THE STARTING CONFIGURATION

6) Positions: randomly in the box. For each particle

\[ x_i = L \times \text{RAN}(\cdot) \]
\[ y_i = L \times \text{RAN}(\cdot) \]
\[ z_i = L \times \text{RAN}(\cdot) \]

- Velocities. Two requirements:
  (a) \( \vec{P} = 0 \) (center-of-mass momentum)
      This relation should be satisfied exactly.
  (b) We would like a velocity distribution such that the temperature is approximately \( T_{ini} \). (approximate requirement)

A simple algorithm

(a) generate for each particle

\[ v_{ix} = \text{RAN} - 0.5 \]
\[ v_{iy} = \text{RAN} - 0.5 \]
\[ v_{iz} = \text{RAN} - 0.5 \]

(b) compute

\[ V_x = \sum_i v_{ix} \]
\[ V_y = \sum_i v_{iy} \]
\[ V_z = \sum_i v_{iz} \]
(c) redefine for all \( i; 1 \ldots N \)

\[
\begin{align*}
  \nu_{i\,x} &= \nu_{i\,x} - \frac{1}{N} \nu_x \\
  \nu_{i\,y} &= \nu_{i\,y} - \frac{1}{N} \nu_y \\
  \nu_{i\,z} &= \nu_{i\,z} - \frac{1}{N} \nu_z
\end{align*}
\]

\( \uparrow \) (\( = \) in the "C-language" meaning)

Now condition (a) is satisfied

(d) We would like to have (reduced units)

\[
\sum \frac{1}{2} \nu_i^2 = \frac{3}{2} N T_{\text{ini}}
\]

Now this is obtained by a rescaling of the velocities, i.e. \( \bar{v} \) is replaced by \( \alpha \bar{v} \).

Let us compute \( \alpha \): define \( \bar{v}_i' = \alpha \bar{v}_i \)

where \( \bar{v}_i \) is the result of step (c) and \( \nu_i' \) is such that

\[
\sum \frac{1}{2} \nu_i'^2 = \frac{3}{2} N T_{\text{ini}}
\]

We have

\[
\alpha^2 \sum_i \nu_i^2 = 3 N T_{\text{ini}}
\]

\[
\alpha = \left( \frac{3 N T_{\text{ini}}}{\sum_i \nu_i^2} \right)^{1/2}
\]

The velocities \( \nu_i' \) are the starting velocities.