

OPEN Scaling and universality in glass transition

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Kinetic facilitated models and the Mode Coupling Theory (MCT) model B are within those systems known to exhibit a discontinuous dynamical transition with a two step relaxation. We consider a general scaling approach, within mean field theory, for such systems by considering the behavior of the density correlator $\langle q(t) \rangle$ and the dynamical susceptibility $\langle q^2(t) \rangle - \langle q(t) \rangle^2$. Focusing on the Fredrickson and Andersen (FA) facilitated spin model on the Bethe lattice, we extend a cluster approach that was previously developed for continuous glass transitions by Arenzon et al. (Phys. Rev. E 90, 020301(R) (2014)) to describe the decay to the plateau, and consider a damage spreading mechanism to describe the departure from the plateau. We predict scaling laws, which relate dynamical exponents to the static exponents of mean field bootstrap percolation. The dynamical behavior and the scaling laws for both density correlator and dynamical susceptibility coincide with those predicted by MCT. These results explain the origin of scaling laws and the universal behavior associated with the glass transition in mean field, which is characterized by the divergence of the static length of the bootstrap percolation model with an upper critical dimension $d_c = 8$.

Many physical systems and models exhibit a sudden slowing down of their dynamics, followed by a dynamical transition associated with a structural arrest. Roughly, we can distinguish two type of transitions, continuous and discontinuous, depending whether or not there is a jump at the threshold of the dynamical correlator in the infinite time limit. An example of the first category is given by the sol-gel transition (e.g. refs 1-3). This dynamical transition was studied using a cluster approach, based on percolation theory4. An explicit scaling form for the dynamical correlator was found, and general scaling laws connecting the dynamical exponents with the random percolation exponents were derived. Recently, it was shown^{5,6} that using mean field percolation exponents, the same scaling form for the correlator and the same scaling relations were also valid for the continuous transition of MCT model A⁷, suggesting that the origin of the continuous MCT scaling relations is due to an underlying static transition in the same universality class of random percolation. In the MCT schematic model, the correlator $\phi(t)$ obeys the integro-differential equation: $\phi(t) + t_0\dot{\phi}(t) + v\int_0^t\phi^q(t-s)\dot{\phi}(s)\,\mathrm{d}s = 0$, where q=1 in the continuous model A and q=2 in the discontinuous model B, v is the controlling parameter and t_0 is a characteristic microscopic timescale⁷.

The glass transition instead belongs to the second category, characterized by discontinuous transition. A great advance in glass theory was provided by MCT developed by Götze and collaborators⁷⁻⁹. This theory starting from first principles, under some mean field approximations, predicts a dynamical arrest at a finite temperature $T_{\mathcal{O}}$ characterized by power law behavior and universal scaling laws. These theoretical predictions have been tested in great detail both experimentally and numerically 10-15. A schematic version is given by the MCT discontinuous model B, introduced above. Other models, like p-spin glass models (e.g. refs 16,17), Random Field Ising model in an external field (e.g. refs 18-21), kinetic facilitated models (e.g. refs 22-24), reproduce in mean field the same dynamical behavior and scaling laws. However the transition described by MCT does not seem to exhibit any critical change in the structure and no diverging static length. How can we then explain the scaling laws and universal behavior found at mean field level? In this paper we consider as paradigmatic example the Fredrickson and Andersen facilitated Ising model²² on a Bethe lattice²⁵. The infinite time limit of the persistence of this model, $\Phi(t)$, tends²⁵ to the order parameter of the bootstrap percolation (BP) model^{26–28}. The BP model exhibits a mixed order transition with an order parameter which jumps discontinuously at the transition, nevertheless the fluctuations, and the critical length associated to it, diverge as the transition is approached from the glassy phase.

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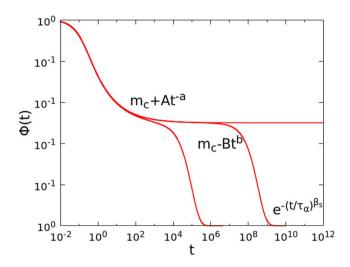


Figure 1. Correlators in MCT schematic model B. Each curve corresponds to a different value of ϵ . The correlator reaches the plateau with a power law decay, $\Phi(t) - m_c \sim t^{-a}$, and the departure from the plateau is given by $\Phi(t) - m_c \sim -(t/\tau_\beta)^b$. At long times, a crossover is observed to a new regime, well fitted by stretched exponential function.

Generalizing the cluster approach considered for the continuous dynamic transition^{5,6}, we are able to predict the dynamical behavior for the correlator and for the dynamical susceptibility of the FA facilitated model, including universal scaling laws that relate dynamical exponents with the static universal exponents of BP. Using the mean field values of these static exponents, we find that the dynamical behavior and the scaling laws are the same as predicted by MCT model B, what validates the early suggestion^{25,29–32} that the facilitated model and the MCT model B have a similar dynamical behavior. Akin the results found for the continuous transition^{5,6}, using the cluster approach we find a new more precise form for the approach of the correlator to the plateau, characterized by a power law, followed by a stretched exponential divided by a power law. These new predictions are verified numerically on both FA facilitated model and MCT model B. All these results suggest a general common mechanism for discontinuous glass transition at mean field level, based on a static transition in the same universality class of bootstrap percolation with a diverging static length, which is responsible for the origin of scaling and universality present in such a wide range of systems, apparently very different from each other.

In the following, using the cluster approach and a damage spreading mechanism, we will derive on the Bethe lattice the dynamical behavior of the correlator and the dynamical susceptibility in terms of critical exponents of the BP model, and compare with MCT results. In the supplementary information, we calculate the critical exponents of the BP model, where in particular it is stressed the difference between the behavior of the mean cluster size of the corona clusters, which diverges with an exponent $\gamma=1/2$, and the fluctuation of the percolation order parameter, which diverges with an exponent $\gamma=1$.

Results

Kinetic facilitated models and bootstrap percolation. Kinetic facilitated models²⁴ like Fredrickson and Andersen²² or Kob and Andersen models²³ on the Bethe lattice have been suggested²⁵ to have a discontinuous MCT-like transition (see Fig. 1)⁷⁻⁹. Our objective is to use a physical picture to understand the origin and the mechanism leading to such peculiar dynamical behavior. In order to do so, we consider, in particular, the Fredrickson and Andersen (FA) kinetic facilitated model²² (FA) on a Bethe lattice. The FA model is defined on a lattice, where an Ising variable, $S_i = \pm 1$, is assigned to each of the N sites, with Hamiltonian, $H = -\frac{1}{2} \sum_{i=1}^{N} S_i$. The

spins variables are updated according to the standard spin flip dynamics, along with the constraint that a spin can only flip if the number of nearest neighbors in the down state $(S_i = -1)$ is larger than or equal to f.

The dynamics of the system can be characterized by the correlator, $\Phi(t) = \langle q(t) \rangle$, a quantitative measure of how the system configuration at time t is correlated to the configuration at time t = 0, the dynamical susceptibility, $\chi_4(t) = N(\langle q^2(t) \rangle - \langle q(t) \rangle^2)$, and the dynamical pair correlation function, $g_{ij}(t)$, where

$$q(t) = \frac{1}{N} \sum_{i} n_{i}(t), \quad g_{ij}(t) = \langle n_{i}(t) n_{j}(t) \rangle - \langle n_{i}(t) \rangle \langle n_{j}(t) \rangle, \quad \chi_{4}(t) = \frac{1}{N} \sum_{ij} g_{ij}(t), \tag{1}$$

with $n_i(t) = 0$, 1 depending whether a spin at site *i* has flipped or not during time interval (0, t), respectively³³.

On a Bethe lattice of coordination number z=k+1, the model, for 0 < f < k-1, has a transition from a liquid phase at high temperatures (where the density of down spins is large), to a frozen phase at low temperatures, where down spins are few and an infinite cluster of blocked spins appears^{34–36}. It was shown²⁵ that in the $t \to \infty$ limit, this transition corresponds exactly to that of BP. Bootstrap percolation has a mixed order transition: while the percolation order parameter P of BP jumps discontinuously at the threshold from zero to P_c , the fluctuation χ of the order parameter with respect to the initial configuration, and the associated length ξ diverge according to:

$$P - P_c \sim \epsilon^{\beta}, \quad \chi \sim \epsilon^{-\gamma}, \quad \xi \sim \epsilon^{-\nu},$$
 (2)

where

$$\beta = 1/2, \quad \gamma = 1, \quad \nu = 1/4.$$
 (3)

The behavior of the order parameter characterized by the exponent $\beta=1/2$ was first derived in the original paper where BP was first introduced²⁶, Note that the fluctuation of the order parameter χ must not be confused with the mean cluster size of the "corona". These are clusters made of sites belonging to the percolating cluster, surrounded by a number of facilitated sites exactly equal to $f-1^{27}$. The mean cluster size of the corona in fact diverges with an exponent $1/2^{27,28}$. In ref. 27 a second correlation function was introduced leading to a second "susceptibility" diverging with an exponent 1, but it is not clear whether this quantity is related to the fluctuation of the percolation order parameter. In the Supplementary Information, we calculate explicitly the fluctuation of the order parameter and show that it diverges with an exponent $\gamma=1$ along with the associated correlation length $\nu=1/4$.

In summary, for the FA model we have, in the glassy phase, m = P, $\chi_4(\infty) = \chi$, and $\xi_4(\infty) = \xi$, where $m = \lim_{t \to \infty} \Phi(t)$, $\chi_4(\infty) = \lim_{t \to \infty} N(\langle q(t)^2 \rangle - \langle q(t) \rangle^2)$ are the FA order parameter and its fluctuation, respectively, and $\xi_4(\infty)$ is the associated length.

Decay to the plateau using the cluster approach. We note that coming from the glassy phase $T < T_{\mathcal{O}}$ the static properties of the FA model exhibits a mixed order transition at the critical temperature $T_{\mathcal{O}}$ whose critical behavior is given by Eq. (2). However, by re-defining the order parameter as $m - m_{\mathcal{O}}$, the transition can be considered as a continuous one. Therefore, we can apply the cluster formalism developed for the continuous transition, such as the sol-gel transition and the dynamical transition of the MCT model A^{4-6} .

In the cluster approach, it is assumed that the system can be described by a distribution of clusters n(s), where each cluster of size s decays with a simple exponential

$$\phi_s(t) \sim e^{-t/\tau_s},\tag{4}$$

where τ_s is the relaxation time of a cluster of size s. The larger the size of the cluster, the larger is the relaxation time. It is natural to assume the following power law relation, as usually found for polymer systems:

$$\tau_s \sim s^x$$
 (5)

where *x* is a constant exponent. The density correlator of the entire system is given by the sum over all clusters

$$\Phi(t) - m \sim \sum_{s} sn(s) e^{-t/\tau_{s}}$$
(6)

where

$$n(s) \sim s^{-\tau} e^{-s/s^*} \tag{7}$$

is the cluster distribution associated to the fluctuation of BP with $\tau=2+\beta/(\beta+\gamma)$ and $s^*=e^{-(\beta+\gamma)}$, where $\beta=1/2$ and $\gamma=1$ are the mean field BP exponents. In the sol-gel transition and MCT model A, the cluster distribution is given by random percolation theory with $\beta=1$ and $\gamma=1^{37}$. Note that this approach is rather general, it is based only under the assumption that the system configuration can be partitioned in a distribution of clusters, each decaying with a relaxation time proportional to s^x . Even if we do not know precisely the cluster definition, the approach is still valid, just like in a liquid-gas transition close to the critical point it is appropriate to describe the critical properties in terms of a distribution of droplets, in the spirit of Fisher's droplet model³⁸⁻⁴⁰.

Provided that we are in the glassy phase, $T \le T_o$ we can apply the cluster formalism of the continuous transition, which predicts a pure power law decay⁴⁻⁶ for the entire range of times at the transition, $T = T_o$, and the same power law below T_o provided that $t \ll \tau_B$.

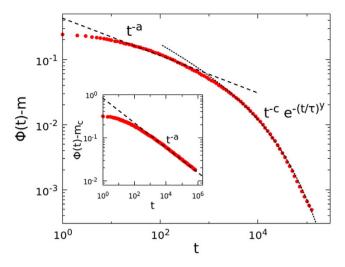


Figure 2. The correlator of the FA model on the Bethe lattice in the glassy phase at $T_c - T = 2^{-7}$ (main frame) and at the transition (inset). The dashed line is the power law t^{-a} with exponent a = 0.29. The dotted line in the glassy phase is given by Eq. (11), with y = 0.46 and c = 0.39.

 $\Phi(t) - m \sim t^{-a}, \quad t \ll \tau_{\beta}, \quad \tau_{\beta} \sim \epsilon^{-z_1}$ (8)

$$a = \frac{1}{x} \frac{\beta}{\beta + \gamma}, \quad z_1 = x(\beta + \gamma) = \frac{\beta}{a},$$
 (9)

where *x* is related to the relaxation time of a fluctuation of size *s* by Eq. (5). Inserting BP mean field exponents $\beta = 1/2$ and $\gamma = 1$, we obtain

$$a = \frac{1}{3x}, \quad z_1 = \frac{3x}{2} = \frac{1}{2a}.$$
 (10)

Moreover, as in the continuous case, close to T_c the power law is followed by a transient, whose behavior is given by a stretched exponential combined with a power law⁴⁻⁶:

$$\Phi(t) - m \sim \epsilon^{\beta} \left(\frac{\tau_{\beta}}{t}\right)^{c} e^{-(t/\tau_{\beta})^{y}}, \tag{11}$$

with

$$c = \frac{3\beta + \gamma}{2(x+1)(\beta + \gamma)} = \frac{5}{6(x+1)} = \frac{5a}{2(1+3a)}$$
(12)

and

$$y = \frac{1}{x+1} = \frac{3a}{1+3a} \tag{13}$$

$$\frac{c}{y} = \frac{3\beta + \gamma}{2(\beta + \gamma)} = \frac{5}{6} \tag{14}$$

we have performed large scale numerical simulations of the FA model on the Bethe lattice with k=3, f=2 and $N=2^{18}$. Figure 2 shows the correlator in the glassy phase (main frame) and at the transition (inset). The value of $a\approx 0.29$ is obtained from the power law decay at the critical temperature. From this value, using Eqs (12) and (13), we predict the exponents $y\approx 0.46$ and $c\approx 0.39$, defined in Eq. (11). Figure 2 shows that the data are in excellent agreement with the cluster approach predictions.

In the liquid phase, we have the same approach to the plateau, Eq. (8) replacing m by m_o and the same power law, Eq. (9), provided that the system is close enough to T_c and $t \ll \tau_\beta$. Note that the behavior given by Eq. (11) is much less pronounced in the liquid phase, since for large t the regime corresponding to the departure from the plateau will become dominant and interfere with it.

Departure from the plateau using the damage spreading mechanism. In the liquid phase, all the clusters (fluctuations) vanish in the long time limit, but they survive on time scales of the order of τ_{β} , when the plateau is still present. The small clusters start to decay first, the last clusters to relax are the largest clusters, i.e. the critical clusters.

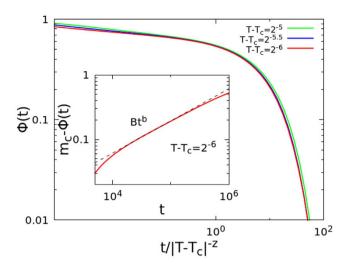


Figure 3. Main frame: Scaling collapse of the correlator of the FA model on the Bethe lattice, in the liquid phase $T > T_c$ Eq. (17), with z = 2.72. Inset: Departure from the plateau, the dashed line is the power law with b = 0.50.

z	a	b	с	у
2.7 ± 0.1	0.29 ± 0.01	0.50 ± 0.02	0.39 ± 0.01	0.46 ± 0.01

Table 1. Numerical exponents obtained for the FA model on the Bethe lattice, the values of c and y are consistent with the scaling obtained from the cluster approach Eqs (12) and (13), the values of c, c and c are consistent with the MCT scaling relations Eqs (18) and (20).

Once the sites in the critical clusters have moved (relaxed), they act as initial damaged sites to "free" the sites of the potential bootstrap percolating cluster represented by the plateau. As the time increases, the damage spreads through a branching cascade process⁴¹. The physical picture behind it is that the potential infinite cluster, which contributes to the plateau, is made of a sea of quasi frozen sites, surrounded by critical clusters. Just above the critical temperature the critical clusters eventually decay, whereas just below the critical temperature, the critical clusters themselves become frozen and part of the infinite cluster. The number of sites m(t) in the core, which are liberated by the damage spreading, is related to the correlator by

$$\Phi(t) \simeq m_c - m(t), \tag{15}$$

$$m(t) \sim \epsilon^{\beta} (t/\tau_{\beta})^{b}, \quad \beta = 1/2,$$
 (16)

where e^{β} is the density of sites in the critical clusters and therefore the density of initial damaged sites, and $1/\tau_{\beta}$ is, according to the cluster picture, the diffusion coefficient of the sites in the critical cluster, and b is a dynamical exponent related to the spreading damage mechanism.

Finally, in the α regime,

$$\Phi(t) \simeq g(t/\tau_{\alpha}), \quad \tau_{\alpha} \sim \epsilon^{-z},$$
(17)

and, like in MCT, using the matching conditions with the previous regime

$$z = \frac{\beta}{a} + \frac{\beta}{b} = \frac{1}{2a} + \frac{1}{2b}.$$
 (18)

In Fig. 3, we have reported the scaling collapse of the correlator in the α regime, Eq. (17), from which the exponent $z\approx 2.72$ of the relaxation time τ_{α} has been evaluated. This value is consistent with the value found in ref. 25. In the inset we have also reported the departure from the plateau Eq. (16) and the value of $b\approx 0.50$ has been evaluated. The exponents z, a and b satisfy not only the scaling relation (16), but a and b are also found to satisfy the other MCT relation, Eq. (20), with $\lambda=0.785$. For convenience, we have reported in Table 1 all the exponents found numerically for the FA model on the Bethe lattice with the estimated errors.

Given two critical times τ_{β} and τ_{α} , in the liquid phase it may be more convenient to express the density correlator $\Phi(t)$ as a scaling function of two variables:

$$\Phi(t) - m_c \simeq \epsilon^{\beta} F\left(\frac{t}{\tau_{\beta}}, \frac{t}{\tau_{\alpha}}\right), \tag{19}$$

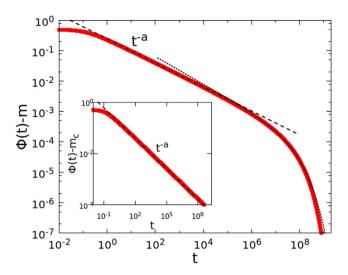


Figure 4. Numerical solution of the MCT schematic model B in the glassy phase (red continuous line), with $\lambda = 0.5$. Dashed line is the power law t^{-a} , with a = 0.40, obtained from Eq. (20). The data are in excellent agreement with the cluster approach prediction (dotted line is the stretched exponential-like decay, Eq. (11), with c = 0.45 and y = 0.54, obtained using x = 1/3a = 0.84).

 $F(x,y)=F_1(x)$ for $y\ll 1$, where $F_1(x)=x^{-\beta/z_1}$ for $x\ll 1$ and $F_1(x)=-x^b$ for x>1, and $F(x,y)=-x^bF_2(y)$ for $x\gg 1$ and y>1. The requirement that $\Phi(t)$ for $t>\tau_\alpha$ is a function of t/τ_α only, Eq. (17), implies that $\epsilon_\beta x^b=y^b$, which in turn leads to $\tau_\alpha=\tau^b\tau_\beta$ where $\tau_b\sim\epsilon^{-z_b}$ with $z_b=1/2b$. Taking into account that $\tau_\beta\sim\epsilon^{-z_1}$, it follows the scaling relation Eq. (18).

Comparison with discontinuous MCT model B. Interestingly, the correlator of the MCT model B satisfies the same scaling forms Eqs (8), (16) and (17) and scaling relations Eqs (9) and (18), suggesting that the above picture is consistent with MCT. This is further validated if we consider that the mean field static BP exponents coincide with those found in the Random Field Ising (RFI) model in an external field^{18–21}, which was shown to be mapped on the MCT theory, and that both BP and RFI model have an upper critical dimension d_c = 8, which coincides with the value found for MCT⁴².

MCT also predicts a relation between the exponent a and b and the MCT parameter λ :

$$\frac{\Gamma^2(1-a)}{\Gamma(1-2a)} = \frac{\Gamma^2(1+b)}{\Gamma(1+2b)} = \lambda.$$
 (20)

The parameter λ for the discontinuous model B is 0.5.

In our approach instead of λ we have x as parameter, which is related to a through

$$a = \frac{1}{x} \frac{\beta}{\beta + \gamma} = \frac{1}{3x}.\tag{21}$$

If our approach applies to MCT, x can be related to λ and consequently to b through Eq. (20)

$$\frac{\Gamma^2(1+b)}{\Gamma(1+2b)} = \frac{\Gamma^2(1-1/3x)}{\Gamma(1-2/3x)} = \lambda.$$
 (22)

At the moment, we do not have an intuitive physical picture of why x and b should be related in such a manner. Interestingly, our data show that the MCT relation Eq. (20) is well verified on the FA model, strongly supporting the idea that the FA model in mean field reproduces entirely MCT^{29–31}.

Our approach predicts that the approach to the plateau, after a power law behavior, should be described by the stretched exponential Eq. (11) with exponents given by Eqs (12) and (13), before becoming an exponential decay. By numerically solving the MCT schematic model, we found that the approach to the plateau is very well described by the above predictions (see Fig. 4).

Fluctuations of the order parameter. Dynamical heterogeneities play an important role in understanding the nature of the glass transition^{43–55}. They are described through the dynamical susceptibility, $\chi_4(t)$, defined as the fluctuations of the dynamical order parameter: $\chi_4(t) = N(\langle q(t)^2 \rangle - \langle q(t) \rangle^2)$. In the following, we will refer to the FA model, however the same predictions apply to the MCT model as well, if the two models behave in the same way, as shown already for the decay of the correlator. As for the correlator, we express $\chi_4(t)$ as a scaling function of two variables. Since in the glassy phase for t going to infinity $\chi_4(t)$ coincides with the fluctuation of the BP order parameter, which diverges with an exponent $\gamma=1$ as the glass transition is approached we can write:

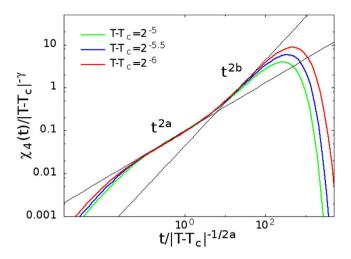


Figure 5. Data collapse in the β regime of the dynamical susceptibility, $\chi_4(t)$, for the FA model on the Bethe lattice, showing the scaling relation Eq. (27) with $\gamma = 1$, $\tau_{\beta} \sim e^{-1/2a}$. Straight lines show the power law behaviors in the early (t^{2a}) and late β regime (t^{2b}), with a = 0.29 and b = 0.50.

$$\chi_4(t) \simeq \epsilon^{-\gamma} G_{\pm} \left(\frac{t}{\tau_{\beta}}, \frac{t}{\tau_{\alpha}} \right).$$
 (23)

where $G_+(x, y)$ is a two variables scaling function in the glassy (+) and liquid (-) phase.

Glassy phase. Given that in the glassy phase $\tau_{\alpha} = \infty$, we have

$$\chi_4(t) \simeq \epsilon^{-\gamma} F_+ \left(\frac{t}{\tau_\beta} \right).$$
 (24)

$$\text{where } F_+\!\!\left(\frac{t}{\tau_\beta}\right) = G_+\!\!\left(\frac{t}{\tau_\beta},\,0\right)\!\!.\, F_+\!=\!\mathrm{const \,for}\; t \to \infty \text{ and } F_+\!\!\left(\frac{t}{\tau_\beta}\right) = \left(\frac{t}{\tau_\beta}\right)^{\!a\gamma/\beta} \text{ for } t < \tau_\beta\text{, so that since } \tau_\beta \sim e^{-\beta/a},$$

$$\chi_4(t) \sim t^{a\gamma/\beta} = t^{2a} \quad \text{for } t < \tau_\beta,$$
 (25)

is independent on ϵ , and

$$\chi_4(t) \sim \epsilon^{-\gamma} = \epsilon^{-1} \quad \text{for } t \to \infty,$$
 (26)

In conclusion in the glassy phase $\chi_4(t)$ grows as a power law t^{2a} until it reaches a plateau at $t \sim \tau_\beta$, whose value diverges with an exponent $\gamma = 1$.

Liquid phase. In the liquid phase, we have:

$$\chi_4(t) \simeq \epsilon^{-\gamma} F_- \left(\frac{t}{\tau_\beta} \right) \quad \text{for } t \ll \tau_\alpha.$$
 (27)

where $F_{-}\left(\frac{t}{\tau_{\beta}}\right) = G_{-}\left(\frac{t}{\tau_{\beta}}, 0\right)$. In the early regime, $t \le \tau_{\beta}$, the behavior is the same as in the glassy phase,

$$\chi_4(t) \sim t^{a\gamma/\beta} = t^{2a} \quad \text{for } t < \tau_\beta,$$
 (28)

$$\chi_4 \sim \epsilon^{-\gamma} = \epsilon^{-1} \quad \text{for } t = \tau_\beta,$$
 (29)

we have numerically verified on FA model on the Bethe lattice the scaling relation Eq. (27). In Fig. 5, we have reported the rescaled susceptibility, showing that in the β regime $t \ll \tau_{\alpha}$ all curves rescale onto a unique function corresponding to $F_{-}(x)$ (with $x = t/\tau_{\beta}$), and that $\chi_{4}(t) \sim e^{-\gamma}$ for $t = \tau_{\beta}$ (with $\gamma = 1$).

In the late β regime, $\tau_{\beta} < t \ll \tau_{\alpha}$, as the dynamical process is due to the damage spreading mechanism, $\chi_4(t)$ must be proportional to the square of the number of visited sites $m^2(t) \sim t^{2b\,56}$ similar to what is found in the diffusing defects mechanism (see refs 33,57), therefore

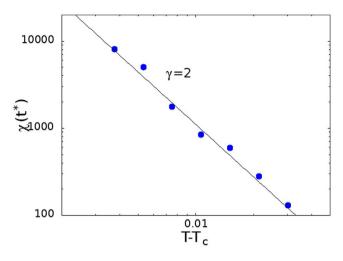


Figure 6. Maximum of the dynamical susceptibility $\chi_4(t^*)$ for the FA model on the Bethe lattice as a function of $T - T_c$. The maximum diverges as $|T - T_c|^2$, in agreement with the prediction of Eq. (33).

$$F_{-}\left(\frac{t}{\tau_{\beta}}\right) = \left(\frac{t}{\tau_{\beta}}\right)^{2b} \quad \text{for } \tau_{\beta} < t \ll \tau_{\alpha}$$
(30)

From Eqs (27) and (30)

$$\chi_4(t) \sim \epsilon^{-\gamma - 2\beta} \left(\frac{t}{\tau_{\alpha}}\right)^{2b} \quad \text{for } \tau_{\beta} < t \ll \tau_{\alpha},$$
 (31)

where $\tau_{\alpha} \sim \epsilon^{-z}$, $\tau_{\beta} \sim \epsilon^{-\beta/a}$ and the scaling relation Eq. (18) has been taken into account.

In general, in the late β and α regime $t > \tau_{\beta}$, from Eq. (27) we have $G_{-}\left(\frac{t}{\tau_{\beta}}, \frac{t}{\tau_{\alpha}}\right) = \left(\frac{t}{\tau_{\beta}}\right)^{2b} H_{-}\left(\frac{t}{\tau_{\alpha}}\right)$, where $H_{-}(y) = \text{const.}$, for $y \le 1$ in order to match the behavior in the late β regime Eq. (30), and goes to zero for $y \gg 1$, as $\chi_{4}(t)$ in the infinite time limit tends to the value of the BP susceptibility χ , which is zero in the liquid phase. Therefore

$$\chi_4(t) = \epsilon^{-\gamma - 2\beta} \left(\frac{t}{\tau_{\alpha}} \right)^{2b} H_{-} \left(\frac{t}{\tau_{\alpha}} \right) \quad \text{for } \tau_{\beta} < t, \tag{32}$$

$$\chi_4 \sim \epsilon^{-\gamma - 2\beta} \sim \epsilon^{-2}$$
 for $t = \tau_{\alpha}$, (33)

where $\beta=1/2, \gamma=1$, have been taken into account. We have found good agreement for the FA model as shown in Fig. 6, where the maximum of $\chi_4(t)$ is plotted for $t=t^*\sim\tau_\alpha$, and in Fig. 5, where it is shown $\chi_4(t)\sim t^{2a}$ in the early β regime and $\chi_4(t)\sim t^{2b}$ in the late β regime.

Comparison with MCT- $\chi_4(t)$ was studied within the p-spin model by Franz and Parisi⁴⁶ and within the MCT theory by Biroli and Bouchaud⁵⁸ using a diagrammatic approach. The MCT results⁵⁷ predicted for $\chi_4(t)$ a growth respectively t^a and t^b for the early and late β regime and a growth of the maximum at t^* with an exponent 1. Later it was argued⁵⁹ that this behavior is valid only for ensembles where all conserved degrees of freedom are fixed, e.g. Newtonian dynamics in the NVE ensemble or Brownian dynamics, in the NVT ensemble, otherwise other diagrams would contribute to $\chi_4(t)$ leading to a behavior t^{2a} and t^{2b} and an exponent 2 for the growth of the maximum of $\chi_4(t)$ at t^* . The same found in our approach. More recently in⁶⁰, this last behavior was found to be much more general, being due to self induced disorder. Changing the initial condition induces fluctuation in the induced disorder leading to the new dynamical behavior.

Discussion

In conclusion, we have shown that a cluster approach and a damage spreading mechanism, applied to the FA kinetic facilitated model in mean field, predict a discontinuous dynamical transition with the same scaling behavior found in the discontinuous MCT transition and Random Field Ising model in a field. The dynamical transition is characterized by a static mixed order transition, in the same universality class of bootstrap percolation. This static transition is characterized by static critical fluctuations diverging only in the glassy phase, being absent in the liquid phase. Nevertheless the dynamics even in the liquid phase is strongly influenced by this static transition, as shown by the behavior of the dynamical heterogeneities, characterized by $\chi_4(t)$. The presence of the static transition, at least at mean field level, characterized by a diverging static length, is responsible for the scaling laws

and universality present in a wide range of dynamical critical phenomena, and sets the value of the upper critical dimensionality $d_c = 8$. In this scenario the sol-gel transition, which in mean field has been shown to be described by the continuous MCT model A^{5,6}, can be considered as dynamical transition in a different universality class, characterized by the static random percolation transition with upper critical dimensionality $d_c = 6$.

Methods

We performed Monte Carlo simulations of the FA kinetic facilitated model on a Bethe lattice. The Bethe lattice is a lattice extracted randomly from the set of lattices where each site is connected to z=k+1 other sites. We consider a random lattice with $N=2^{18}$ sites, fixed coordination number z=k+1=4, and f=2. For each temperature we extract 32 different random lattices and initial configurations, and we start from a random configuration of the spins with density $p=(1+e^{-1/T})^{-1}$ of the up spins. Each Monte Carlo step is given by N spin flip trials. A spin flip trial consists in taking a random spin, and flipping it if it has f or more neighboring down spins, and with probabilities given by $p(-\to +) = \frac{e^{1/2T}}{e^{1/2T}+e^{-1/2T}}$ and $p(+\to -) = \frac{e^{-1/2T}}{e^{1/2T}+e^{-1/2T}}$. For k=3 and f=2 the critical temperature is $T_c = \left[\ln\left(\frac{p_c}{1-p_c}\right)\right]^{-1} \approx 0.480898$, with $p_c=8/9$ and a fraction of blocked spins equal to $m_c\approx 0.673$. The relaxation function is defined as

$$\Phi(t) = \langle q(t) \rangle$$

where $q(t) = \frac{1}{N} \sum_{i} n_i(t)$, and $n_i(t) = 0$, 1 depending whether a spin at site *i* has flipped or not during time interval (0, t), while the fluctuations are defined as

$$\chi_4(t) = N[\langle q(t)^2 \rangle - \langle q(t) \rangle^2]$$

where $\langle \cdots \rangle$ is the average over the thermal noise, the initial configurations and the random lattice.

References

- 1. Flory, P. J. The Physics of Polymer Chemistry (Cornell University Press 1954).
- 2. de Gennes, P. G. Scaling Concepts in Polymer Physics (Cornell University Press 1993).
- 3. Zaccarelli, E. Colloidal gels: equilibrium and non-equilibrium routes. J. Phys.: Condens. Matter 19, 323101 (2007).
- Fierro, A., Abete, T. & Coniglio, A. Static and Dynamic Heterogeneities in a Model for Irreversible Gelation. J. Chem. Phys. 131(19), 194906 (2009).
- 5. Arenzon, J. J., Coniglio, A., Fierro, A. & Sellitto, M. Percolation approach to glassy dynamics with continuously broken ergodicity. *Phys. Rev. E* 90, 020301(R) (2014).
- Coniglio, A., Arenzon, J. J., Fierro, A. & Sellitto, M. Relaxation dynamics near the sol-gel transition: From cluster approach to mode-coupling theory, Eur. Phys. J. Special Topics 223, 2297–2306 (2014).
- 7. Götze, W. Complex dynamics of glass-forming liquids (Oxford University Press, 2009).
- 8. Götze, W. & Sjogren, L. Relaxation processes in supercooled liquids. Rep. Prog. Phys. 55, 241 (1992).
- 9. Götze, W. Recent tests of the mode-coupling theory for glassy dynamics. J. Phys. Cond. Matt. 11, A1 (1999).
- Pusey, P. N. & van Megen, W. Observation of a glass transition in suspensions of spherical colloidal particles. Phys. Rev. Lett 59, 2083 (1987).
- 11. Kob, W. & Andersen, H. C., Testing mode-coupling theory for a supercooled binary Lennard-Jones mixture I: The van Hove correlation function. *Phys. Rev. E* **51**, 4626 (1995).
- 12. Kob, W. & Andersen, H. C., Testing mode-coupling theory for a supercooled binary Lennard-Jones mixture. II. Intermediate scattering function and dynamic susceptibility. *Phys. Rev. E* **52**, 4134 (1995).
- Dawson, K. et al. Higher-order glass-transition singularities in colloidal systems with attractive interactions. Phys. Rev. E 63, 011401 (2000).
- 14. Chen, S. H., Chen, W. R. & Mallamace, F. The Glass-to-Glass Transition and Its End Point in a Copolymer Micellar System. *Science* **300**, 619 (2003).
- Mallamace, F., Corsaro, C., Stanley, H. E., Mallamace, D. & Chen, S. H. The dynamical crossover in attractive colloidal systems. J Chem Phys. 139, 214502 (2013).
- 16. Mèzard, M., Parisi, G. & Virasoro, M. A. Spin Glass Theory and Beyond (World Scientific, Singapore 1987).
- 17. Cugliandolo, L. F. & Kurchan, J. Analytical solution of the off-equilibrium dynamics of a long-range spin-glass model. *Phys. Rev. Lett.* **71**, 173 (1993).
- 18. Stevenson, J. D., Walczak, A. M., Hall, R. W. & Wolynes, P. G. Constructing explicit magnetic analogies for the dynamics of glass forming liquids. *J. Chem. Phys.* **129**, 194505 (2008).
- 19. Franz, Š., Parisi, G., Ricci-Tersenghi, F. & Rizzo, T. Properties of the perturbative expansion around the mode-coupling dynamical transition in glasses, arXiv:1001.1746.
- 20. Biroli, G., Cammarota, C., Tarjus, G. & Tarzia, M. Random-field-like criticality in glass-forming liquids, *Phys. Rev. Lett.* 112, 175701 (2014).
- 21. Nandi, S., Biroli, G. & Tarjus, G. Spinodals with Disorder: from Avalanches in Random Magnets to Glassy Dynamics, arXiv:1507.06422.
- 22. Fredrickson, G. H. & Andersen, H. C. Kinetic Ising Model of the Glass Transition. Phys. Rev. Lett. 53, 1244 (1984).
- 23. Kob, W. & Andersen, H. C. Kinetic lattice-gas model of cage effects in high-density liquids and a test of mode-coupling theory of the ideal-glass transition. *Phys. Rev. E* 48, 4364 (1993).
- 24. Ritort, F. & Sollich, P. Glassy dynamics of kinetically constrained models. Advances in Physics 52, 219 (2003).
- 25. Sellitto, M., Biroli, G. & Toninelli, C. Facilitated spin models on Bethe lattice: bootstrap percolation, mode coupling transition and glassy dynamics. *Europhys. Lett.* **69**, 496 (2005).
- 26. Chalupa, J., Leath, P. L. & Reich, R. Bootstrap percolation on a Bethe lattice. J. Phys. C: Solid State Phys. 12, L31 (1979).
- 27. Schwarz, J. M., Liu, A. J. & Chayes, L. Q. The onset of jamming as the sudden emergence of an infinite *k*-core cluster. *Europhys. Lett.* **73**, 560 (2006).
- Baxter, G. J., Dorogovtsev, S. N., Goltsev, A. V. & Mendes, J. F. F. Heterogeneous k-core versus bootstrap percolation on complex networks. Phys. Rev. E 83, 051134 (2011).
- 29. Arenzon, J. J. & Sellitto, M. Microscopic models of mode-coupling theory: the F_{12} scenario. J. Chem. Phys. 137, 084501 (2012).
- 30. Sellitto, M., De Martino, D., Caccioli, F. & Arenzon, J. J. Dynamic facilitation picture of a higher-order glass singularity. *Phys. Rev. Lett.* 105, 265704 (2010).

- 31. Franz. S. & Sellitto, M. Finite-size critical fluctuations in microscopic models of mode-coupling theory. I. Stat. Mech. P02025 (2013).
- 32. Sellitto, M. Crossover from beta to alpha Relaxation in Cooperative Facilitation Dynamics. Phys. Rev. Lett. 115, 225701 (2015).
- 33. Pastore, R., Coniglio, A. & Pica Ciamarra, M. Dynamical Correlation Length and Relaxation Processes in a Glass Former. *Phys. Rev. Lett.* **107**, 065703 (2011).
- 34. Toninelli, C., Biroli, G. & Fisher, D. S. Spatial structures and dynamics of kinetically constrained models for glasses. *Phys. Rev. Lett.* **92**, 185504 (2004).
- 35. Dorogovtsev, S. N., Goltsev, A. V. & Mendes, J. F. F. K-core organization of complex networks. Phys. Rev. Lett. 96, 040601 (2006).
- 36. Dorogovtsev, S. N., Goltsev, A. V. & Mendes, J. F. F. Critical phenomena in complex networks, Rev. Mod. Phys. 80, 1275 (2008).
- 37. Stauffer, D. & Aharony, A. Introduction to Percolation Theory (Taylor & Francis 1992).
- 38. Fisher, M. E. Magnetic Critical Point Exponents-Their Interrelations and Meaning. J. Appl. Phys. 38, 981 (1967).
- 39. Fisher, M. E. & Widom, B. Decay of Correlations in Linear Systems. J. Chem. Phys. 50, 3756 (1969).
- 40. Fisher, M. E. Critical Phenomena, Proceedings of the International School of Physics "Enrico Fermi" Course LI, Varenna on lake Como (Italy) (eds Green, M. S.) 1 (Academic, New York, 1971).
- 41. Baxier, G. J., Dorogovtsev, S. N., Lee, K.-E., Mendes, J. F. F. & Goltsev, A. V. Critical dynamics of the *k*-core pruning process. *Phys. Rev. X* 5, 031017 (2015).
- 42. Biroli, G. & Bouchaud, J.-P. Critical fluctuations and breakdown of the Stokes-Einstein relation in the mode-coupling theory of glasses. *J. Phys: Condens.* 19, 205101 (2007).
- 43. Cicerone, M. T., Blackburn, F. R. & Ediger, M. D. Anomalous diffusion of probe molecules in polystyrene: evidence for spatially heterogeneous segmental dynamics. *Macromolecules* 28, 8224 (1995).
- 44. Kob, W., Donati, C., Plimpton, S. J., Poole, P. H. & Glotzer, S. C. Dynamical heterogeneities in a supercooled Lennard-Jones liquid, *Phys. Rev. Lett.* **79**, 2827 (1997).
- 45. Bennemann, C., Donati, C., Baschnagel, J. & Glotzer, S. C. Growing range of correlated motion in a polymer melt on cooling towards the glass transition. *Nature* 399, 246 (1999).
- 46. Franz, S. & Parisi, G. On non-linear susceptibility in supercooled liquids. J. Phys.: Condens. Matter 12, 6335 (2000).
- 47. Widmer-Cooper, A., Harrowell, P. & Fynewever, H. How reproducible are dynamic heterogeneities in a supercooled liquid? *Phys. Rev. Lett.* **93**, 135701 (2004).
- 48. Berthier, L. et al. Direct experimental evidence of a growing length scale accompanying the glass transition. Science 310, 1797 (2005).
- 49. Pan, A. C., Garrahan, J. P. & Chandler, D. Heterogeneity and growing length scales in the dynamics of kinetically constrained lattice gases in two dimensions. *Phys. Rev. E* 72, 041106 (2005).
- 50. Bouchaud, J.-P. & Biroli, G. Nonlinear susceptibility in glassy systems: A probe for cooperative dynamical length scales. *Phys. Rev. B* 72, 064204 (2005).
- 51. Biroli, G., Bouchaud, J.-P., Miyazaki, K. & Reichman, D. R., Inhomogeneous mode-coupling theory and growing dynamic length in supercooled liquids. *Phys. Rev. Lett.* **97**, 195701 (2006).
- 52. Berthier, L. et al. Spontaneous and induced dynamic fluctuations in glass-formers I: General results and dependence on ensemble and dynamics. J. Chem. Phys. 126, 184503 (2007).
- 53. Berthier, L. et al. Spontaneous and induced dynamic correlations in glass formers. II. Model calculations and comparison to numerical simulations. J. Chem. Phys. 126, 184504 (2007).
- 54. Chaudhuri, P., Berthier, L. & Kob, W. Universal nature of particle displacements close to glass and jamming transitions. *Phys. Rev.* Lett. **99**, 060604 (2007)
- Dalle-Ferrier, C. et al. Spatial correlations in the dynamics of glassforming liquids: Experimental determination of their temperature dependence. Phys. Rev. E 76, 041510 (2007).
- 56. Coniglio, A., de Arcangelis, L., Herrmann, H. & Jan, N. Exact relations between damage spreading and thermodynamical properties. Europhysics Lett. 8, 315 (1989)
- 57. Toninelli, C., Wyart, M., Berthier, L., Biroli, G. & Bouchaud, J.-P. Dynamical susceptibility of glass formers: Contrasting the predictions of theoretical scenarios. *Phys. Rev. E* 71, 041505 (2005).
- 58. Biroli, G. & Bouchaud, J.-P. Diverging length scale and upper critical dimension in the Mode-Coupling Theory of the glass transition. *Europhys. Lett.* **67**, 21 (2004).
- 59. Berthier, L. et al. Spontaneous and induced dynamic correlations in glass formers. II. Model calculations and comparison to numerical simulations. J. Chem. Phys. 126, 184504 (2007).
- 60. Franz, S., Parisi, G., Ricci Tersenghi, F. & Rizzo, T. Field theory of fluctuations in glasses. Eur. Phys. J. E. 34, 1-17 (2011).

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Author Contributions

A.d.C., A.F. and A.C. conceived the project, A.d.C. and A.F. carried out simulations and analyzed the data, A.d.C., A.F. and A.C. wrote the paper.

Additional Information

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