Organizatihon of the code

Input parameters:
\[
\begin{align*}
N \text{ (number of particles)} \\
\Delta V \text{ (shift in the Metropolis routine)} \\
\frac{1}{\sigma} \text{ (derive it from } \rho \sigma^3) \\
\beta = \frac{\epsilon}{kT}
\end{align*}
\]

Define a vector \text{position}[N][3] \leftarrow \text{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) \text{ in the last point)

1) Starting conf
   
   for } i = 1 \ldots N
   \begin{align*}
   x_i = L \ast RAN( ) \\
y_i = L \ast RAN( ) \\
z_i = L \ast RAN( )
   \end{align*}
   \text{endfor}

2) Iteration
   
   for } i = 1 \ldots N
   \begin{align*}
   \text{generate } \vec{r} \text{ in box around } \vec{r}_i \text{ (cube } \Delta^3) \\
   \text{perform acceptance check, compute } \Delta U \text{ and use Metropolis acceptance} \\
   \text{if accepted, } \vec{r}_i = \vec{r}
   \end{align*}
   \text{endfor}
measure

\text{energy} = 0 = \text{vreal}

\text{for } i : 2, N \quad (\text{we sum } i \leq j)

\text{for } j : 1 \ldots i - 1

\text{energy} = \text{energy} + \mathcal{V}(i - j)

\text{vreal} = \text{vreal} + \text{vreal}(i - j)

\text{endfor}

\text{endfor}

---

program

generate starting conf (routine 2)

for \text{ } i : 1, \ldots \text{ number of iterahions}

perform an iteration (routine 3)

perform a measure (routine 3)

save on disk, energy, vreal, number of accepted moves

\text{endfor}

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\textbf{BASIC ROUTING: RAN( )}

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

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