PRACTICAL TRICKS: TRUNCATION OF THE POTENTIAL

For systems with potentials that have long tails [this is typical for fluid systems] the update requires a significant amount of CPU-time

In Metropolis $(r_i \to r_i')$ requires computing

$$\Delta U = \sum_{j \neq i} V(|r_i' - r_j|) - V(|r_i - r_j|) \qquad \begin{bmatrix}\text{two-body} \\ \text{interactions}\end{bmatrix}$$

↑ CPU $\propto$ Number of particles

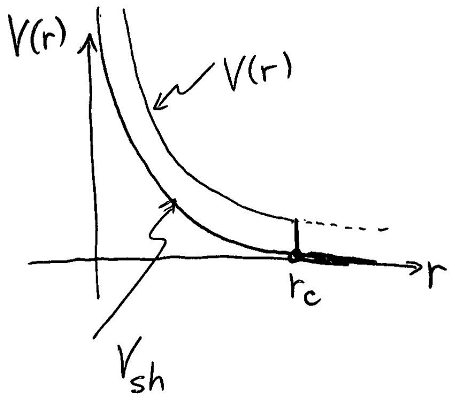
Therefore the update of 1 particle requires a CPU time that increases with N.

A way out. Introduce

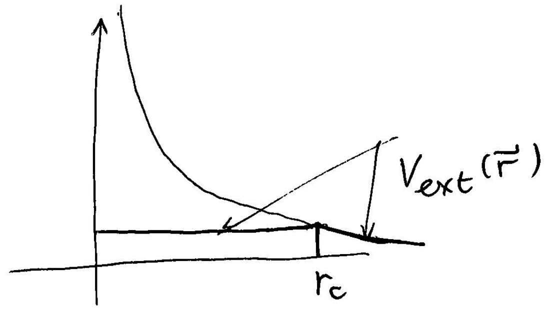
$$V_{sh}(\vec{r}) = \begin{cases} V(r) - V_0(r_c) & r < r_c \\ 0 & r > r_c \end{cases}$$

$\boxed{r_c = \text{CUTOFF}}$

$$V_{ext}(\vec{r}) = \begin{cases} V(r_c) & r < r_c \\ V(r) & r > r_c \end{cases}$$



V_{sh} is SHIFTED so that $V_{sh}(r_c) = 0$



If r_c is sufficiently large $V_{ext}(\vec{r})$ is small

Clearly

$$V(\vec{r}) = V_{sh}(\vec{r}) + V_{ext}(\vec{r})$$
$$\Downarrow$$
$$U(\vec{r}) = U_{sh}(\vec{r}) + U_{ext}(\vec{r})$$

$$U_{sh} = \sum_{i<j} V_{sh}(|r_i - r_j|)$$
$$U_{ext} = \sum_{i<j} V_{ext}(|r_i - r_j|)$$

Now we rewrite

$$\int d^{3N}r\, A(r_1 \dots r_N)\, e^{-\beta U} = \int d^{3N}r\, e^{-\beta U_{sh}} \left(A\, e^{-\beta U_{ext}}\right)$$
$$\int d^{3N}r\, e^{-\beta U} = \int d^{3N}r\, e^{-\beta U_{sh}} \left(e^{-\beta U_{ext}}\right)$$

If we define $Z_{sh} = \int d^{3N}r\, e^{-\beta U_{sh}}$

$$\langle B \rangle_{sh} = \frac{1}{Z_{sh}} \int d^{3N}r\, B\, e^{-\beta U_{sh}}$$

we obtain

$$\langle A \rangle = \frac{\langle A e^{-\beta U_{ext}} \rangle_{sh}}{\langle e^{-\beta U_{ext}} \rangle_{sh}}$$

This expression is EXACT

This expression represents an improvement with respect to the original formulation.

In the update we use $V_{sh}(\vec{r})$ and thus we should only consider particles satisfying $r < r_c$.

It is possible to write codes such that the update of 1 particle requires a CPU time that is constant as N increases.

Measurement: it is still a calculation of order N^2

THE COMPUTATION of U_{ext} requires a sum over all pairs of particles.

If we perform approximations we can speed up also the calculation of the mean values.

FIRST APPROX:

$$\langle A \rangle \approx \langle A \rangle_{sh}$$

we neglect U_{ext} in the mean values.

SECOND APPROX:

We use that A is a two-body observable

$$A = \sum_{i<j} a(|r_i - r_j|)$$

potential energy and virials are observables of this type. We write

$$a_{cut}(r) = \begin{cases} a(r) & r<r_c \\ 0 & r>r_c \end{cases} \qquad A_{cut} = \sum_{i<j} a_{cut}(r_{ij})$$

$$a_{ext}(r) = \begin{cases} 0 & r<r_c \\ a(r) & r>r_c \end{cases} \qquad A_{ext} = \sum_{i<j} a_{ext}(r_{ij})$$

$$\langle A \rangle_{sh} = \langle A_{cut} \rangle_{sh} + \langle A_{ext} \rangle_{sh}$$

$\langle A_{cut} \rangle_{sh}$ is computed in the MC simulation.

$\langle A_{ext} \rangle_{sh}$ is ESTIMATED (approximated) as follows

$$\langle A_{ext} \rangle_{sh} = \sum_{i<j} \langle a_{ext}(|r_i - r_j|) \rangle_{sh}$$

$$= \sum_{i<j} \int d^3R \, \langle \delta(\vec{R} - \vec{r}_{ij}) \, a_{ext}(|r_{ij}|) \rangle_{sh}$$

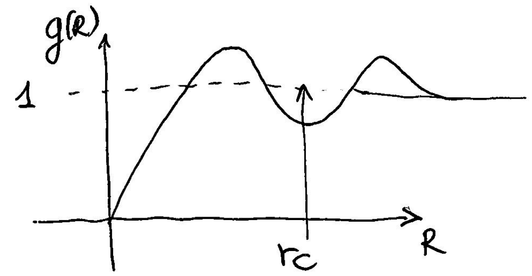
$$= \sum_{i<j} \int d^3R \, a_{ext}(|R|) \, \frac{1}{V} \, g^{(2)}(R)$$

pair correlation function

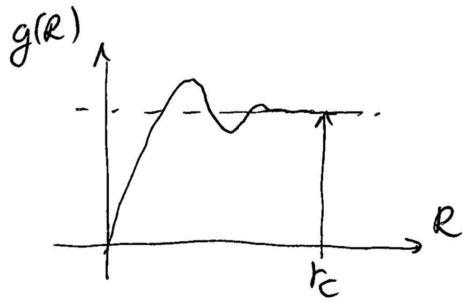
$$= \frac{1}{V} \frac{N(N-1)}{2} \int d\Omega \, R^2 dR \, a_{ext}(R) \, g^{(2)}(R)$$

$$= 2\pi \frac{N(N-1)}{V} \int_{r_c}^{\infty} R^2 dR \, a_{ext}(R) \, g^{(2)}(R)$$

Now we assume that r_c is such that $g^{(2)}(R) \simeq 1$ for $R > r_c$



NOT GOOD



GOOD

NEVER TAKE r_c
in the region where
interactions are
relevant

$$\langle A_{ext} \rangle_{sh} = 2\pi \frac{N(N-1)}{V} \int_{r_c}^{\infty} R^2 dR \, a_{ext}(R)$$

Everything is known.

Example $V(r) = \frac{B}{r^p}$ $\quad$ p some parameter >3

We estimate

$$\langle V \rangle_{sh} = \langle V_{cut} \rangle + 2\pi \frac{N(N-1)}{V} \int_{r_c}^{\infty} R^2 dR \, \frac{B}{R^p}$$

$$= \langle V_{cut} \rangle + \underbrace{2\pi \frac{N(N-1)}{V} \frac{B}{p-3} r_c^{3-p}}_{\text{This is called ``tail correction''}}$$

computed from the MC data