Supplementary Information for manuscript

On standardised moments of force distribution in simple liquids

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Molecular dynamics (MD) data presented in the main manuscript are provided as data files, which are described in this document. We also include plots of additional statistics of interest which have been sampled during the same MD simulations. Units of data presented are standard reduced units, which are discussed in Section II of the manuscript.

Supporting information for **Figure 1**

Data presented in Figure 1 are included as Supplementary File `figure1.dat`, where the first column gives the length of the box width, L, and the second column includes the calculated values of kurtosis, α_4. For this simulation we utilised Langevin dynamics with frictional parameter of $\gamma = 0.1$, the simulation length was 1.1×10^8 time steps, each of size $\Delta t = 0.01$. The first 0.1×10^8 time steps were for initialisation, and the remaining $t_{\text{sim}} = 10^8$ time steps were used to calculate statistics from the simulation. We calculated the temperature of our system at points in time separated by $r = 10^4$ time steps and plotted them in Figure S1(a). While some fluctuations are relatively large, the average temperature ($T = 1.003$) is near the target temperate $T = 1$ (the red dashed line) in Figure S1(a). To illustrate that the large values of temperature are rare, we have included a histogram in Figure S1(b) created from the same $t_{\text{sim}}/r = 10^4$ results, which we have plotted as a time series in Figure S1(a). This histogram has been normalized and presented as a probability distribution function, $p(T)$, in Figure S1(b).

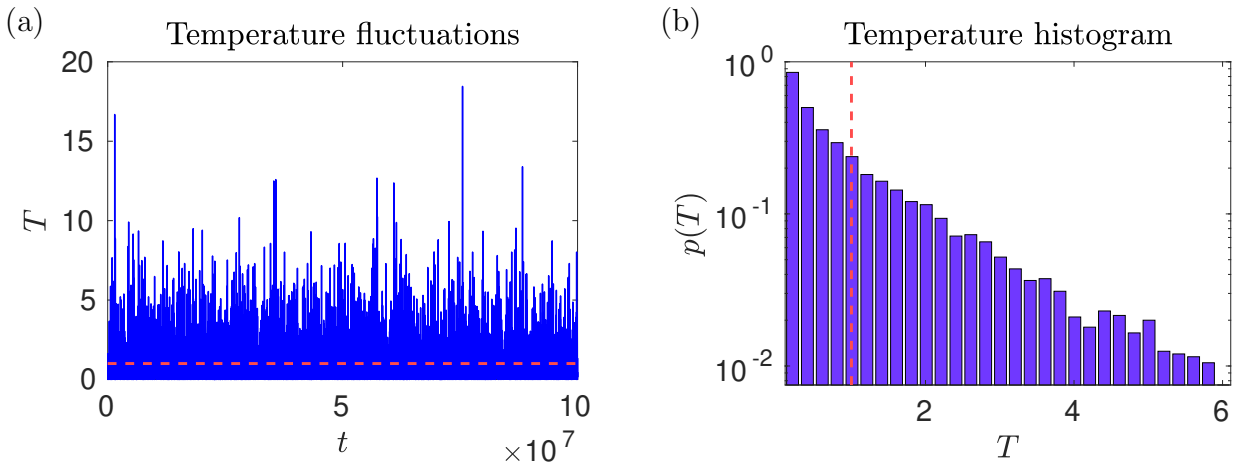

Figure S1: (a) *Temperature fluctuations between times separated by* 10^4 *time steps are shown in blue;* (b) *histogram of the sampled temperature values, normalized as a probability density function and visualized using a log-scale. The red dashed lines on both panels correspond to the average temperature calculated over the whole* t_{sim} *simulation length* ($T \approx 1$).

Supporting information for **Figure 2**

Data presented in Figure 2 of the manuscript are included as Supplementary File `figure2.dat`, where the first column gives the length of the box width, L, and the second column includes the calculated values of kurtosis, α_4. The third, fourth, fifth and sixth columns give the calculated values of α_6, α_8, α_{10} and α_{12} respectively. We include data from simulations of length $t_{\rm sim} = 10^{11}$ time steps at different box widths $L = 1.2^{i-1} \times 10$ for $i = 1, 2, \ldots, 30$. We use the velocity Verlet algorithm with the Nosé-Hoover thermostat, relaxation parameter $Q = 10$, time step $\Delta t = 0.01$ and target temperature $T = 1$. In Figure S2, we present illustrative figures of temperature fluctuations for three of these simulations, using box widths $L = 10$, $L = 154$ and $L = 1978$. We plot the instantaneous temperatures at points in time separated by $r = 10^6$ time steps, visualizing $t_{\rm sim}/r$ data points. We have included the average temperature for each simulation as a red dashed line in each of the panels in Figure S2, these are $T = 1.0003$, $T = 1.00002$, $T = 0.999997$ for $L = 10$, $L = 154$ and $L = 1978$, respectively.

Supporting information for **Figure 3**

Data presented in Figure 3 of the manuscript are included as Supplementary File `figure3.dat`, where the first column gives the temperature, T, and the second column includes the calculated values of kurtosis, α_4. The third, fourth, fifth and sixth columns give the calculated values of α_6, α_8, α_{10} and α_{12}, respectively. The statistics are calculated over the whole simulation. We include data for simulations with target temperature $T = i/100$ for $i = 1, 2, \ldots, 300$. We use the velocity Verlet algorithm with the Nosé-Hoover thermostat with temperature dependent relaxation parameter $Q = T$ to simulate each system over $t_{\rm sim} = 10^{11}$ time steps of length $\Delta t = 0.01$. In Figure S3, we present illustrative figures of temperature fluctuations for three of these simulations, using target temperatures $T = 0.01$, $T = 0.1$ and $T = 0.15$, and visualizing the instantaneous temperatures at points in time separated by $r = 10^6$ time steps. We have included the sampled average temperature for each simulation as a red dashed line in each of the panels in Figure S3.

Supporting information for **Figure 4**, **Figure 5** and **Figure 6**

Data presented in Figures 4, 5 and 6 are included in the Supplementary File `figures456.xlsx`. To obtain our results in Figures 4 and 5, we use the velocity Verlet algorithm with the Nosé-Hoover thermostat with relaxation parameter $Q = 10$ and target temperature $T = 1$. We simulate systems involving $N = 2$, 8, 64, 512 particles at various number densities. We do this by performing each simulation with a box width of $L = L_0 \times (6/5)^{i-1}$, where $i = 1, 2, \ldots, 20$ labels the simulation number and L_0 is the smallest cubic box width, included in Table I of the manuscript. To obtain our results in Figure 6, we have implemented the velocity Verlet algorithm with the Nosé-Hoover thermostat with a relaxation parameter proportional to temperature, $Q = 10T$. Each simulation is run at a similar number density, n_0, given in Table I in the manuscript.

Temperature fluctuations for systems of comparative densities are shown in Figure S4. Temperature fluctuations for the $N = 2$ system, that is simulated with $L_0 = 5$, are shown in Figure S4(a). These are still comparatively large, as expected with few particles, however the

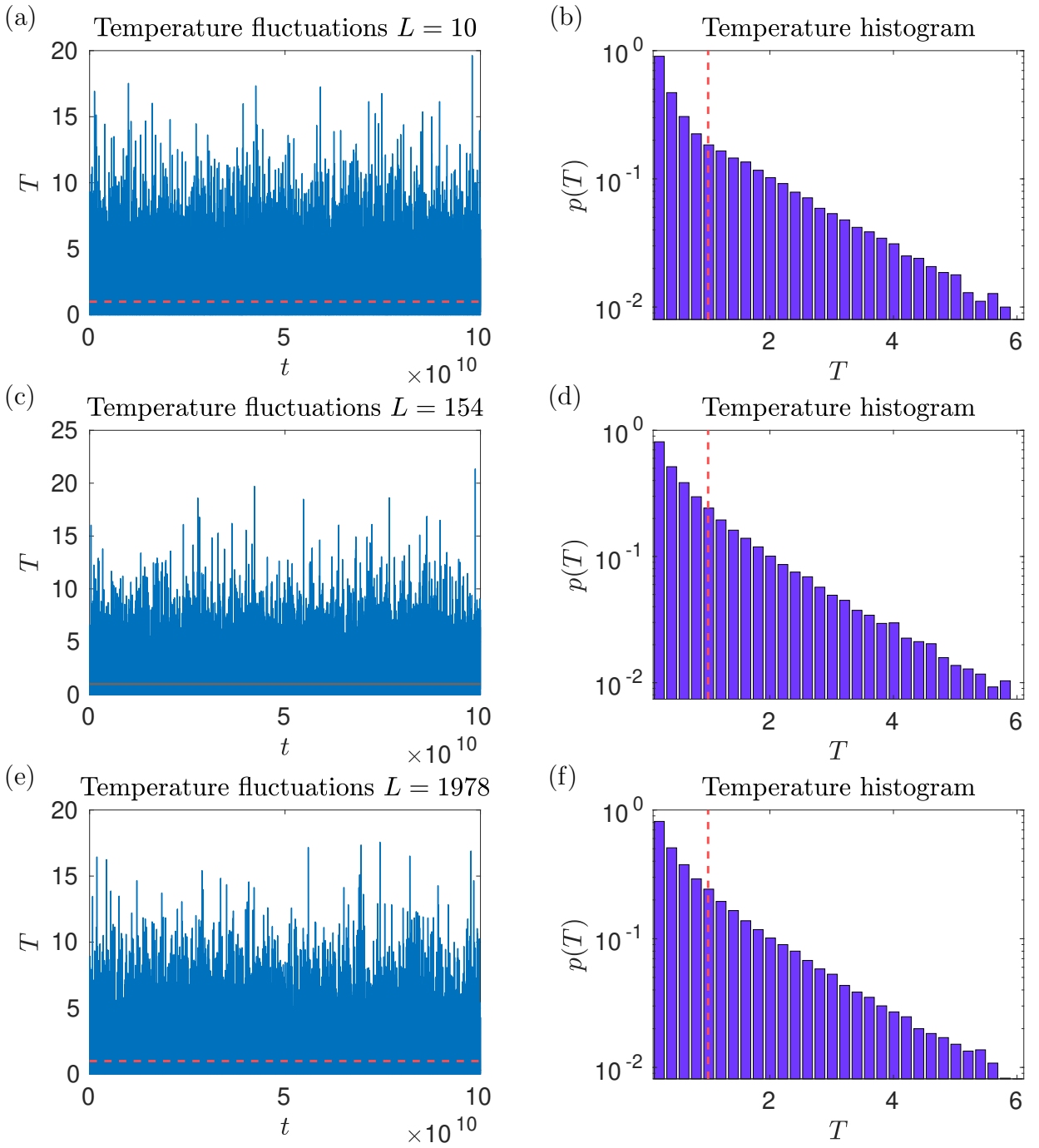

Figure S2: *Temperature fluctuations for MD simulations with box width* (a) $L = 10$, (c) $L = 154$ *and* (e) $L = 1978$, *which are presented in the manuscript in Figure* 2. *Panels* (b), (d) *and* (f) *show the corresponding histograms of temperature values visualized as probability density functions using the log scale. The red dashed line in each panel represents the average temperature for the whole simulation, which is* $T \approx 1$ *in each case.*

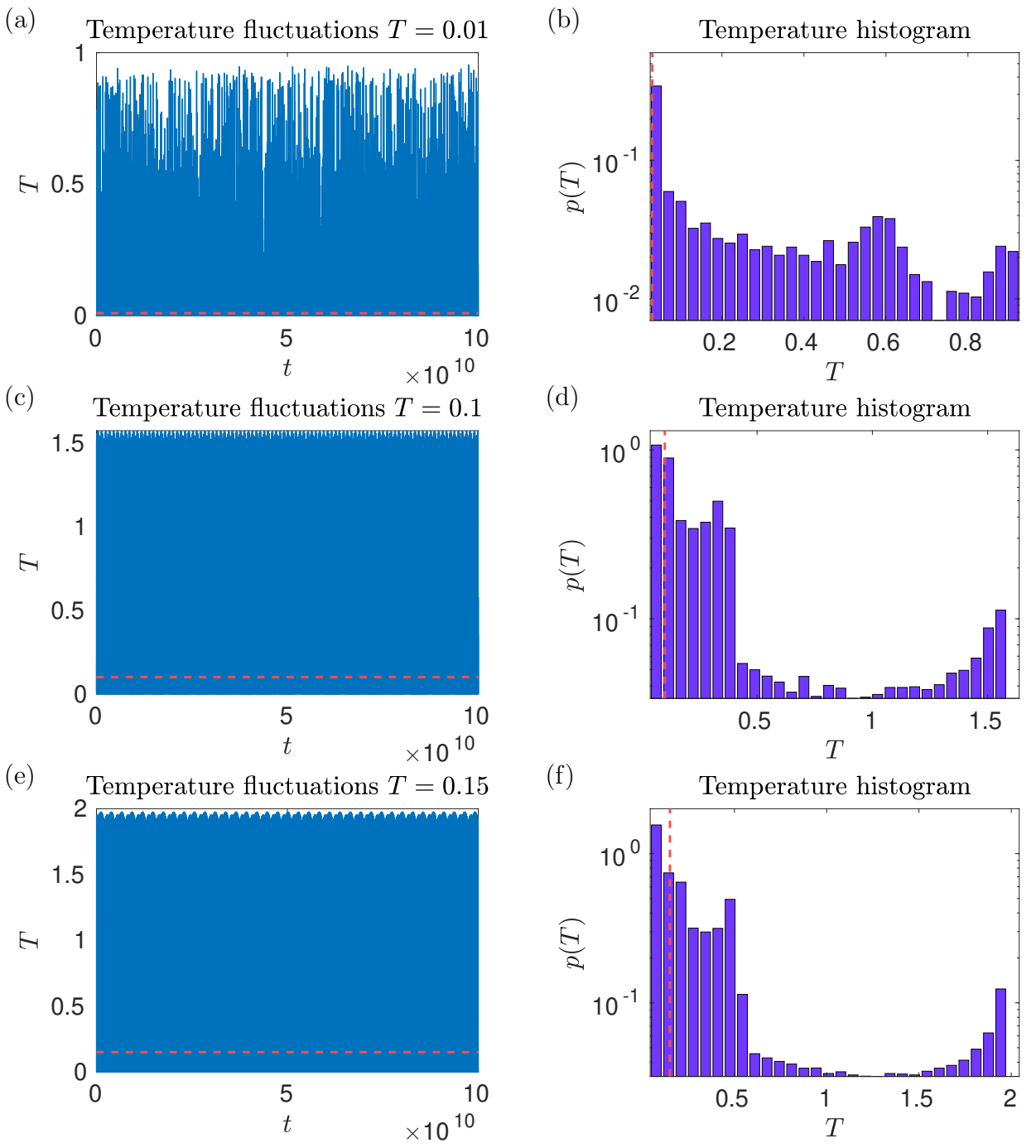

Figure S3: *Temperature fluctuations for MD simulations with target temperatures* (a) $T = 0.01$, (c) $T = 0.1$ *and* (e) $T = 0.15$, *which are presented in the manuscript in Figure* 3. *Panels* (b), (d) *and* (f) *show the corresponding histograms of temperature values visualized as probability density functions using the log scale. The red dashed lines in panels* (a)/(b), (c)/(d) *and* (e)/(f) *correspond to the sampled average temperatures, which are equal to* $T = 0.01001$, $T = 0.1001$ *and* $T = 0.1502$, *respectively.*

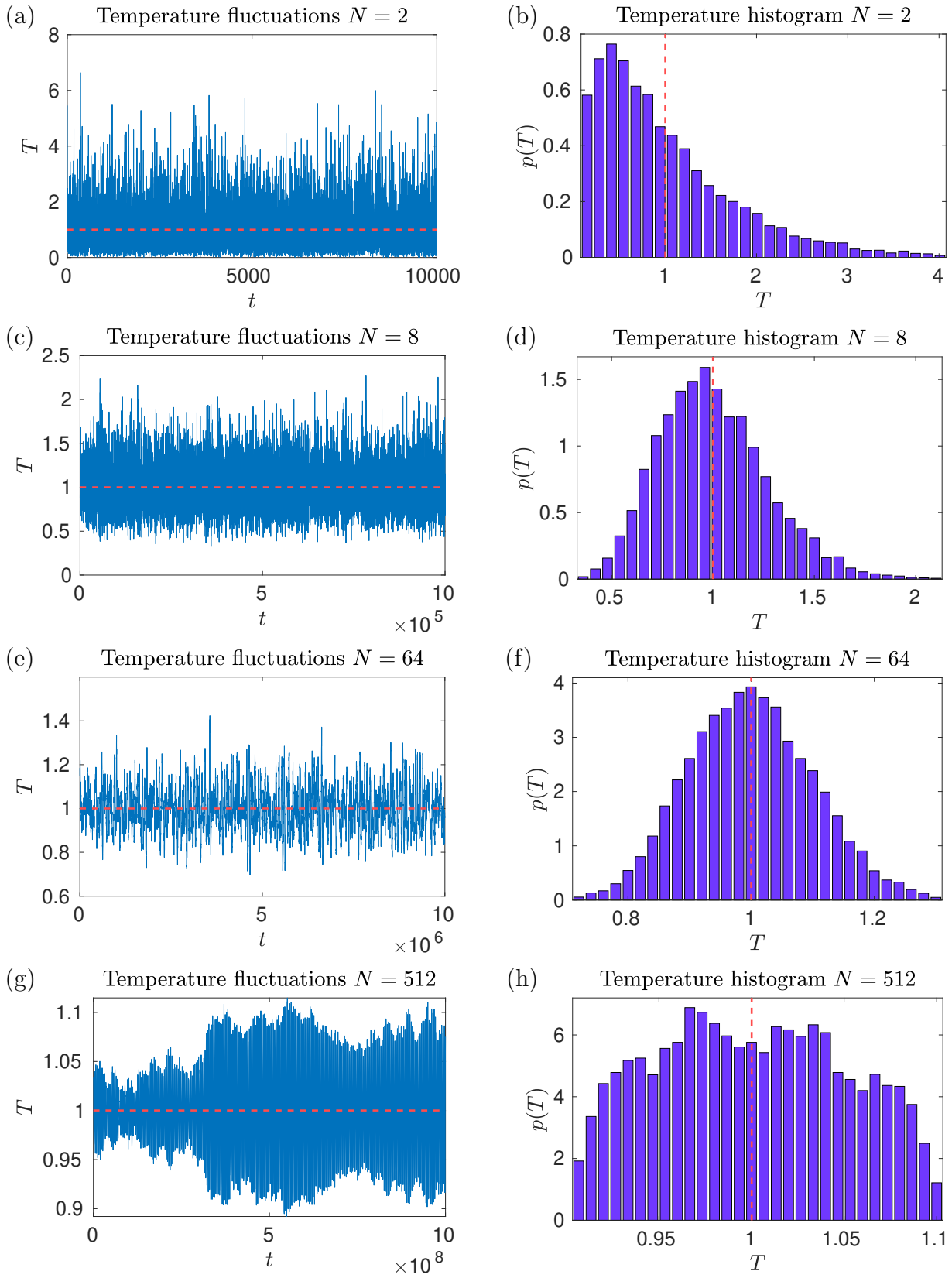

Figure S4: *Temperature fluctuations in the* 3D *case for simulations with different particle numbers, visualized as time series (left panels) and probability density functions (right panels).*

histogram in Figure S4(b) verifies that these outlier temperatures are rarely seen and the sampled average temperature is $T = 1 + O(10^{-5})$. Typical temperature fluctuations for the many particles systems are shown in Figures S4(c), S4(e) and S4(g) for the $N = 8$, $N = 64$ and $N = 512$ particle systems, respectively. We observe that the magnitude of temperature fluctuations is smaller than for the two particle system and also the distribution of temperatures is more symmetric, as shown by accompanying histograms in Figures S4(d), S4(f) and S4(h). The sampled average temperature is plotted as the red dashed line in each panel. It is equal to $T = 1 + O(10^{-5})$ in all MD simulations presented in Figure S4.

Supporting information for **Figure 8**

To create Figure 8 in the manuscript: we carry out $12 \times 16 = 192$ MD simulations corresponding to phase plane points (n, T) with $n = 10^{-2} + (i-1)/10$ and $T = 10^{-1} + j/10$, where $i = 1, 2, \ldots, 12$ and $j = 1, 2, \ldots, 16$. These simulations use $N = 512$, relaxation parameter $Q = 10$, time step $\Delta t = 0.01$ and simulation time $t_{\text{sim}} = 3 \times 10^5$ time steps. Supplementary File `figure8.xlsx` contains all statistics calculated from these 192 simulations, including the total simulation averages of simulated temperature, pressure, internal energy and kurtosis. In Figure S5, we plot the pressure and internal energy in a similar way to Figure 8 in the manuscript (which displays the MD data for kurtosis).

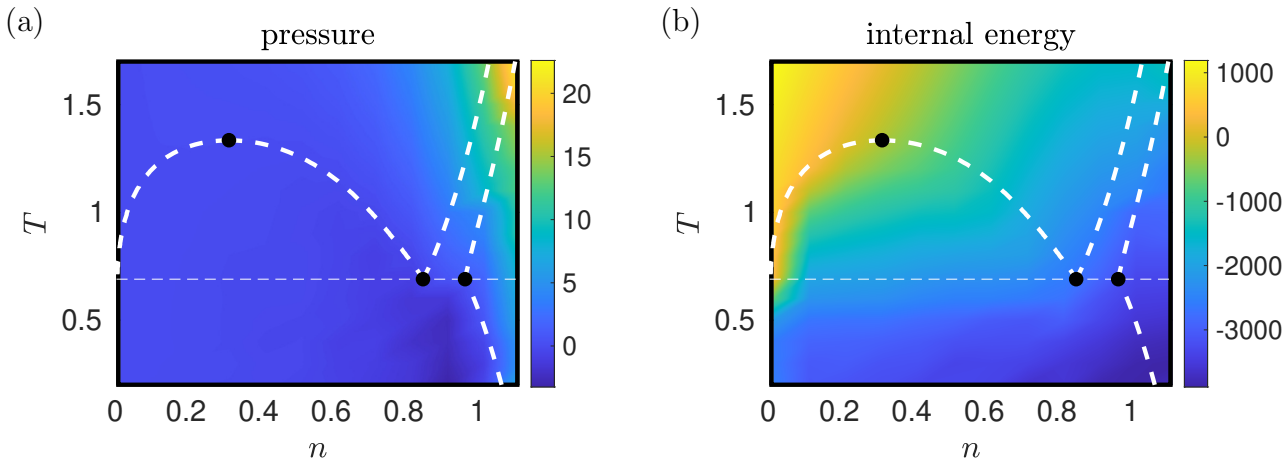

Figure S5: *Additional statistics obtained using the MD simulations in Figure* 8. *We present:* (a) *pressure*, (b) *internal energy, calculated from MD simulations at* 192 *phase points* (n, T).