HOMEWORK II

Organization of the code

input parameters : $\begin{cases} N \text{ (number of particles)} \\ \Delta/\sigma \text{ (shift in the Metropolis routine)} \\ L/\sigma \text{ (derive it from } \rho\sigma^3) \\ \beta_r = \epsilon/kT \end{cases}$

Define a vector position[N][3] ← the coordinates

3 routines

1. a routine that creates the starting conf
2. a routine that performs an iteration
3. a routine that measures virial and pot. energy (also the histograms needed for $g(r)$ in the last point)

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1 starting conf

for i :... N
$x_i = L*RAN()$ $y_i = L*RAN()$ $z_i = L*RAN()$
endfor

2 iteration

for i : 1 ... N
generate $\vec{r}$ in box around $\vec{r}_i$ (cube Δ^3)
perform acceptance check : compute ΔU and use Metropolis acceptance
if accepted $\vec{r}_i = \vec{r}$
endfor

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(3) measure
energy = 0 = virial
for i : 2, N (we sum i<j)
for j : 1 ... i-1
energy = energy + V(|i-j|)
virial = virial + virial (i-j)
endfor
endfor

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program

generate starting conf (routine (1))
for i : 1, ... number of iterations
perform an iteration (routine (2))
perform a measure (routine (3))
save on disk, energy, virial, number of accepted moves
endfor

BASIC ROUTINE : RAN( )

Any routine is good for our purposes
For "professional" simulations, RAN( ) should be chosen very carefully

Before using it perform a short run and verify, e.g., $\langle x \rangle = \frac{1}{2}$, $\langle x^2 \rangle = \frac{1}{3}$, $\langle x^3 \rangle = \frac{1}{4}$ ...
