Soft Matter

SUPPORTING INFORMATION

Particle dispersion through porous media with heterogeneous attractions

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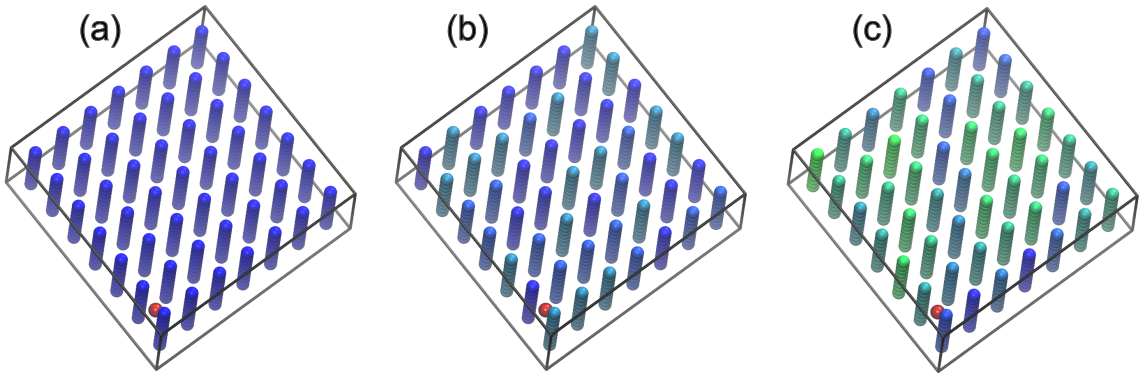

Fig. S1 Schematic illustration of 7×7 subsections of 100×100 nanopost arrays with well depth $u_0 = 5$ and heterogeneity parameter $\beta =$ (a) 0, (b) 2, and (c) 5.

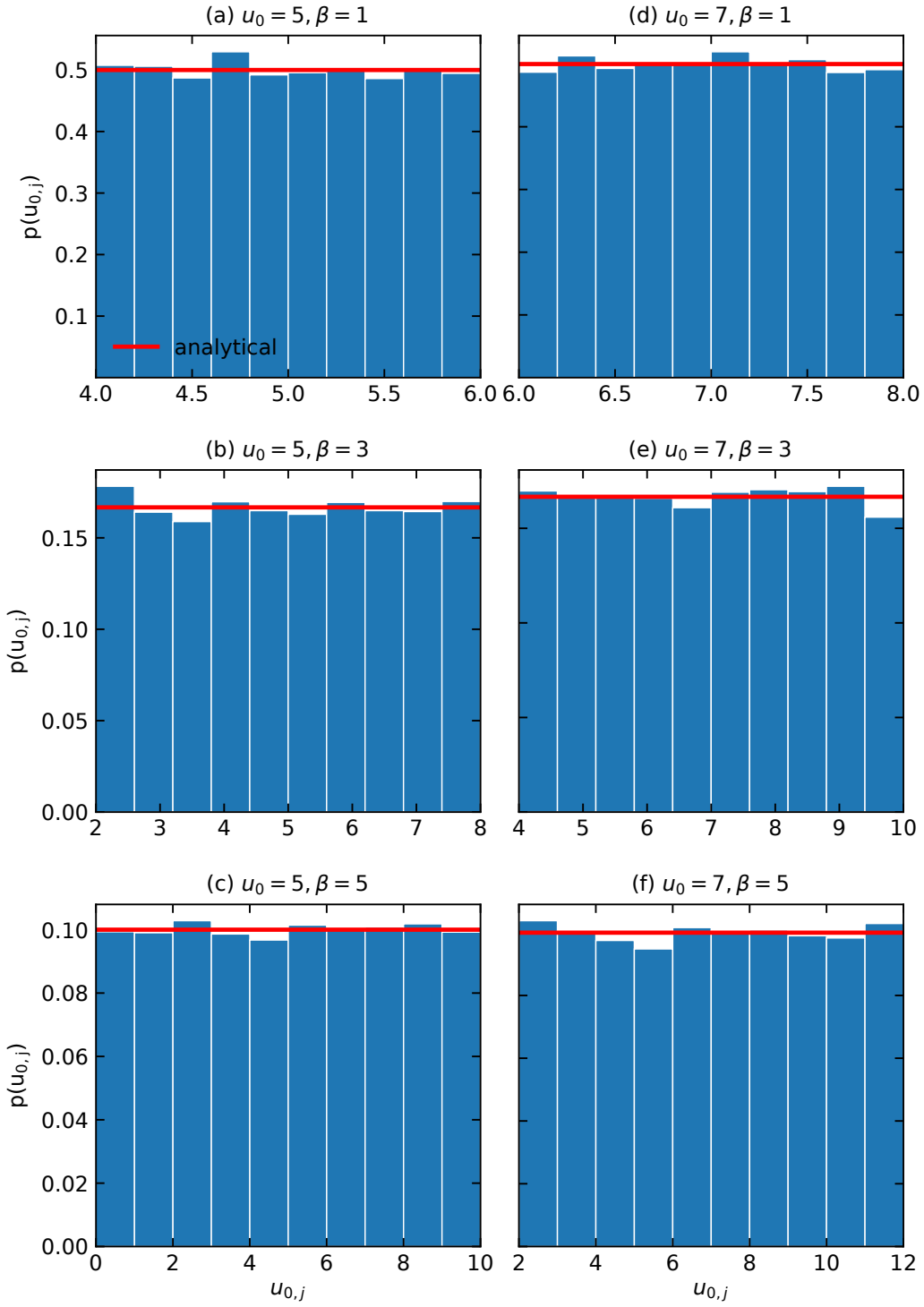

Fig. S2 Histograms of the interaction energy distributions for (a),(b),(c) $u_0 = 5$, and (d),(e),(f) $u_0 = 7$ for (a),(d) $\beta = 1$, (b),(e) $\beta = 3$ and (c),(f) $\beta = 5$. The red line is the analytical result for a uniform distribution $u_0 \mathscr{U}(1-\beta, 1+\beta)$.

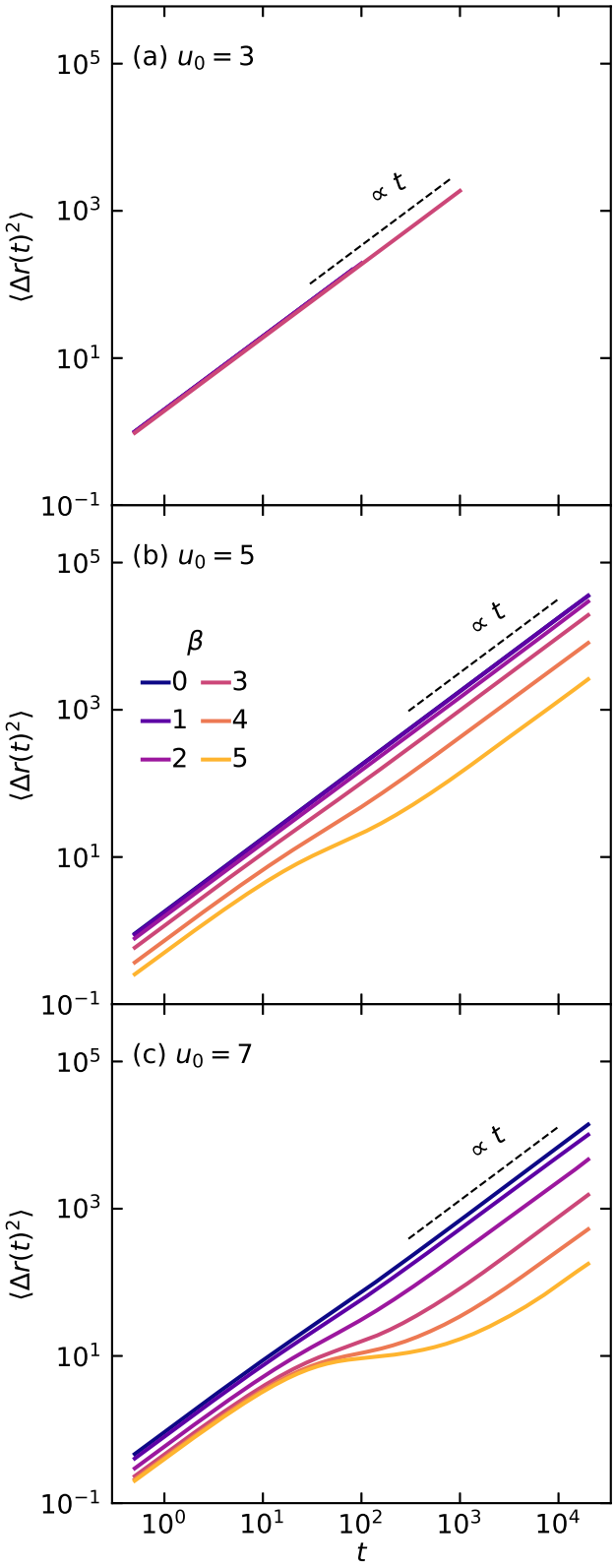

Fig. S3 Mean-squared displacements $\langle \Delta r^2(t) \rangle$ as functions of lag time t in nanopost arrays with $\phi = 0.014$ and $u_0 =$ (a) 3, (b) 5, and (c) 7. The dashed lines are references indicating $\propto t$ scaling. The legend in (b) applies to all panels.

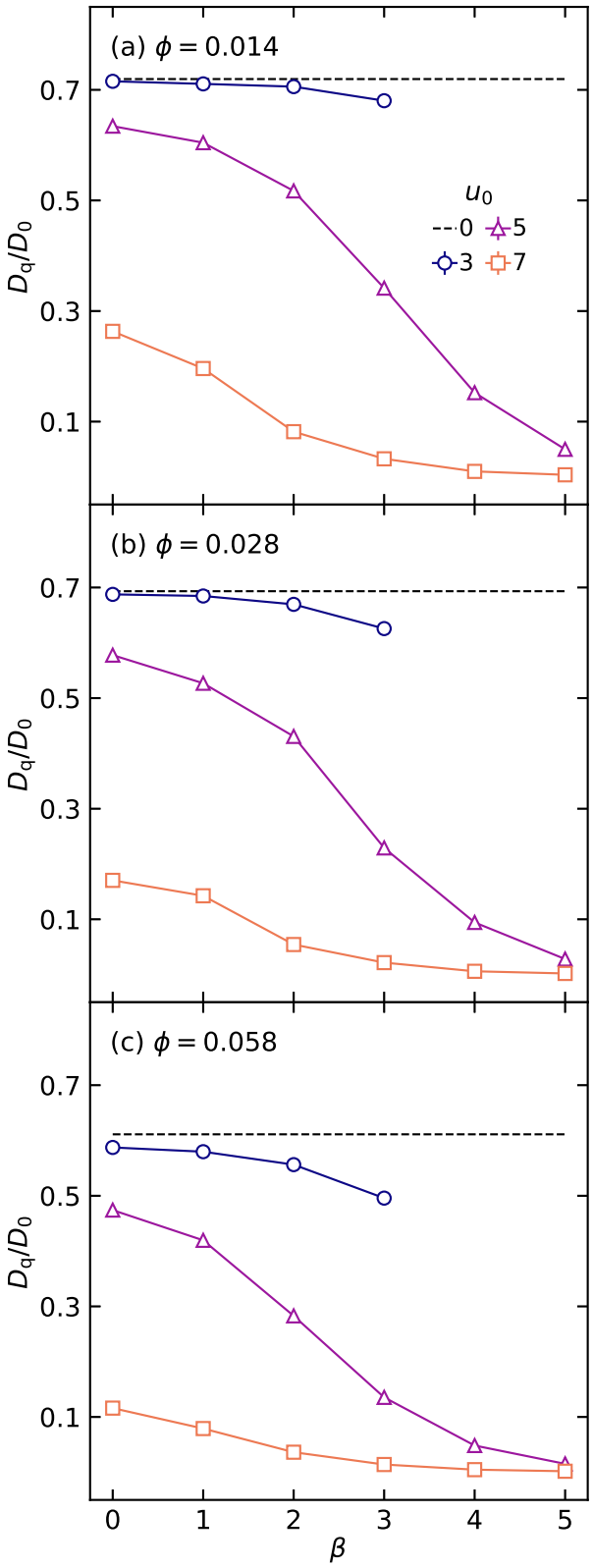

Fig. S4 Normalized diffusion coefficients D_q/D_0 as functions of the heterogeneity parameter β in nanopost arrays with $\phi =$ (a) 0.014, (b) 0.028, and (c) 0.058. The dashed lines indicate the values of D_q/D_0 for cases where $u_0 = 0$. The legend in (a) applies to all panels. Estimated uncertainties are smaller than the symbol sizes.

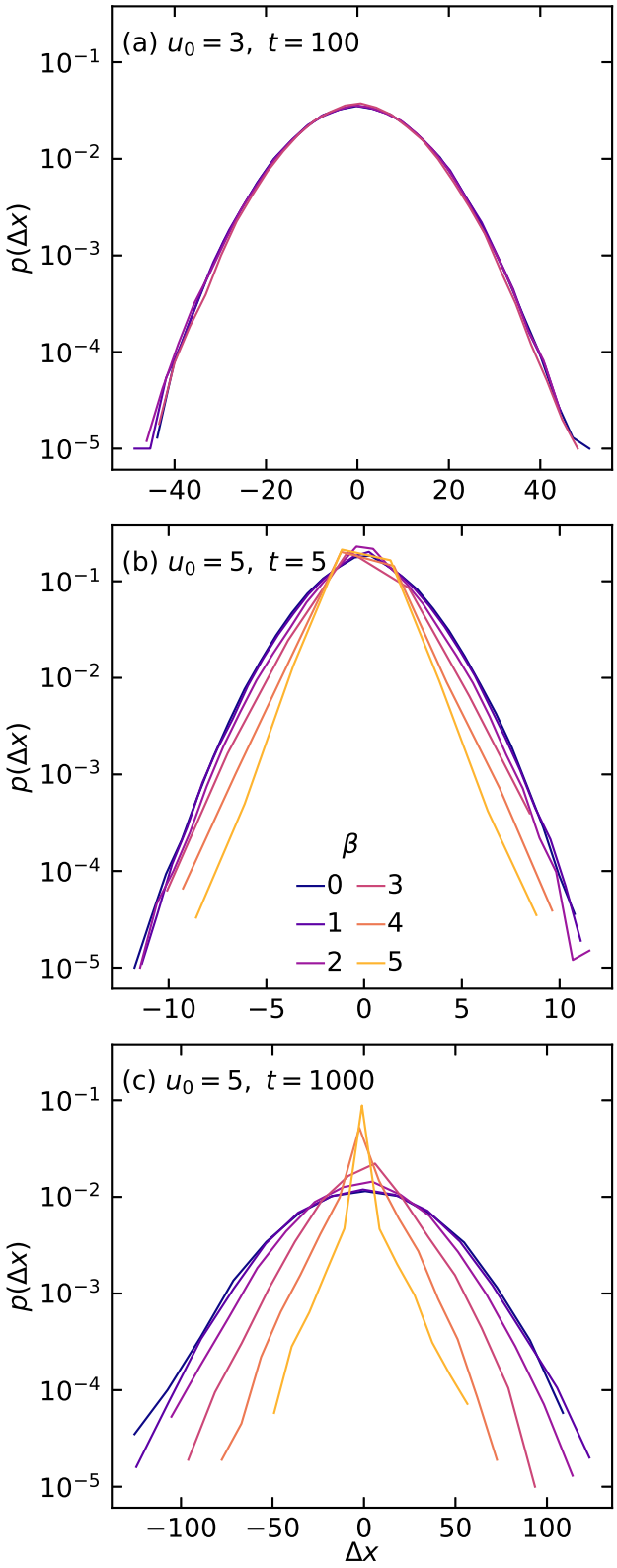

Fig. S5 Particle displacement distributions at different lag times t for nanopost arrays with $\phi = 0.028$ and $u_0 =$ (a) 3 and (b),(c) 5. The lag times are chosen to lie within the different diffusive regimes observed in the corresponding MSDs. The legend in (b) applies to all panels.

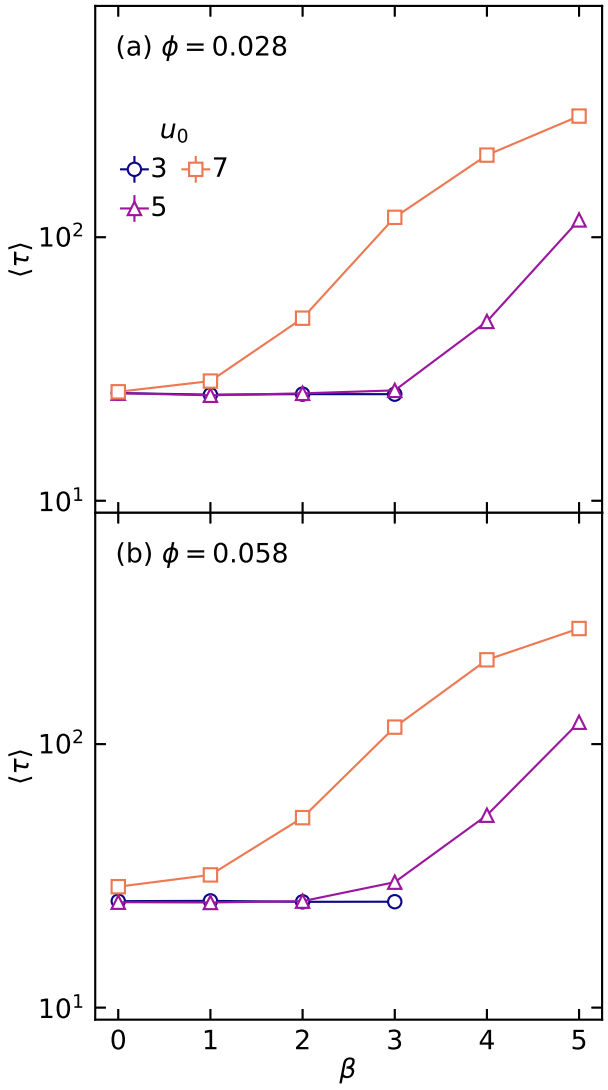

Fig. S6 Tortuosities $\langle\tau\rangle$ as functions of the heterogeneity parameter β in nanopost arrays with $\phi =$ (a) 0.028 and (b) 0.058. The legend in (a) applies to both panels. Estimated uncertainties are smaller than the symbol sizes.

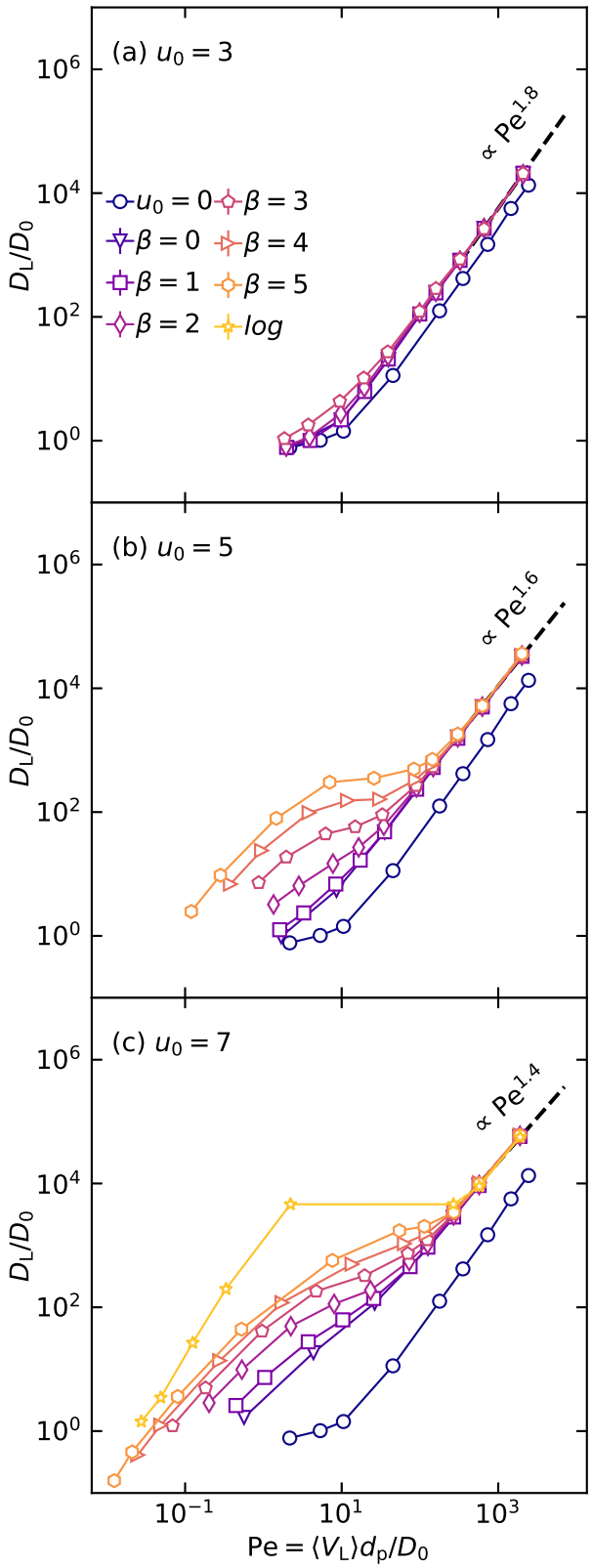

Fig. S7 Normalized longitudinal dispersion coefficients D_L/D_0 as functions of Pe for nanopost arrays with $\phi = 0.028$ and $u_0 =$ (a) 3, (b) 5, and (c) 7. Panel (c) also shows the results for the case where the system's heterogeneity follows a lognormal distribution, $Y \sim Lognormal(u_0, \beta^2)$, and $\beta = 2$ in this instance. The legend in (a) applies to all panels. Estimated uncertainties are smaller than the symbol sizes.

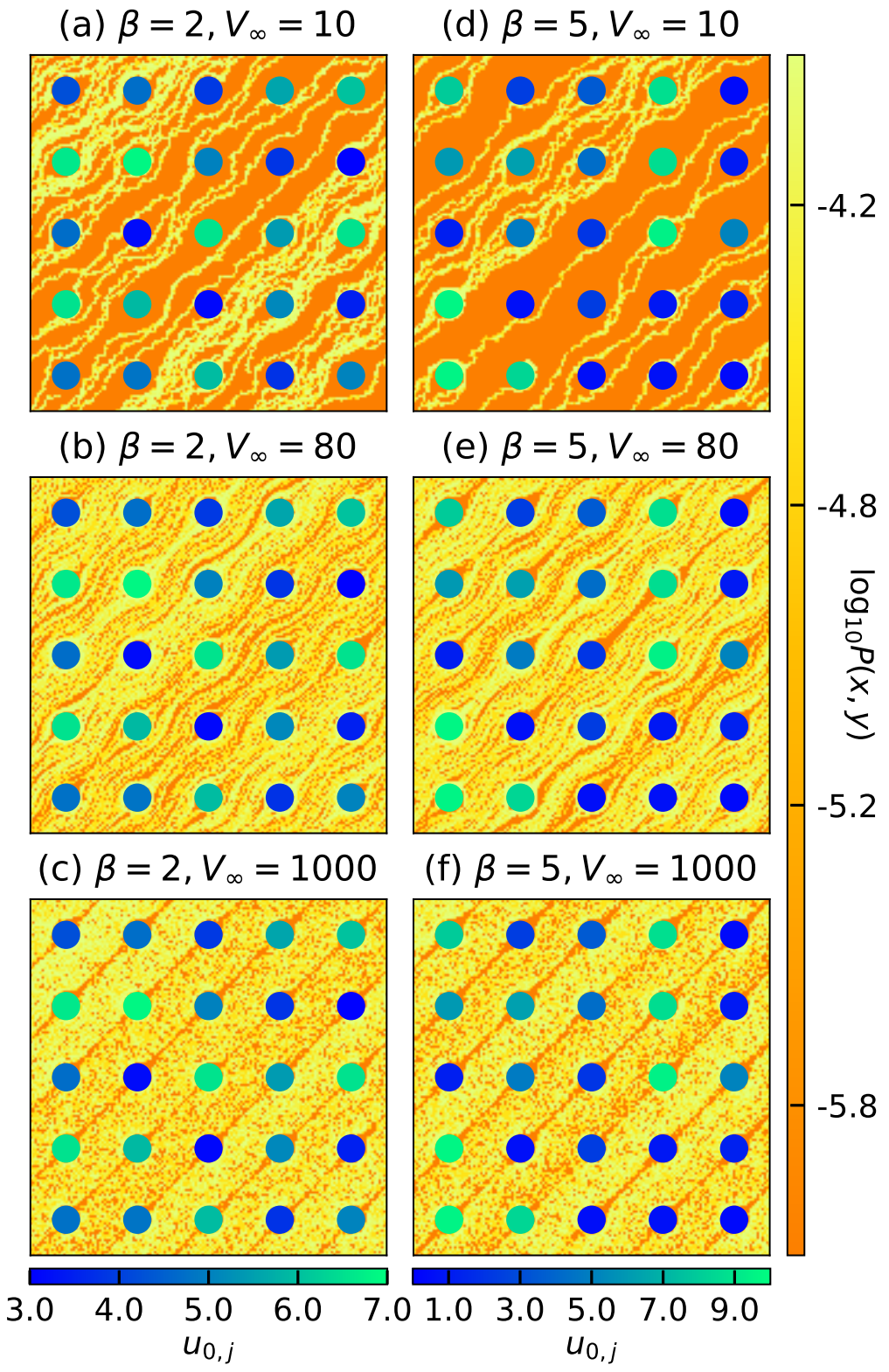

Fig. S8 Log-probability density distributions of particle positions $\log_{10} P(x, y)$ at flow rates $V_\infty =$ (a),(d) 10, (b),(e) 80, and (c),(f) 1000 in 5×5 subsections of nanopost arrays with $\phi = 0.028$, $u_0 = 5$, and heterogeneity parameter $\beta =$ (a),(b),(c) 2 and (d),(e),(f) 5. The nanoposts are colored using a blue-to-green scheme to indicate increasing well depth $u_{0,j}$.

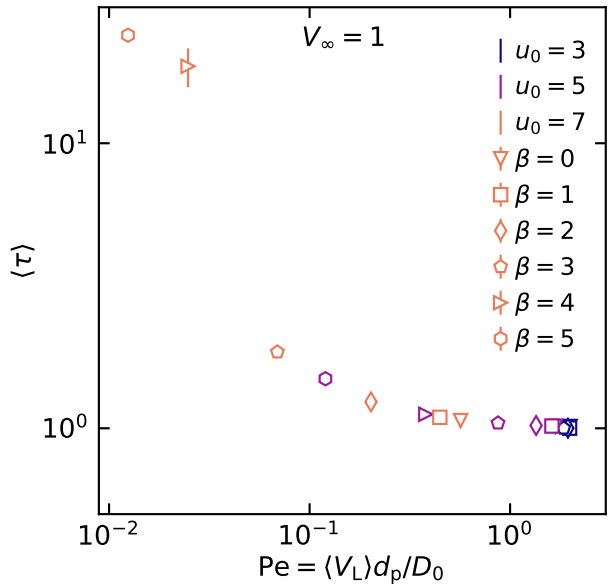

Fig. S9 Tortuosities $\langle\tau\rangle$ as functions of Pe for low flow rate $V_\infty = 1$ in nanopost arrays with $\phi = 0.028$. The symbols correspond to β and are the same across u_0. The symbols and colors denote different values of β and u_0, respectively.

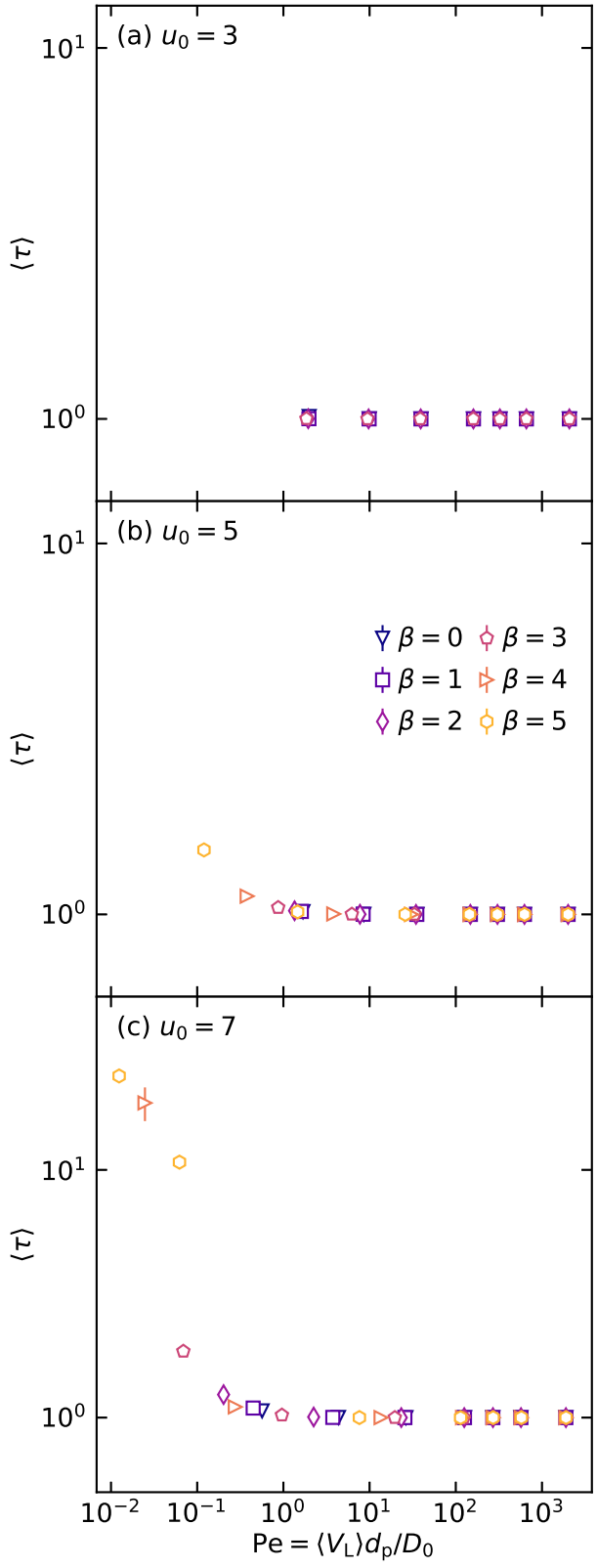

Fig. S10 Tortuosities $\langle\tau\rangle$ as functions of Pe in nanopost arrays with $\phi = 0.028$ and $u_0 =$ (a) 3, (b) 5, and (c) 7. The legend in (b) applies to all panels.

Supporting Movie 1: This movie has been referred as ESI Movie 1 in the main text and has the file name Movie1.mpg. It shows normal diffusion through the void space in a nanopost array with $u_0 = 0$ and $\beta = 0$. As described in the main text, the simulations were performed under dilute conditions, and the movie shows trajectories for multiple independent simulations that have been overlaid.

Supporting Movie 2: This movie has been referred as ESI Movie 2 in the main text and has the file name Movie2.mpg. It shows hopping diffusion between nanoposts in a system with $u_0 = 5$ and $\beta = 0$. As described in the main text, the simulations were performed under dilute conditions, and the movie shows trajectories for multiple independent simulations that have been overlaid.