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Supporting Information

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Simulation Details

Planting Method. We generate the initial configuration as follows:

- We generate randomly the positions $\underline{x}$ of the N spheres, with a uniform probability distribution over the simulation box.
- For each sphere i, we generate its shifts $\mathbf{l_{ij}}$ with uniform distribution in the simulation box. Each shift $\mathbf{l_{ij}}$ is accepted if and only if

$$|\mathbf{x_i}-\mathbf{x_j}+\mathbf{l_{ij}}|>1, \qquad \textbf{[S1]}$$

otherwise it is generated again until condition **S1** is satisfied.

It can be shown (1) that in the infinite volume limit this procedure generates a thermalized initial configuration where the annealed average of entropy is equal to the quenched one (i.e., a configuration in the liquid phase) (1).

We have tested that the procedure works, that the configurations that we generate are at equilibrium and their properties are independent from time (as long as the density remains constant). The result for the observable $g(r,0)$ for planting density $\varphi_0=2.5$ is shown in Fig. S1. We can see in the low r region a behavior compatible with the equilibrium one:

$$g(\mathbf{x}-\mathbf{y})=\exp(-v(\mathbf{x}-\mathbf{y}))=\begin{cases}0 & \text{if } |\mathbf{x}-\mathbf{y}|<D\\ 1 & \text{if } |\mathbf{x}-\mathbf{y}|>D\end{cases} \qquad \textbf{[S2]}$$

within 1 or 2 SDs. For example, for the contact point we have $g(1)=0.987\pm0.019$. We do not study the large r behavior of $g(r,0)$, which shows a decay caused by the finite size of the simulation box and cannot be compared with the infinite-volume analytical result (Eq. **S2**).

Monte Carlo Evolution Algorithm and Verlet Lists. We used a Monte Carlo evolution algorithm. At each step t we propose a displacement $\Delta\mathbf{x_i}(t)$ to each sphere i. The proposed displacement is generated uniformly in a 3D sphere of radius δ, where $\delta=0.2$ is a fixed parameter. The proposed displacement is accepted if and only if the condition

$$|\mathbf{x_i}+\Delta\mathbf{x_i}-\mathbf{x_j}+\mathbf{l_{ij}}|>1 \qquad \textbf{[S3]}$$

is satisfied for all other spheres $j\neq i$; otherwise it is rejected. This stochastic dynamics satisfies the detailed balance property, thus implying relaxation toward equilibrium. To reduce computational time we use Verlet lists (see, e.g., ref. 2).

Radial Distribution Function Computation. We denote by $\Omega_{\Delta,\underline{l}}(r,t)$ the number of sphere couples such that

$$|\mathbf{x_i}(t)-\mathbf{x_j}(t)+l_{ij}|\in[r,r+\Delta]$$

and we define a fixed time radial distribution function

$$g_{\Delta,\underline{l}}(r,t)=\frac{1}{4N\varphi}\,\frac{\Omega_{\Delta,\underline{l}}(r,t)}{(r+\Delta r)^3-r^3}.$$

The parameter Δ is fixed and corresponds to the histogram bin length. We choose $\Delta=0.05$. To gain central processing unit time we perform measurements at equispaced intervals in time (typically every 20 Montecarlo sweeps). In our simulation we further average over the different starting configuration. The number of configurations is $M=6$, a reasonable value for a self-averaging quantity. The statistical error is estimated from sample-to-sample fluctuations.

Decompression Protocol. In the following we denote by k the logarithm in base 2 of the number of Monte Carlo steps performed for each density value. We are interested in a decompression protocol that mimics the physical heating of a glass. We start from a planted initial configuration at a density φ_0 in the glassy region ($\varphi_0>\varphi_d$) in the liquid phase ($\varphi_0<\varphi_k$), equivalent to the supercooled liquid region in real glass formers. To be safe we choose φ_0 values between 2 and 3. After planting, we decompress the system changing the box size, leaving the integer sphere positions unchanged, causing a jump $\varphi_0\to\varphi_1$ of density, with $\varphi_1<\varphi_0$. The system evolves for 2^k Monte Carlo steps at density φ_1, then density jumps again to a lower value $\varphi_2<\varphi_1$, the system evolves for 2^k steps at density φ_2, and so on.

Compression Protocol. To compress the system, we increase the particle radius until the particles touch. When this happens, Monte Carlo steps are performed to separate the particles; afterward, the radius is increased again, until the final density is reached.

The procedure is slow and therefore the final system is nearly thermalized. After the final density is reached, we run a long simulation for final thermalization and we take measurements only in the second half of the run.

Mean Square Displacement

For each density value φ we measured the relaxation time by fitting the plateau escape region of the MSD $\Delta(t)$ with the power law

$$\Delta(t)=a\left(1+ct^b\right).$$

We discarded the fast relaxation region. We considered for each density value only points with $t>2^{11}$. We defined the relaxation time using the relation $\Delta(\tau_R)=1.5\ \Delta(2^{11})$. The value 1.5 is somewhat arbitrary: It should be neither too small, to reduce noise effects, nor too large, to allow us to obtain relaxation time values not too large compared with the typical time scales of our simulations. Using this procedure we obtained the value of relaxation time for each value of density. For the highest studied values of density (i.e., $\varphi=1.7,1.68,1.66$), we obtained $\tau_R>2^{22}$, meaning that 2^{22} steps were not sufficient to observe relaxation: These are extrapolated points and we discarded them.

Computation of Isocomplexity Lines

The first step is the computation of the replicated entropy $S(m,\varphi)$ as a functional of the replicated density. Denoting by $\underline{x}=\{\mathbf{x}^{(a)}\}$ the set of the positions of the m replicas, by $\rho(\underline{x})$ the replicated density, for the mean-field MK model we have

$$S(m,\varphi)[\rho]=-\int d\underline{x}\,\rho(\underline{x})\log(\rho(\underline{x}))+\frac{1}{2}\int d\underline{x}\ \underline{y}\,\rho(\underline{x})\rho(\underline{y})f(\underline{x}-\underline{y})+N\log(N), \qquad \textbf{[S4]}$$

where

$$f(\underline{x}-\underline{y})=\overline{\exp\left(\sum_{a=1}^{m}v\left(\mathbf{x}^{(a)}-\mathbf{y}^{(a)}+\mathbf{l}\right)\right)}-1$$

is the replicated Mayer function. In practice, the replicated density is usually parameterized as

$$\rho(\underline{x}) = \frac{N}{V} \int d\mathbf{X} \prod_{a=1}^{m} g_A\left(\mathbf{x}^{(a)} - \mathbf{X}\right), \qquad \textbf{[S5]}$$

where $\mathbf{x}^{(a)}$ is the position of replica a and g_A is the Gaussian function with variance A. The parameter A represents the average cage radius and can be also interpreted as the plateau value of the mean square displacement of particles in the caging regime. For the mean-field MK model of hard spheres, combining results presented in appendix A of ref. 3 and in section VI of ref. 4, putting parameterization **S5** in **S4** we obtain

$$\begin{aligned} S(m,\varphi,A) &= \log(N) - \log\left(\frac{\varphi}{\mathcal{V}_d(1)}\right) \\ &\quad + S_{harm}(m,A) - 2^{d-1}\varphi(1-\mathcal{G}(m,A)), \end{aligned} \qquad \textbf{[S6]}$$

where $\mathcal{G}(m,A)$ and $S_{harm}(m,A)$ are defined in ref. 4. We stress that Eq. **S6** is the same of a pure hard-sphere system (that is, without shifts) in infinite dimension. We must then optimize this with respect to A (4), getting the equation

$$\frac{1}{\hat{\varphi}} = \mathcal{F}(m, A(m,\varphi)), \qquad \textbf{[S7]}$$

where $\hat{\varphi} = 2^d\varphi/d$ and

$$\mathcal{F}(m,A) = \frac{A}{1-m}\frac{\partial \mathcal{G}(m,A)}{\partial A}. \qquad \textbf{[S8]}$$

Eq. **S16** and the form of the function $\mathcal{F}$ (4) imply a first-order transition at the endpoint of metastable curves, both in the (m,φ) plane and in the pressure-density plane. We discuss this result in *Singularity of Cage Radius and Pressure at the Clustering Line*.

We plug the solution $A(m,\varphi)$ of Eq. **S16** in Eq. **S6**, obtaining $S(m,\varphi)$. Using then the replica relations

$$s_{eq}(m,\varphi) = \frac{\partial S(m,\varphi)}{\partial m}, \qquad \textbf{[S9]}$$

$$\Sigma_{eq}(m,\varphi) = m^2\frac{\partial\left[m^{-1}S(m,\varphi)\right]}{\partial m}, \qquad \textbf{[S10]}$$

on Eq. **S6** we get the following expression for the complexity:

$$\begin{aligned} \Sigma(m,\varphi,A) &= S(m,\varphi,A) \\ &\quad -\frac{d}{2}(1+m+m\log(2\pi A)) + 2^{d-1}\varphi\mathcal{H}(m,A), \end{aligned} \qquad \textbf{[S11]}$$

where

$$\mathcal{H}(m,A) = -m\frac{\partial \mathcal{G}(m,A)}{\partial m}.$$

The only remaining task is now to solve the equation

$$\Sigma(m,\varphi) = \Sigma_0 = \Sigma(1,\varphi_0)$$

with respect to m, for various values of φ. Because in the clustering region Σ is a decreasing function of m at fixed φ, the solution $m_{\Sigma_0}(\varphi)$ of the isocomplexity condition can be found with a simple bisection algorithm. We start at φ_0, then we change the density of a small amount $\Delta\varphi$, and we use bisection to find the solution m_{Σ_0} of the equation

$$\Sigma(m_{\Sigma_0}, \varphi_0 + \Delta\varphi) = \Sigma_0. \qquad \textbf{[S12]}$$

Once it has been found, we change the density again and the procedure is repeated until the clustering line is reached and the solution for A disappears.

In-State Pressure

In principle the ratio $p(\varphi)$ between physical pressure $P(\varphi)$ of a state of complexity Σ_0 and density φ can be computed using the relation

$$p(\varphi) = \rho^{-1}P(\varphi) = -\varphi\frac{d}{d\varphi}s_{eq}(m(\varphi),\varphi), \qquad \textbf{[S13]}$$

where $m(\varphi)$ solves Eq. **S12** for a given complexity value Σ_0. Eq. **S13** is uncomfortable because it involves also the partial derivative with respect to m. Instead of directly using Eq. **S13** we define a modified replicated entropy for each complexity value Σ_0:

$$\tilde{S}(m,\varphi) = S(m,\varphi) - \Sigma_0 = ms_{eq}(m,\varphi) + \Sigma_{eq}(m,\varphi) - \Sigma_0.$$

Isocomplexity Eq. **S12** is then equivalent to the equation

$$m^2\frac{\partial}{\partial m}\left(m^{-1}\tilde{S}(m,\varphi)\right)\Big|_{m=m(\varphi)} = 0. \qquad \textbf{[S14]}$$

Therefore, the pressure of a metastable state can be expressed in terms of total entropy S:

$$\begin{aligned} p(\varphi) &= -\frac{\varphi}{m(\varphi)}\frac{\partial}{\partial\varphi}\left(\tilde{S}(m,\varphi)\right)\Big|_{m=m(\varphi)} \\ &= -\frac{\varphi}{m(\varphi)}\frac{\partial}{\partial\varphi}\left(S(m,\varphi)\right)\Big|_{m=m(\varphi)}. \end{aligned} \qquad \textbf{[S15]}$$

Eq. **S15** is all we need to pass from (m,φ) plane to the pressure-density plane. It is also easy to pass to the contact value of radial distribution function through the relation (5) $g(1) = (p-1)/(4\varphi)$.

Singularity of Cage Radius and Pressure at the Clustering Line

For each metastable curve $m(\varphi)$ the clustering point φ_d is defined as the lowest φ value for which equation

$$\frac{1}{\hat{\varphi}} = \mathcal{F}(m, A(m,\varphi)) \qquad \textbf{[S16]}$$

admits a finite solution $A(m(\varphi),\varphi)$. The corresponding cage radius A_{max} is the value of A for which $\mathcal{F}(m(\varphi_d),A)$ has a maximum (4). Expanding $\mathcal{F}(m,A)$ in Taylor power series near φ_d and rearranging terms we obtain from Eq. **S16**

$$A(\varphi) - A_{max} = C\sqrt{\hat{\varphi} - \hat{\varphi}_d} + \mathcal{O}(\varphi - \varphi_d), \qquad \textbf{[S17]}$$

where $A_{max} = A(m(\varphi_d),\varphi_d)$, $\hat{\varphi} \equiv \frac{2^d}{d}\varphi$ and the constant C is given by

$$C = \sqrt{-\frac{1}{2}\frac{\partial^2\mathcal{F}(m(\varphi_d),A_{max})}{\partial A^2}\left(\frac{1}{\widehat{\varphi_d}^2} + \frac{\partial\mathcal{F}(m(\varphi_d),A_{max})}{\partial m}\frac{\partial m(\varphi_d)}{\partial\hat{\varphi}}\right)}.$$

Eq. **S17** implies that

$$\frac{dA(\varphi)}{d\varphi} = -\frac{C/2}{(\hat{\varphi}-\hat{\varphi}_d)^{1/2}} + \text{regular terms}, \qquad \textbf{[S18]}$$

that is, $A'(\varphi)$ has a square-root singularity at $\varphi = \varphi_d$.

We show now that this square-root singularity is transmitted to compressibility. Expanding the expression for the pressure

$$p(\varphi) = \frac{1}{m(\varphi)}\left(1 + 2^{d-1}\varphi(1 - \mathcal{G}(m_{db}A(m(\varphi;\Sigma_0),\varphi)))\right), \qquad \textbf{[S19]}$$

in $\varphi = \varphi_d$ we obtain

$$p(\hat{\varphi}) = p(\hat{\varphi}_d) - B(\hat{\varphi})\sqrt{\hat{\varphi} - \hat{\varphi}_d} + \mathcal{O}(\hat{\varphi} - \hat{\varphi}_d), \qquad \textbf{[S20]}$$

where we defined the (positive) constant

$$B(\hat{\varphi}) = -\frac{d(1 - m(\hat{\varphi}))}{2m(\hat{\varphi})A_{max}}\frac{\hat{\varphi}}{\hat{\varphi}_d}C.$$

Deriving Eq. **S20** we obtain

$$\frac{dp(\hat{\varphi})}{d\hat{\varphi}} = -\frac{B(\hat{\varphi}_d)/2}{(\hat{\varphi} - \hat{\varphi}_d)^{1/2}} + \text{regular terms}, \qquad \textbf{[S21]}$$

that is, the derivative $p'(\hat{\varphi})$ of the pressure has a singularity in $\hat{\varphi} = \hat{\varphi}_d$ with the same critical exponent of $A'(\hat{\varphi})$. This fact implies an overshoot in the pressure as the system escapes from the metastable state. Indeed, the same overshoot can be seen also in the state-following method (6), not only in the pressure vs. density plane, but also in the shear stress vs. shear strain plane.

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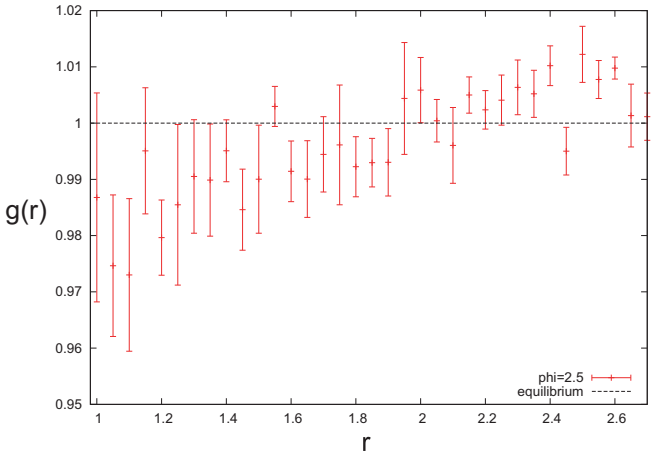

Fig. S1. Radial distribution function $g(r)$ of the planted configuration at density $\varphi_0 = 2.5$.