Better than counting: Density profiles from force sampling

Daniel de las Heras and Matthias Schmidt
Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany

The one-body density distribution plays a central role in statistical physics. Accurate measurements of the density profile are very valuable to study, e.g., wetting properties, crystal nucleation, the liquid-vapor interface, and capillary effects, as well as to assess the validity of new density functional theories. Traditionally, the density profile is measured experimentally, or calculated in computer simulations, by literally counting the number of particles in each bin of a predefined spatial grid.

We have developed an alternative method [1] based on a histogram of the local force density. Using the exact force balance equation of an equilibrium system, the density profile can be obtained from the local force density profile via a simple spatial integration. The method eliminates the ideal gas fluctuations, reducing therefore the statistical uncertainty and the computation time as compared to the traditional counting method.

We have tested the method in Monte Carlo, Brownian dynamics, and molecular dynamics. In all cases, obtaining the density profile via the force density profile performs significantly better than just counting the number of particles in a given bin. A representative example is shown in the figure.

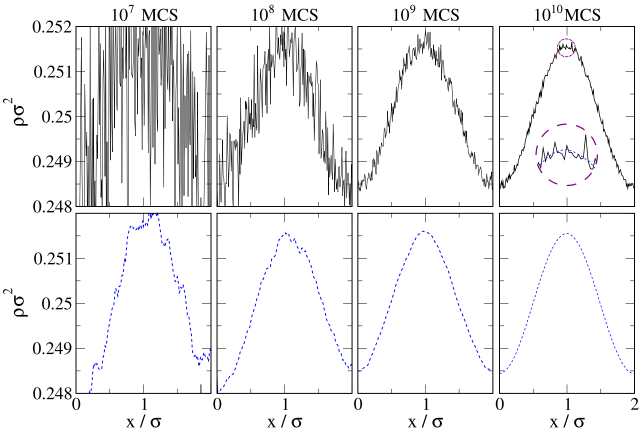

Fig. 1. Density profiles obtained with Monte Carlo simulations for different number of Monte Carlo steps (MCS), as indicated. The profiles have been obtained with the traditional counting method (top profiles) and the force sampling method (bottom profiles). The bin size is $\Delta x/\sigma = 0.01$ with σ the particle length. The profiles correspond to an equilibrium system of Lennard-Jones particles in an external potential.

[1] D. de las Heras and M. Schmidt, Phys. Rev. Lett. **120**, 218001 (2018).