THE STARTING CONFIGURATION

- Positions: randomly in the box. For each particle

$$x_1 = L * RAN(\,)$$
$$y_1 = L * RAN(\,)$$
$$z_i = L * RAN(\,)$$

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

A simple algorithm

(a) generate for each particle

$$v_{1x} = RAN - 0.5$$
$$v_{1y} = RAN - 0.5$$
$$v_{1z} = RAN - 0.5$$

(b) compute

$$V_x = \Sigma_i v_{1x}$$
$$V_y = \Sigma_i v_{1y}$$
$$V_z = \Sigma_i v_{1z}$$

(c) redefine for all $i; 1 \dots N$

$$\begin{cases} v_{ix} = v_{ix} - \frac{1}{N} V_x \\ v_{iy} = v_{iy} - \frac{1}{N} V_y \\ v_{iz} = v_{iz} - \frac{1}{N} V_z \end{cases}$$

(= in the "C-language" meaning)

Now condition (a) is satisfied

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

$$\boxed{\sum \frac{1}{2} v_i^2 = \frac{3}{2} N T_{ini}}$$

~~Now~~ This is obtained by a rescaling of the velocities, i.e. $\vec{v}$ is replaced by $\alpha \vec{v}$

Let us compute α: define $\vec{v}_i' = \alpha \vec{v}_i$ and where $\vec{v}_i$ is the result of step (c) and v_i' is such that

$$\sum \frac{1}{2} v_i'^2 = \frac{3}{2} N T_{ini}$$

We have

$$\alpha^2 \sum_i v_i^2 = 3 N T_{ini}$$

$$\alpha = \left(\frac{3 N T_{ini}}{\sum_i v_i^2} \right)^{1/2}$$

The velocities v_i' are the STARTING VELOCITIES