universität innsbruck
Institut für
Theoretische Physik

Prof. Dr. T. Franosch

Dr. Michele Caraglio

Institut für Theoretische Physik

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Computer Simulations in Statistical Physics
Prof. Dr. T. Franosch

Problem set 6

Proseminar

Problem 6.1 *NPT ensemble for MC simulation of hard spheres*

In order to implement NPT ensemble in MC simulation we have to allow trial moves to change the volume. As discussed at lesson, this can be done, through the following algorithm:

- perform a trial volume change $V_{\text{old}} \to V_{\text{new}} = V_{\text{old}}(1+\varepsilon)$ with ε a random variable uniformly distribuited into the interval $[-\varepsilon_{\max}, \varepsilon_{\max}]$.
- accept the trial move with probability:

$$\min\left(1, \exp\left\{-\beta\left[\mathcal{U}_{\text{new}} - \mathcal{U}_{\text{old}} + pV_{\text{old}}\varepsilon - \frac{N+1}{\beta}\ln(1+\varepsilon)\right]\right\}\right) \ ,$$

where $\mathcal{U}_{\text{new}}$ and $\mathcal{U}_{\text{old}}$ are respectively the energies of the new and the old configuration, p is the pressure and β the inverse temperature.
It is commom practice to perform one volume trial move for every cycle of positional trial moves. However, note that in order to guarantee the symmetry of the underlying Markov chain, volume moves should not be attempted periodically after a fixed number (say N) of positional trial moves. Rather, at every step there should be a probability $1/N$ to attempt a volume move instead of a particle move.

a) Starting from the code snippet "MC_hard_spheres_npt_snippet.cpp" complete the functions "mc_step_npt()" and "mc_volume_move()" according to the above algorithm; Note that in order to perform trial volume moves you will have also to complete the function "determine_global_overlap(Ln)".

b) Starting with $N = 7^3$ particles (diameter of particles $\sigma = 1$), packing fraction $\varphi = 0.5$, temperature $T = 1$ and $p = 2$ find a good value of ε_{max} in order to have an acceptance ratio of volume trial moves of about $0.2 - 0.4$ under equilibrium conditions.

   <u>Attention:</u> at low pressure the volume becomes very large. As a consequence, the particle position trial moves are almost always accepted and one can be tempted to increase the typical size of particle positional updates. However, it is important that this does not become bigger than about $\sigma/4$ because, otherwise, numerical instabilities leading to an excessive non-physical expansion could arise.

c) Fix $T = 1$ and $p = 2$ and plot the volume as a function of time. Repeat for $p = 32$

d) By changing the pressure in the range $[0.5 : 32]$, plot the average value of fraction $\beta p/\varrho$ (average at equilibrium) as a function of the packing fraction $\eta = \pi\varrho\sigma^3/6$.

e) Compute and plot the volume fluctuations $\langle(\delta V)^2\rangle = \langle V^2\rangle - \langle V\rangle^2$ as a function of the pressure.