log(\rho(t_1)) - \log(\rho(t_2))}{\log(t_1) - \log(t_2)},
\]

and a similar expression for the effective exponent \( \delta_{\text{eff},p} \) for the pair density. Substituting the asymptotic behavior as given in equation (1), we retrieve that \( \delta_{\text{eff}} \to \delta \) as \( t \) goes to infinity. The procedure is equivalent to numerical differentiation of \( \partial \log(\rho) / \partial \log(t) \).

Equation (3) shows that there is still freedom in choosing \( t_1 \) and \( t_2 \). The trade-off is as follows. If we choose \( t_1 \) closer to \( t_2 \), the plot is generally more accurate, in the sense that features present in the analytical \( \delta_{\text{eff}} \) curve are less smoothed out and lost in that way. On the other hand, the curve is much noisier. We found that in our case choosing \( t_1 / t_2 \approx \exp(3) \) gives good results.

We find an estimate for \( p_c \) by a manual binary search, which sounds more cumbersome than it is, because far from \( p_c \) the \( \delta_{\text{eff}} \) plots are very clearly recognizable as either sub- or super-critical. Closer to \( p_c \) it gets much harder to estimate \( p_c \), because of the drift in the effective exponent, which gives our estimate for \( p_c \) a larger error bar. Apart from the density \( \rho \) of the system, we can also measure the pair density \( \rho_p \). This is especially useful for testing the validity of mean field theory, as it predicts that \( \rho_p = \rho^2 \), and thus also \( \delta_{\text{eff},p} = 2\delta_{\text{eff}} \).

For each value of \( p \) we performed at least \( N = 200 \) independent simulations of runs up to \( T = 8 \times 10^8 \), with a lattice size of \( L = 2^{21} = 2097152 \). We simulated at annihilation rates between \( p = 0.095 \), \( 0.095 04 \), \( 0.095 08 \), \( 0.095 11 \), \( 0.095 12 \), \( 0.095 125 \), \( 0.095 13 \), always with \( d = 0.5 \). Our estimate for the critical annihilation rate is \( p_c = 0.095 10^{+0.000 02}_{-0.000 05} \).

3. Simulation results

First, in figure 1 we present the raw simulation data for the average particle density \( \rho \) and the pair density \( \rho_p \) as a function of time, starting from a random initial state with density \( \rho = 1/2 \) (and \( \rho_p = 1/4 \)). The particle density shows an approximately straight line in a double logarithmic plot, indicating power-law behavior. At the same \( p \) values, the pair density shows strong curvature, which indicates strong finite-time corrections to power-law behavior. We note that the curves close to the critical point look qualitatively similar to the ones found in [8], although the slope is different: we find 0.33, whereas they reported 0.27(1). In our opinion, this discrepancy can be attributed to differences in the
The density $\rho$ (black curves) and the pair density $\rho_p$ (gray curves) as a function of time in a double logarithmic plot. The lattice size is $L = 2^{21}$, with 200 independent runs for each value of $p$ and $0.095 < p < 0.09513$.

The effective exponents $\delta_{\text{eff}}$ and $\delta_{\text{eff},p}$, describing the decay of particles and of pairs of particles, are plotted against $t^{-\alpha}$ in figure 2, with values for $p$ close to $p_c$. We chose $\alpha = 0.2$, as this is a rough estimate of the exponent governing the leading finite-time corrections, due to details of the models. Because our data have very small error bars, we can use $\delta_{\text{eff}}$ to investigate the ‘power-law’ like behavior of the density and the pair density in more detail.
Figure 3. The ratio $\rho_p/\rho$ between the pair density $\rho_p$ and the particle density $\rho$ as a function of $t^{-\alpha}$, with $\alpha = 0.2$. The precise value of $\alpha$ is not important here. At criticality the curve seems to arrive at the vertical axis at a value higher than 0, which means that eventually $\rho/\rho_p$ will reach a constant value.

corrections. As we will not use any extrapolation method, the choice for $\alpha$ does not affect our conclusions.

It is clear from the plot that $\delta_{eff,p} \neq 2\delta_{eff}$, even at short times $t$, and thus we conclude that mean field theory does not correctly describe the TCPD model.

The figure also shows that some curves first ascend to the value for $\delta_{eff}$ of mean field theory (1/3), then turn slightly downwards to values of around 0.32, and then ascend above 1/3 again. We interpret this behavior as a signature of a $p$-value that is close to, but slightly below, $p_c$, as the data roughly follow the critical curve, before reaching the inactive regime. Our main reason is that we find it very unlikely that the critical curve makes more than one bend on these time scales. Thus, we find a lower bound: $\delta < 0.32$. Obviously, if our assumption is not correct this lower bound is also not correct. However, if this were the case we believe that any attempt at numerical analysis would be impossible with the current simulation approach and state of software and hardware. Another important aspect to note is that $\delta_{eff}$ and $\delta_{eff,p}$ are closing in on each other in a way very similar to that in the PCPD model [7].

The ratio $\rho_p/\rho$ is plotted in figure 3 against $t^{-\alpha}$, again with $\alpha = 0.2$, for different values of $p$, including ones that are above $p_c$. We have to be more careful here in our choice of $\alpha$, because we are trying to make a conclusion about the extrapolated value. If we assume that $\rho_p/\rho \sim t^{-\beta}$, then the choice $\alpha = \beta$ combined with linear extrapolation yields the correct constant for $t \to \infty$. On the other hand, choosing $\alpha > \beta$ yields an overestimation, whereas $\alpha < \beta$ gives us a prediction lower than the true value. Since we are not interested in the exact value of the ratio at $t \to \infty$, but only in whether it is equal to 0 or higher, we try to choose $\alpha < \beta$. Since $\beta$ is unknown, we choose a value for $\alpha$ such that the critical curves seem to arrive close to horizontally at the $x$-axis, which is indicative of $\alpha \leq \beta$. In figure 3, all curves are approaching the vertical axis (corresponding to $t \to \infty$) in a way
that strongly suggests that it will go to a finite value. Thus, we conclude that the ratio $\rho_p/\rho$ approaches a non-zero value as $t \to \infty$.

4. Summary and conclusion

We have performed extensive simulations of the one-dimensional TCPD model, using a highly efficient GPU-based simulation approach. We find that the TCPD model is not described by mean field theory, as evidenced by the convergence of the ratio of the pair density and the particle density $\rho_p/\rho$ to a non-zero value at criticality, instead of going to zero as expected by mean field theory. Given the similarities between the PCPD model and the TCPD model with regards to finite-time corrections, we find it not unlikely that they both belong to the DP universality class. Numerical evidence for the PCPD model belonging to the DP universality class was given by us in [7]. We emphasize that there is no solid numerical data on which a value of $\delta$ for the TCPD model can be based. However, we do find an upper bound of $\delta < 0.32$, which excludes most previous literature values for this exponent in the TCPD model, and is also less than the mean field value. Thus a safer conclusion is that numerical data do not exclude the possibility that the TCPD and PCPD belong to the DP universality class, and that this should still be considered as a serious possibility.

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