Mesh based methods

MD Formulation

$$V(x_1, \ldots, x_N) \quad \text{energia potenziale}$$

$$F_i = \nabla_{x_i} V(x_1, \ldots, x_N) \quad \text{forze}$$

$$V = \sum_{i=1}^{N} \sum_{J=i+1}^{N} U(\| x_i - x_J \|)$$

Complessità del calcol delle forze

$$\mathcal{O}(N^c)$$
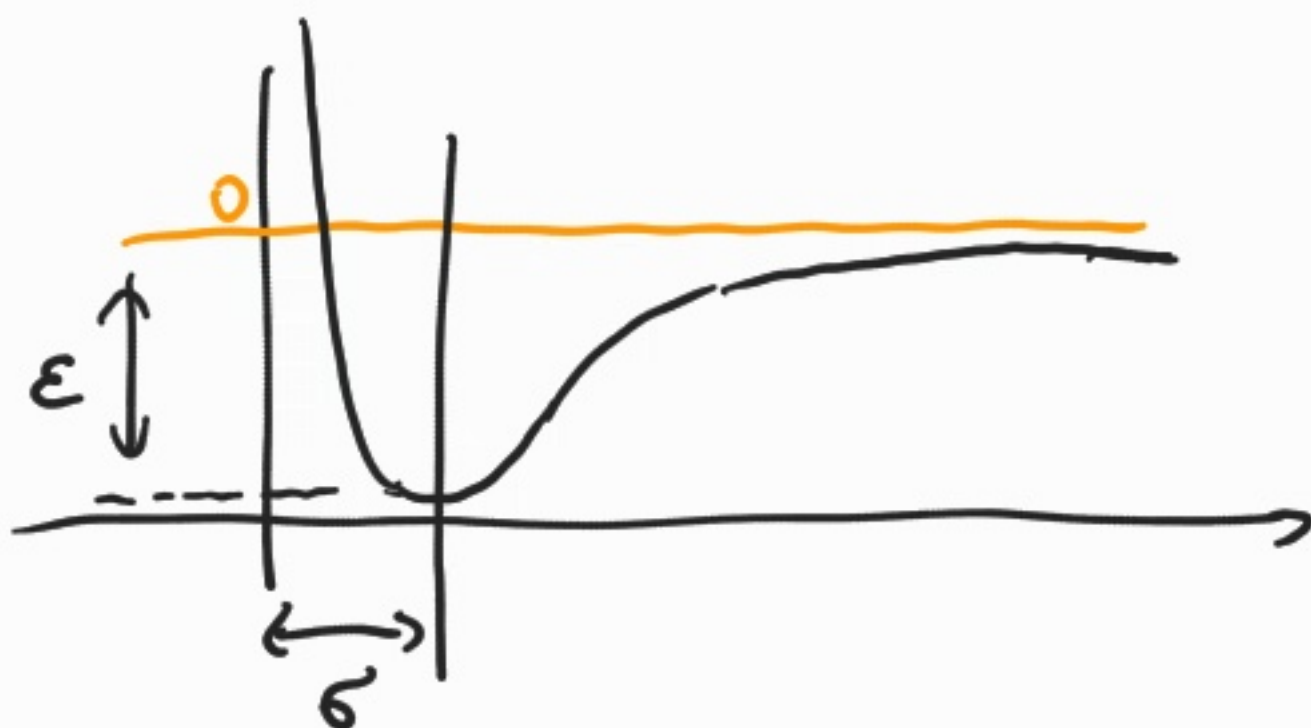
Long - range

Coulomb interaction

$$U\left(\|x_i - x_j\|\right) = \frac{q_1 q_2}{4\pi\varepsilon_0} \frac{1}{\|x_i - x_j\|}$$

Short range

Lennard-Jones potential

$$U\left(\|x_i - x_j\|\right) = 4\varepsilon \left(\frac{\sigma}{\|x_i - x_j\|}\right)^6 \left(\left(\frac{\sigma}{\|x_i - x_j\|}\right)^6 - 1\right)$$

$$F_i = -\nabla_{x_i} V(x_1 \cdots x_N)$$

$$= 24 \varepsilon \sum_{i \neq j} \left(\frac{\sigma}{\| x_i - x_j \|} \right)^6 \left(1 - 2 \left(\frac{\sigma}{\| x_i - x_j \|} \right)^6 \right) (x_i - x_j)$$
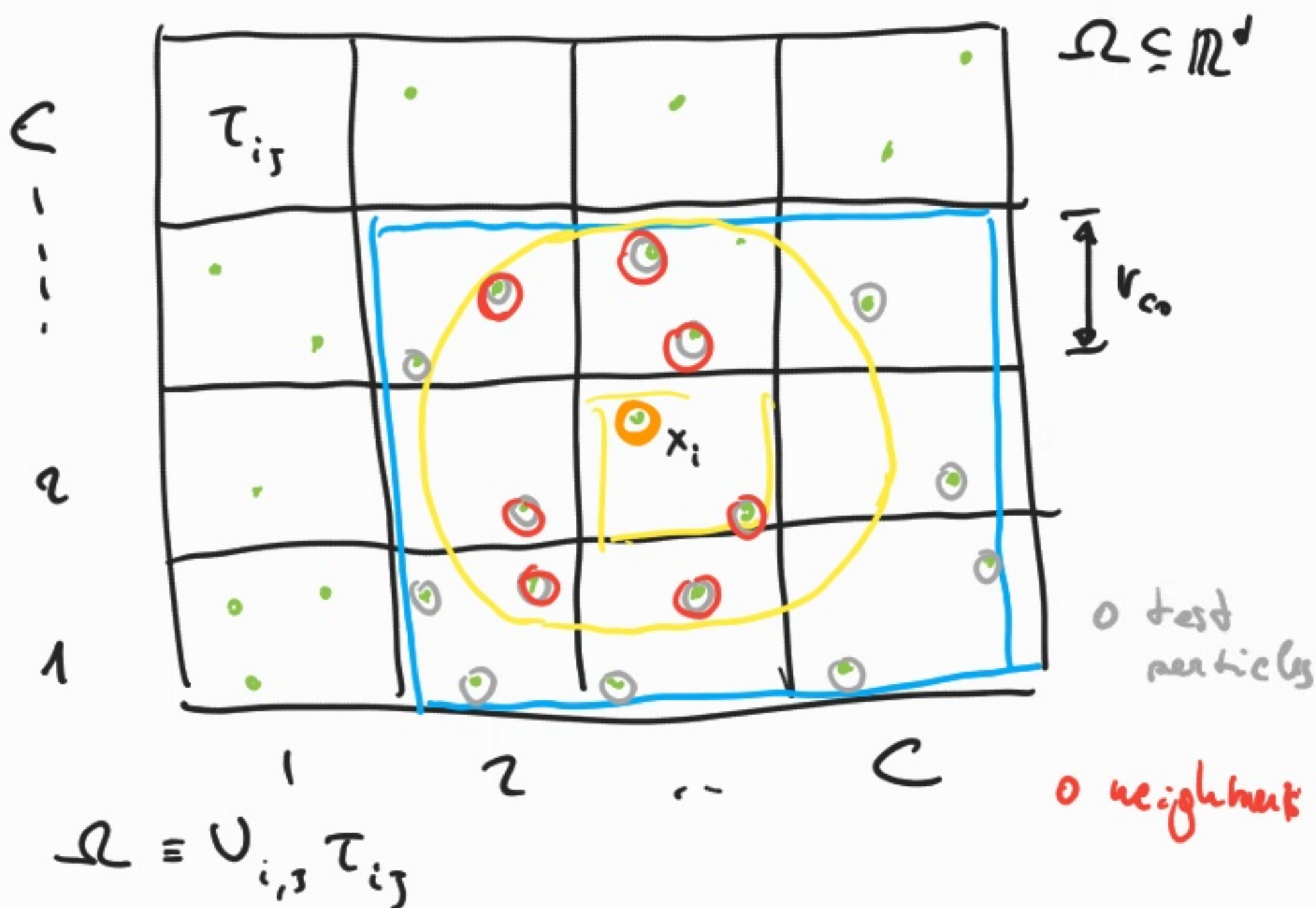
r_{co} <u>cut off radius</u>

$$U(\| x_i - x_j \|) = \begin{cases} 4\varepsilon \left(\frac{\sigma}{\| x_i - x_j \|} \right)^6 \left(\left(\frac{\sigma}{\| x_i - x_j \|} \right)^6 - 1 \right) & \text{se } \| x_i - x_j \| \lesssim r_{co} \\ 0 & \text{se } \| x_i - x_j \| > r_{co} \end{cases}$$

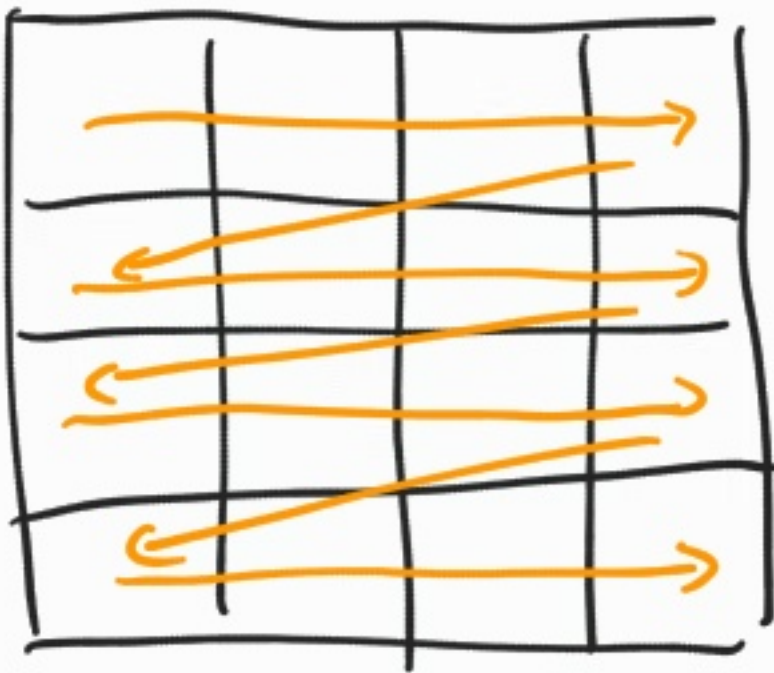$$\Theta(N^2) \longrightarrow \Theta(N \cdot m)$$

$$r_{co} \approx 2.5 \, \delta$$

First neighbour search $\Theta(N^2)$

Linked-cell algorithm

$\Omega \subseteq \mathbb{R}^d$

τ_{ij}

r_{co}

○ test particles

○ neighbours

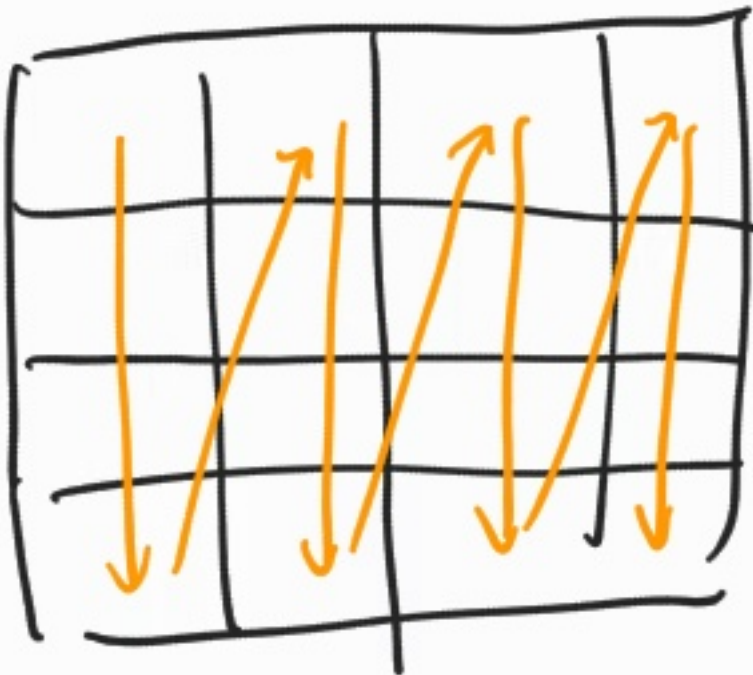$\Omega \equiv \bigcup_{i,j} \tau_{ij}$
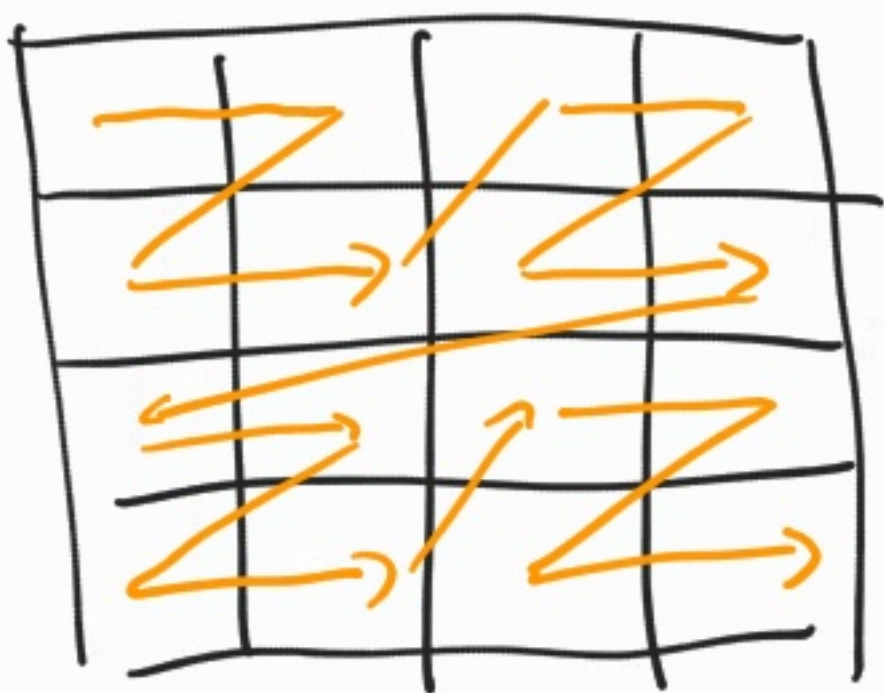
Linked - all algorithm

$$\tau_{ij} \equiv \tau_u$$

row-major ordering

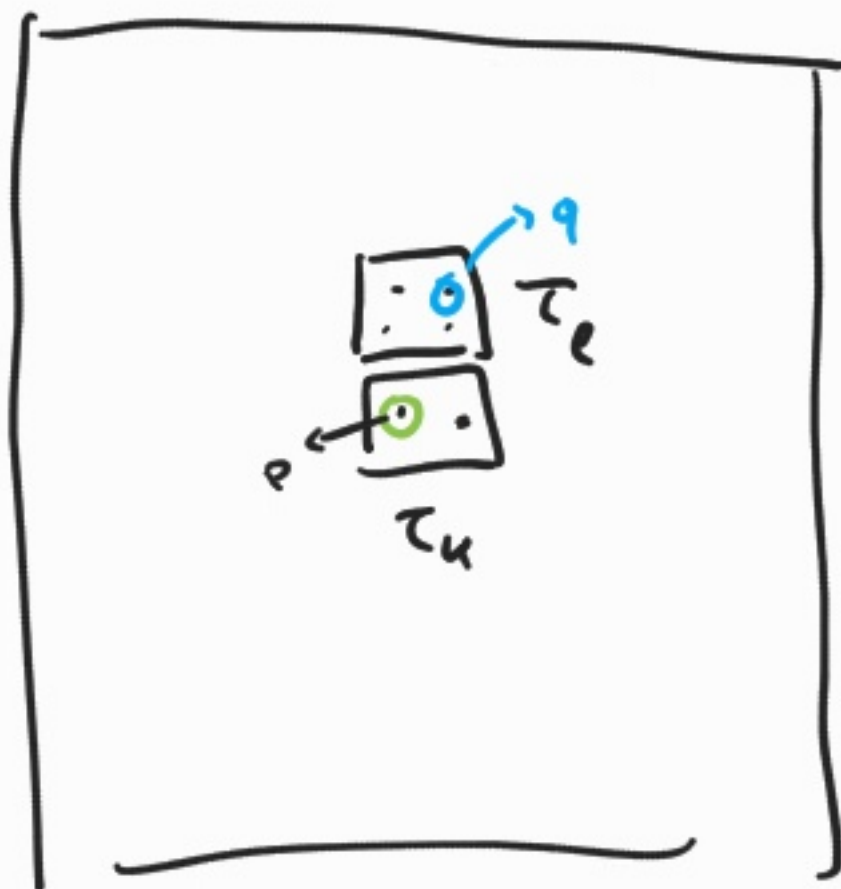column-major ordering

Z-ordering

for $k = 1 \ldots C^2$
  for $p = 1 \ldots P_k$
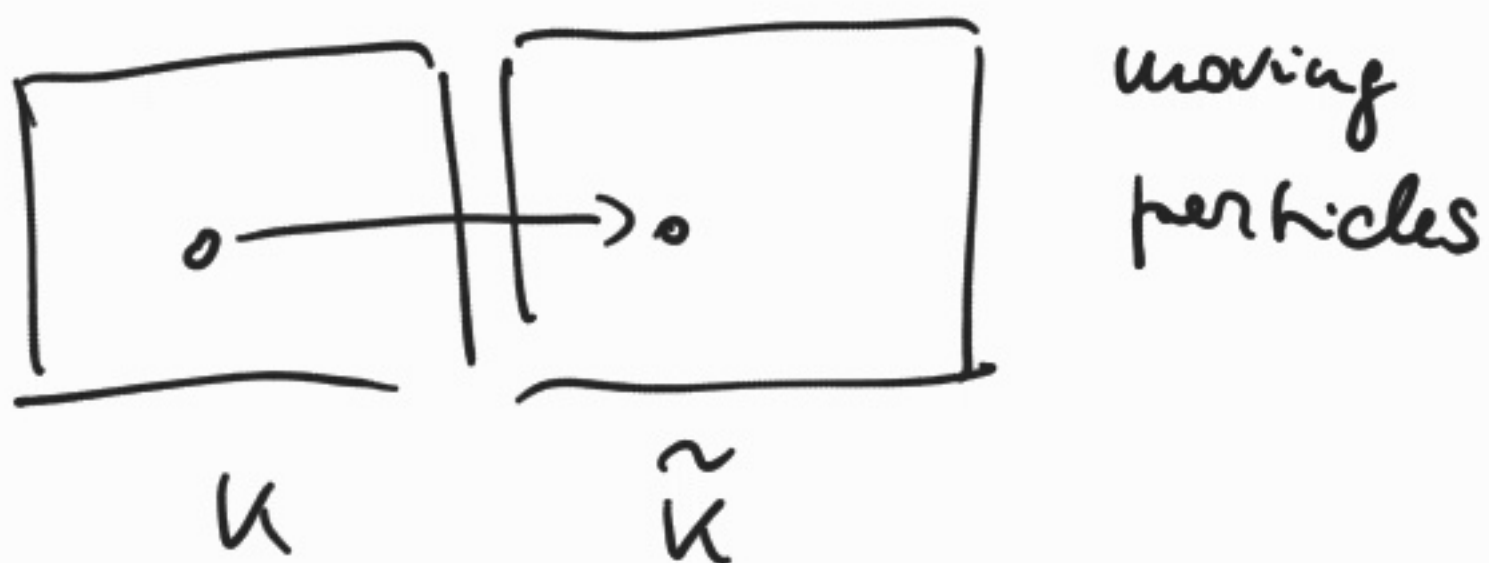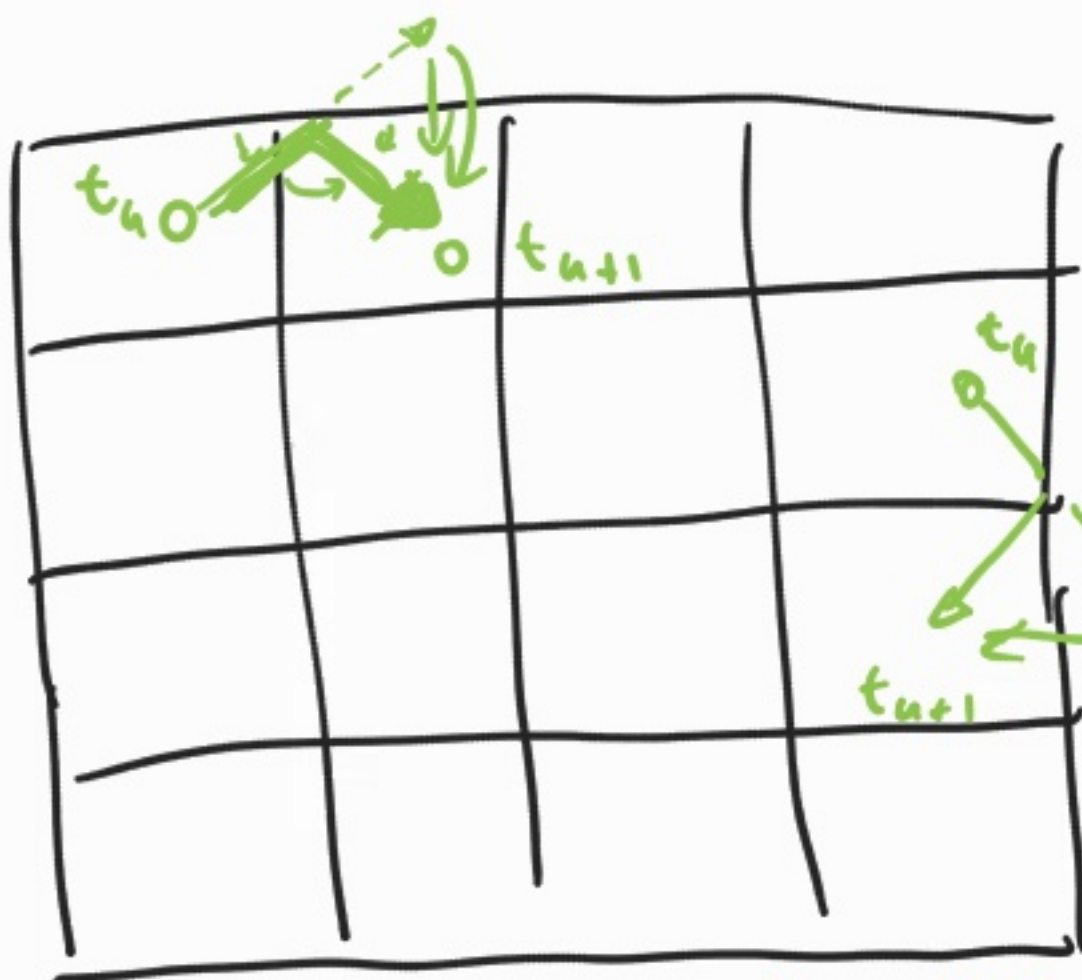   for $l = 1 \ldots nn$
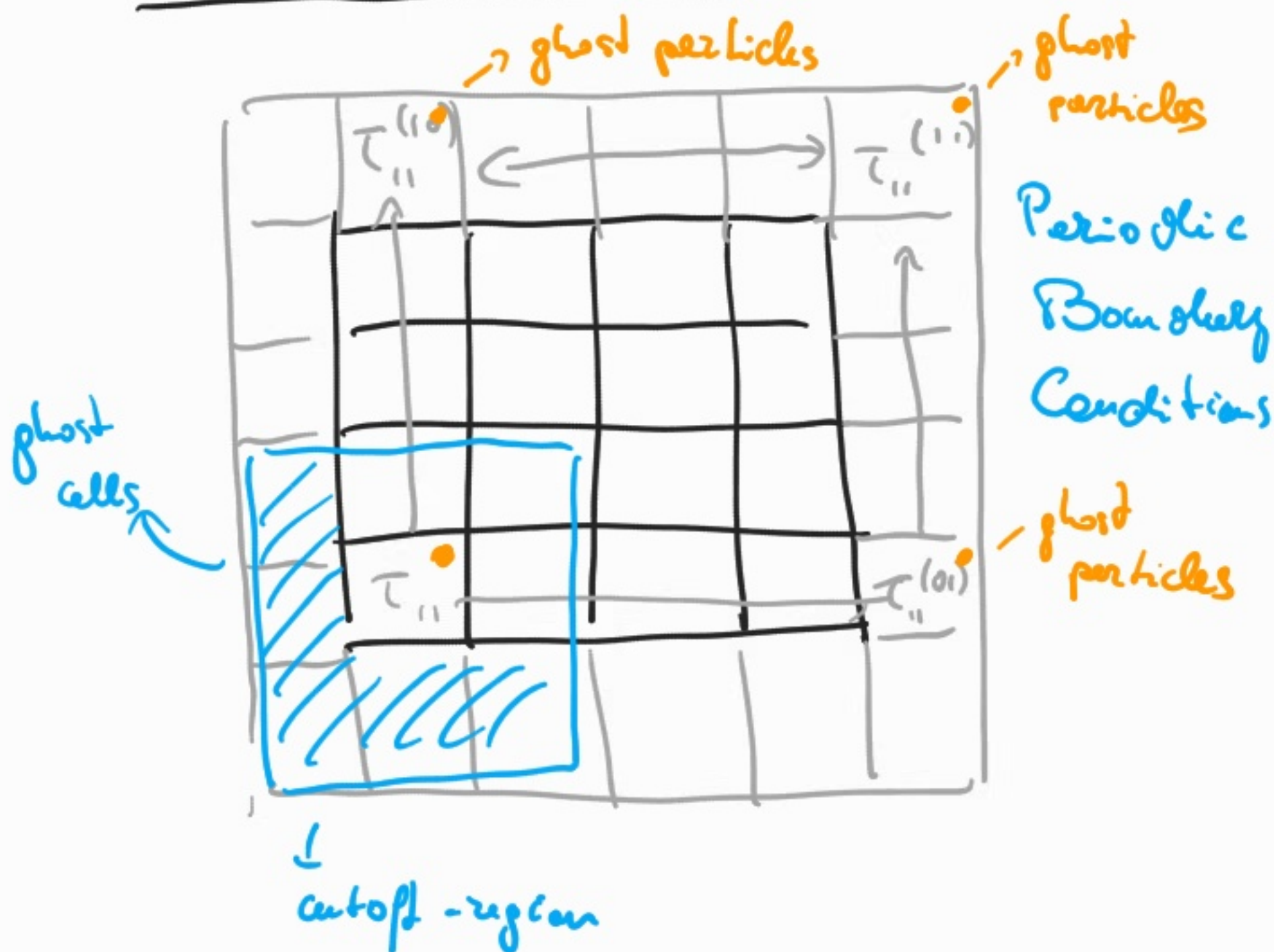   for $q = 1 \ldots P_l$
        compute F_{pq}

moving particles

Boundary conditions

- Reflecting Boundary conditions

- Periodic Boundary conditions

Reflecting
Boundary
Conditions

t_n O
O t_{n+1}

t_n
t_{n+1}

ghost particles

ghost particles

$\tau_{\shortparallel}^{(10)}$

$\tau_{\shortparallel}^{(11)}$

Periodic
Boundary
Conditions

ghost
cells

$\tau_{\shortparallel}$

$\tau_{\shortparallel}^{(01)}$

ghost particles

cutoff-region

Assignement #2

$\Omega \subseteq \mathbb{R}^2$

Reflecty B.C.

L_2

B_1

$\downarrow \underline{v}$

B_2

L_1
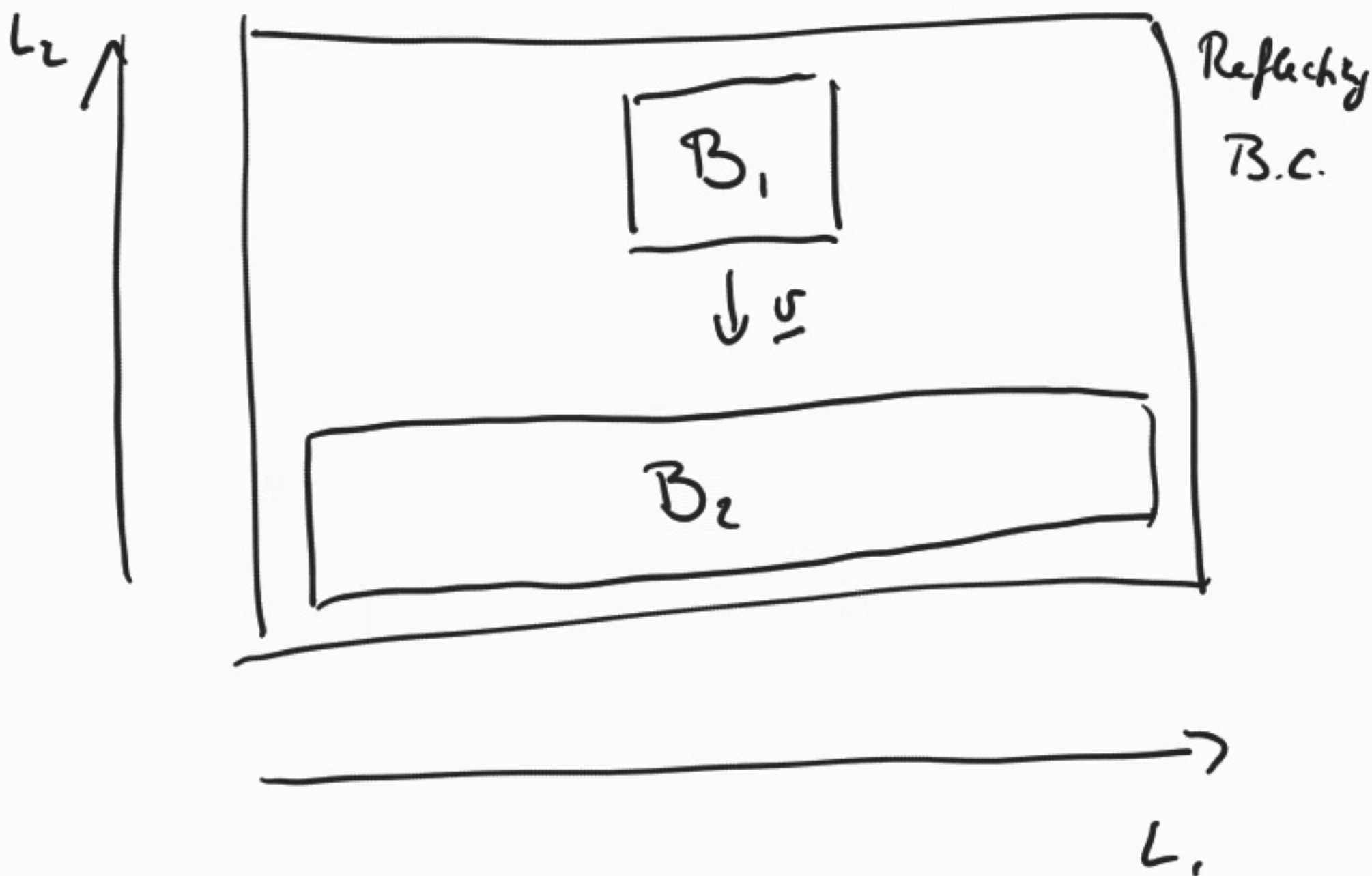
$B_1 : 40 \times 40$ particles

$B_2 : 160 \times 40$ particles

Initial conditions $\begin{cases} \text{interparticle distance} \sqrt[6]{2} \, d \\ \langle v \rangle = 0.1 \end{cases}$