Supplemental Material
Better than Counting: Density Profiles from Force Sampling

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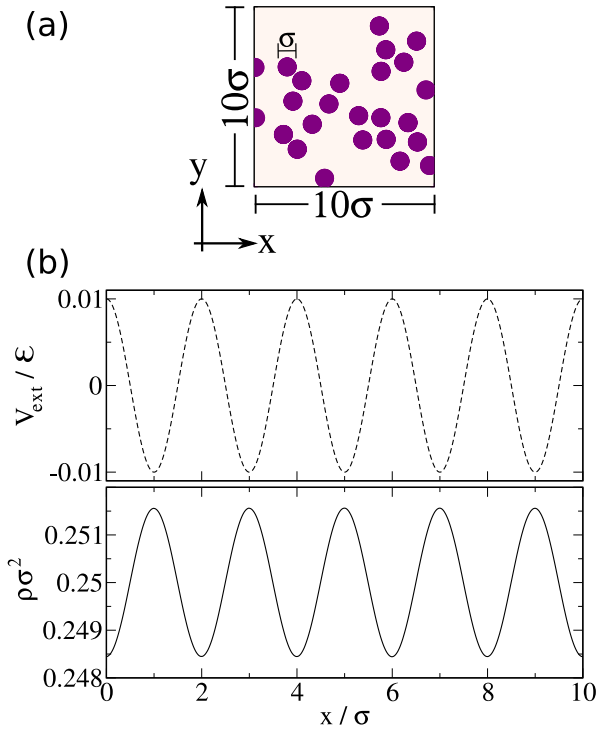
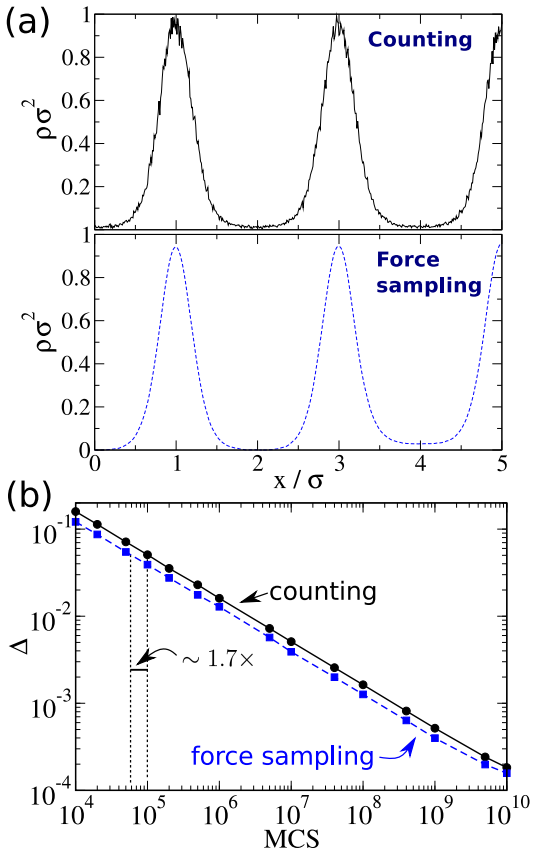


Supplemental Fig. 1. (a) Schematic of the system, $N = 25$ LJ particles of size σ in a square box of side length 10σ with periodic boundary conditions. (b) External potential (top) and corresponding equilibrium density profile (bottom) obtained with MC simulation (10^{12} Monte Carlo steps).



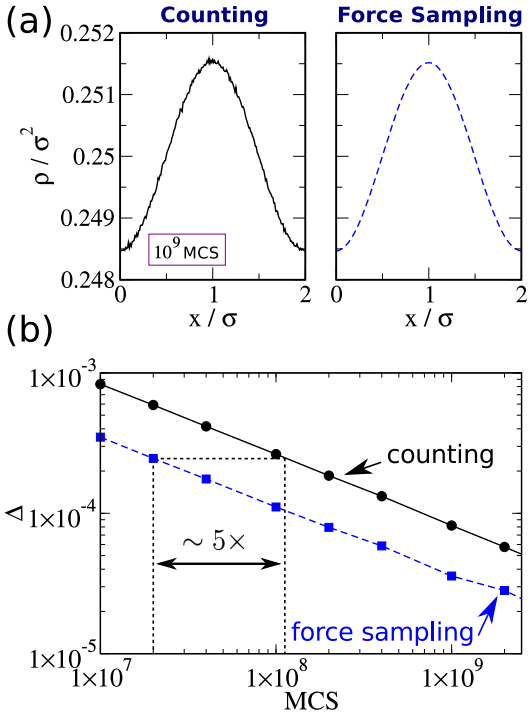
Supplemental Fig. 2. (a) Density profiles obtained with MC simulations using the counting (top) and the force sampling (bottom) method. The number of MCS is 10^4 and the bin size is $\Delta x/\sigma = 0.01$. The size of the box is $L/\sigma = 10$ (only half of the box is shown) and $N = 25$. The particles are in equilibrium in the external potential $V_{\rm ext}(x) = V_0 \sin(2\pi n_w x/L)$ with $n_w = 5$ and $V_0/\epsilon = 3$. The temperature is $k_{\rm B}T/\epsilon = 1$. (b) Logarithmic plot of the sampling error Δ as a function of the number of Monte Carlo steps. Data obtained via counting (black circles) and via force sampling (blue squares). The "true" equilibrium profile used to compute Δ is approximated by the average profile given by both methods after $4 \cdot 10^{11}$ MCS.

System

A schematic of the system is shown in Supplemental Fig. 1a. The external potential and the corresponding equilibrium density profile are shown in Supplemental Fig. 1b and c, respectively.

High density states

An example exhibiting local high density values is shown in Supplemental Fig. 2. The particles are in equilibrium in the same type of external potential as that shown in Fig. 1b of the main text, that is $V_{\rm ext}(x) = V_0 \sin(2\pi n_w x/L)$ with $n_w = 5$, but much stronger, $V_0/\epsilon = 3$. As a result the density profile shows strong oscillations, see Supplemental Fig. 2a. The force sampling method is more accurate and generates smoother profiles than the counting method. The reduction in the sampling error is, however, less pronounced than in cases with smooth density profiles. To achieve a given sampling error Δ with traditional counting we need simulations ~ 2 times longer than using force sampling, see Supplemental Fig. 2b. That is, force sampling reduces the computation time by $\sim 40\%$.



Supplemental Fig. 3. (a) Density profiles (MC simulation with 10^9 MCS) obtained via counting (left) and force sampling (right) in a system with $N = 10^3$ confined in a box with side lengths $L_x/\sigma = 10$ and $L_y/\sigma = 400$. The bin size is $\Delta x/\sigma = 0.01$. The particles are in equilibrium in the external potential $V_{\rm ext}(x) = V_0 \sin(2\pi n_w x/L_x)$, with $V_0/\epsilon = 0.01$ and $n_w = 5$. Only one fifth of the simulation box is shown, $x/\sigma \in [0, 2]$. (b) Logarithmic plot of the sampling error as a function of the number of MCS.

Realistic number of particles

In Supplemental Fig. 3a we show a comparison of the density profiles obtained with MC via counting and force sampling a system with $N = 10^3$. The particles are in a rectangular box with side lengths $L_x/\sigma = 10$ and $L_y/\sigma = 400$ subject to the external potential shown in Fig. 1b. Therefore, the system is homogeneous in the $y-$coordinate. In Supplemental Fig. 3b we show the sampling error Δ of both methods in MC. Force sampling is ~ 5 times more accurate than counting. The "true" equilibrium profile used to compute the sampling error Δ is approximated here by the average profile given by both methods after $2 \cdot 10^{10}$ MCS (obtained by averaging $2 \cdot 10^3$ MC simulations of 10^7 MCS each).

Multidimensional density profiles

If the density profile depends on several spatial coordinates, there are at least three routes to implement the force sampling method. One possibility, as described in Eq. (5) of the main text, is to perform a line integral of the force density. Alternatively, we can invert the force density balance equation and obtain the density profile via a volume integral over the full space, see Eqs. (6) and (7) of the main text. Eq. (7) of the main text can be solved either in real or in Fourier space (see Ref. [21] of the main text) a post processing of the data sampled during the simulation. Finally, we can also obtain the density profile via numerical minimization of the functional

$$H[\rho] = \int d\mathbf{r} ||\nabla\rho(\mathbf{r}) - \mathbf{F}(\mathbf{r})||^2, \qquad (1)$$

which is a standard procedure to numerically find the scalar potential that generates a given curl-free vector field. In practice, inverting the force balance equation via Eq. (7) of the main text, or numerically minimizing $H[\rho]$ results in more accurate density profile than solving the line integral in Eq. (5) of the main text. Note that both inversion of the force balance equation and minimization of $H[\rho]$ use information from the whole system in order to compute the local density profile at position $\mathbf{r}$. The two-dimensional density profiles shown in Fig. 4 (right) of the main text have been obtained via minimization of $H[\rho]$.