Supplementary information: Excitation of vibrational soft modes in disordered systems using active oscillation

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I. NEWTONIAN DYNAMICS WITH FRICTION

In this section, we detail how we perform the Newtonian dynamic simulation (Eq. (2) of the main text) with a friction term $\propto \xi$ and an active oscillation in the particles' diameters (Eq. (3) of the main text).

Our dynamical variables are the positions $\{\mathbf{r}_i(t)\}$, velocities $\{\mathbf{v}_i(t)\}$, and diameters of the particles $\{\sigma_i(t)\}$, where the index $i = 1, 2, \dots N$ labels the particle and $N = 1000$ is the total number of particles in the system. We start our simulation at $t = 0$ with all particles at rest: $\mathbf{v}_i(0) = 0$, $\forall i$. We also assign a random position $\mathbf{r}_i(0)$ for each particle i anywhere inside the simulation box. The initial particles' diameter $\sigma_i(0)$ is either 0.714σ or σ with a ratio $3:2$ to avoid crystallization.

We then update the particles' positions and velocities according to Newtonian dynamics (Eq. (2) of the main text):

$$m\frac{d\mathbf{v}_i}{dt} + \xi\mathbf{v}_i = -\sum_{j=1, j\neq i}^{N} \frac{\partial V(r_{ij})}{\partial \mathbf{r}_i} \tag{1}$$

$$\mathbf{v}_i = \frac{d\mathbf{r}_i}{dt} \tag{2}$$

where m is the mass of each particle, ξ is the friction coefficient between the particles and the friction, and $V(r_{ij})$ is the two body potential, given by:

$$V(r_{ij}) = \frac{\epsilon}{2}\left(1 - \frac{r_{ij}}{\sigma_{ij}}\right)^2 H(r_{ij} - \sigma_{ij}) \tag{3}$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and $\sigma_{ij} = (\sigma_i + \sigma_j)/2$. $H(x)$ is the Heaviside function, defined such that $H(x) = 1$ if $x \geq 0$ and $H(x) = 0$ if $x < 0$. We also update the particles' diameters using a sinusoidal function:

$$\sigma_i(t) = \sigma_i(0)\left[1 + a\cos(\omega_d t + \psi_i)\right] \tag{4}$$

where a is the amplitude of active oscillation and ω_d is the driving frequency. The phase difference ψ_i is chosen to be $\psi_i = 2\pi i/N$ as this will conserve the global volume fraction. Note that by introducing an active oscillation in the particles' diameters (Eq. (4)), we drive the system out-of-equilibrium.

We then non-dimensionalize the equations of motion Eqs. (1,2) by rescaling the position and time by:

$$\begin{aligned} \mathbf{r}_i &\to \mathbf{r}_i/\sigma \\ t &\to \omega_0 t \end{aligned} \tag{5}$$

where $\omega_0 = \sqrt{\frac{\epsilon}{m\sigma^2}}$ is the characteristic frequency defined in the main text. Subsequently Eq. (1) become:

$$\frac{d\mathbf{v}_i}{dt} + \xi\frac{\sigma}{\sqrt{m\epsilon}}\mathbf{v}_i = \mathbf{F}_i \tag{6}$$

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where

$$\mathbf{F}_i = \sum_{j=1, j\neq i}^{N} (1 - r_{ij})\, H(r_{ij} - 1) \frac{\mathbf{r}_{ij}}{r_{ij}}. \tag{7}$$

Finally, putting in the definition of damping coefficient $\zeta = \frac{\xi\sigma}{2\sqrt{m\epsilon}}$ from the main text, the dimensionless equations of motion are:

$$\frac{d\mathbf{v}_i}{dt} + 2\zeta \mathbf{v}_i = \mathbf{F}_i \tag{8}$$

$$\mathbf{v}_i = \frac{d\mathbf{r}_i}{dt} \tag{9}$$

In our simulations, we fix $\zeta = 0.01$.

Eqs. (8,9) are then discretized in time similar to velocity Verlet algorithm [1]:

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t\,(1 - \zeta\Delta t) + \frac{1}{2}\mathbf{F}_i(t)\Delta t^2 \tag{10}$$

$$\mathbf{v}_i\left(t + \frac{\Delta t}{2}\right) = \mathbf{v}_i(t)\,(1 - \zeta\Delta t) + \frac{1}{2}\mathbf{F}_i(t)\Delta t \tag{11}$$

$$\mathbf{v}_i(t + \Delta t) = (1 + \zeta\Delta t)^{-1}\left[\mathbf{v}_i\left(t + \frac{\Delta t}{2}\right) + \frac{1}{2}\mathbf{F}_i(t + \Delta t)\Delta t\right], \tag{12}$$

where $\Delta t \ll 1$ is the time interval. In our simulations, we fix $\Delta t = 0.01$. Thus, given $\{\mathbf{r}_i(0), \mathbf{v}_i(0), \sigma_i(0)\}$, we can update $\{\mathbf{r}_i(t), \mathbf{v}_i(t), \sigma_i(t)\}$ using Eqs. (10,11,12,4).

We now give derivations of Eqs. (10,11,12). To derive Eq. (10), we first Taylor expand $\mathbf{r}_i(t + \Delta t)$:

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t + \frac{1}{2}\frac{d\mathbf{v}_i(t)}{dt}\Delta t^2 + \mathcal{O}\left(\Delta t^3\right).$$

Substituting Eq. (8), we obtain:

$$\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t + \frac{1}{2}\left(\mathbf{F}_i(t) - 2\zeta\mathbf{v}_i(t)\right)\Delta t^2 + \mathcal{O}\left(\Delta t^3\right) \tag{13}$$

$$= \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t\,(1 - \zeta\Delta t) + \frac{1}{2}\mathbf{F}_i(t)\Delta t^2 + \mathcal{O}\left(\Delta t^3\right). \tag{14}$$

To derive Eq. (11), we Taylor expand $\mathbf{v}_i\left(t + \frac{\Delta t}{2}\right)$ to obtain:

$$\mathbf{v}_i\left(t + \frac{\Delta t}{2}\right) = \mathbf{v}_i(t) + \frac{1}{2}\frac{d\mathbf{v}_i(t)}{dt}\Delta t + \mathcal{O}\left(\Delta t^2\right). \tag{15}$$

Substituting Eq. (8), we obtain:

$$\mathbf{v}_i\left(t + \frac{\Delta t}{2}\right) = \mathbf{v}_i(t) + \frac{1}{2}\left(\mathbf{F}_i(t) - 2\zeta\mathbf{v}_i(t)\right)\Delta t + \mathcal{O}\left(\Delta t^2\right) \tag{16}$$

$$= \mathbf{v}_i(t)\,(1 - \zeta\Delta t) + \frac{1}{2}\mathbf{F}_i(t)\Delta t + \mathcal{O}\left(\Delta t^2\right). \tag{17}$$

Finally to derive Eq. (12), we Taylor expand $\mathbf{v}_i\left(t + \frac{\Delta t}{2}\right)$ to obtain:

$$\mathbf{v}_i\left(t + \tfrac{\Delta t}{2}\right) = \mathbf{v}_i(t + \Delta t) - \frac{1}{2}\frac{d\mathbf{v}_i(t + \Delta t)}{dt}\Delta t + \mathcal{O}\left(\Delta t^2\right). \tag{18}$$

Substituting Eq. (8), we obtain:

$$\mathbf{v}_i\left(t + \frac{\Delta t}{2}\right) = \mathbf{v}_i(t + \Delta t) - \frac{1}{2}\left[\mathbf{F}_i(t + \Delta t) - 2\zeta\mathbf{v}_i(t + \Delta t)\right]\Delta t + \mathcal{O}\left(\Delta t^2\right) \tag{19}$$

and thus we recover Eq. (12).

II. NORMAL MODE ANALYSIS

In this section, we detail how to obtain the normal eigenmodes from a static configuration close to a local potential energy minimum [2]. The total potential energy is obtained by summing all the two body potential $V(r_{ij})$:

$$U(\mathbf{r}^N) = \frac{1}{2}\sum_i \sum_{j\neq i} V(r_{ij}) \tag{20}$$

where $\mathbf{r}^N = (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)^T$. The Hessian matrix $\mathbf{H}_{ij}$ is defined to be the second derivative of the total potential energy with respect to the positions of the particles:

$$\mathbf{H}_{ij} = \frac{\partial^2 U}{\partial \mathbf{r}_i \partial \mathbf{r}_j}. \tag{21}$$

More explicitly, the Hessian matrix can be written as:

$$\mathbf{H} = \begin{pmatrix} \frac{\partial^2 U}{\partial x_1 \partial x_1} & \frac{\partial^2 U}{\partial x_1 \partial y_1} & \frac{\partial^2 U}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 U}{\partial x_1 \partial y_N} \\ \frac{\partial^2 U}{\partial y_1 \partial x_1} & \frac{\partial^2 U}{\partial y_1 \partial y_1} & & & \vdots \\ \frac{\partial^2 U}{\partial x_2 \partial x_1} & & \ddots & & \\ \vdots & & & & \\ \frac{\partial^2 U}{\partial y_N \partial x_1} & \cdots & & & \frac{\partial^2 U}{\partial y_N \partial y_N} \end{pmatrix} \tag{22}$$

where (x_i, y_i) are the Cartesian coordinates of $\mathbf{r}_i$. The components of the Hessian matrix can be calculated as follow:

$$\begin{aligned}
\frac{\partial^2 U}{\partial x_i \partial x_i} &= \sum_{j\neq i} \left\{ V''(r_{ij}) \left(\frac{x_i - x_j}{r_{ij}}\right)^2 + V'(r_{ij}) \frac{1}{r_{ij}} \left(1 - \left(\frac{x_i - x_j}{r_{ij}}\right)^2\right) \right\} \\
\frac{\partial^2 U}{\partial y_i \partial y_i} &= \sum_{j\neq i} \left\{ V''(r_{ij}) \left(\frac{y_i - y_j}{r_{ij}}\right)^2 + V'(r_{ij}) \frac{1}{r_{ij}} \left(1 - \left(\frac{y_i - y_j}{r_{ij}}\right)^2\right) \right\} \\
\frac{\partial^2 U}{\partial x_i \partial x_j} &= -V''(r_{ij}) \left(\frac{x_i - x_j}{r_{ij}}\right)^2 + V'(r_{ij}) \frac{1}{r_{ij}} \left(1 + \left(\frac{x_i - x_j}{r_{ij}}\right)^2\right) \\
\frac{\partial^2 U}{\partial y_i \partial y_j} &= -V''(r_{ij}) \left(\frac{y_i - y_j}{r_{ij}}\right)^2 + V'(r_{ij}) \frac{1}{r_{ij}} \left(1 + \left(\frac{y_i - y_j}{r_{ij}}\right)^2\right) \\
\frac{\partial^2 U}{\partial x_i \partial y_i} &= \sum_{j\neq i} \left\{ V''(r_{ij}) \left(\frac{x_i - x_j}{r_{ij}}\right) \left(\frac{y_i - y_j}{r_{ij}}\right) - V'(r_{ij}) \frac{1}{r_{ij}} \left(\frac{x_i - x_j}{r_{ij}}\right) \left(\frac{y_i - y_j}{r_{ij}}\right) \right\} \\
\frac{\partial^2 U}{\partial x_i \partial y_j} &= -V''(r_{ij}) \left(\frac{x_i - x_j}{r_{ij}}\right) \left(\frac{y_i - y_j}{r_{ij}}\right) + V'(r_{ij}) \frac{1}{r_{ij}} \left(\frac{x_i - x_j}{r_{ij}}\right) \left(\frac{y_i - y_j}{r_{ij}}\right)
\end{aligned} \tag{23}$$

where V' and V'' are the first and second derivative of the two body potential respectively. The normal eigenmodes $\{\mathbf{e}_\omega\}$ and eigenfrequencies $\{\omega\}$ are then obtained by solving the eigenvalue equation:

$$\mathbf{H} \cdot \mathbf{e}_\omega = \omega^2 \mathbf{e}_\omega \tag{24}$$

where the Hessian matrix is evaluated at some static configuration $\mathbf{r}_0^N$ close to a local potential energy minimum. Eq. (24) can be solved using standard Jacobi iteration method [3] to obtain a set of eigenmodes $\{\mathbf{e}_\omega\}$ and corresponding eigenfrequencies $\{\omega\}$.

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