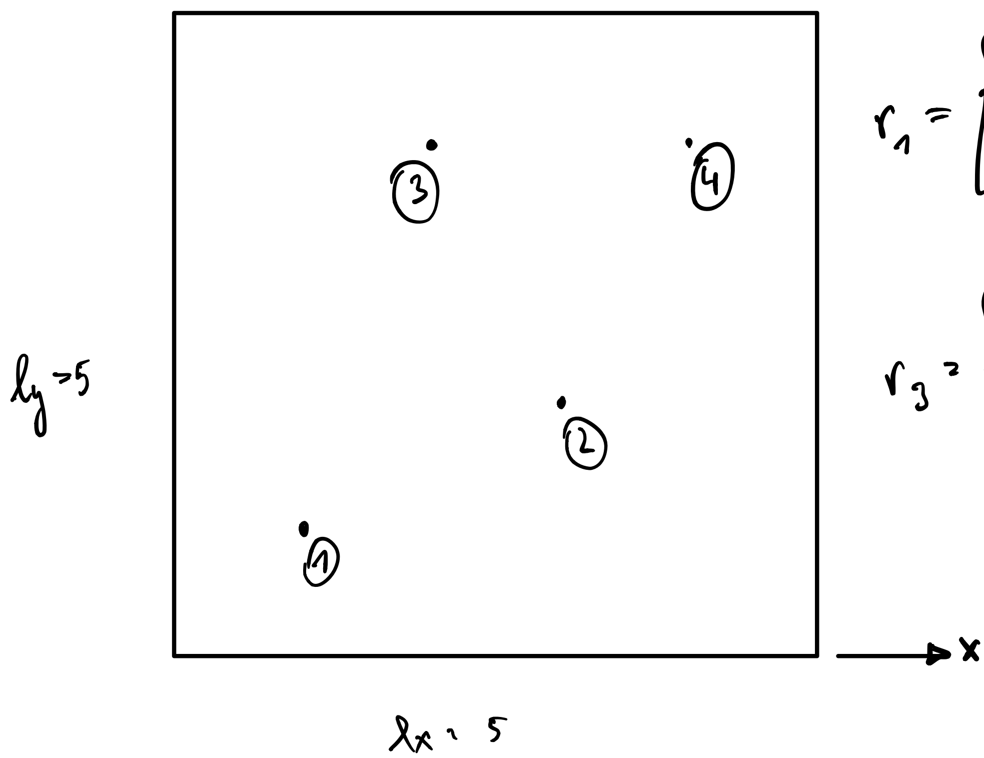
Distance benchmark model



$$r_1 = \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix}, \quad r_2 = \begin{Bmatrix} 3 \\ 2 \\ 0 \end{Bmatrix}$$

$$r_3 = \begin{Bmatrix} 2 \\ 4 \\ 0 \end{Bmatrix}, \quad r_4 = \begin{Bmatrix} 4 \\ 4 \\ 0 \end{Bmatrix}$$

$$\underline{d}_{12} = \begin{Bmatrix} 3 \\ 2 \\ 0 \end{Bmatrix} - \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix} = \begin{Bmatrix} 2 \\ 1 \\ 0 \end{Bmatrix}, \quad |\underline{d}_{12}| = \sqrt{4+1+0} = 2{,}236 \checkmark$$

$$\underline{d}_{13} = \begin{Bmatrix} 2 \\ 4 \\ 0 \end{Bmatrix} - \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 3 \\ 0 \end{Bmatrix}, \quad |\underline{d}_{13}| = \sqrt{1+9+0} = 3{,}163 \checkmark$$

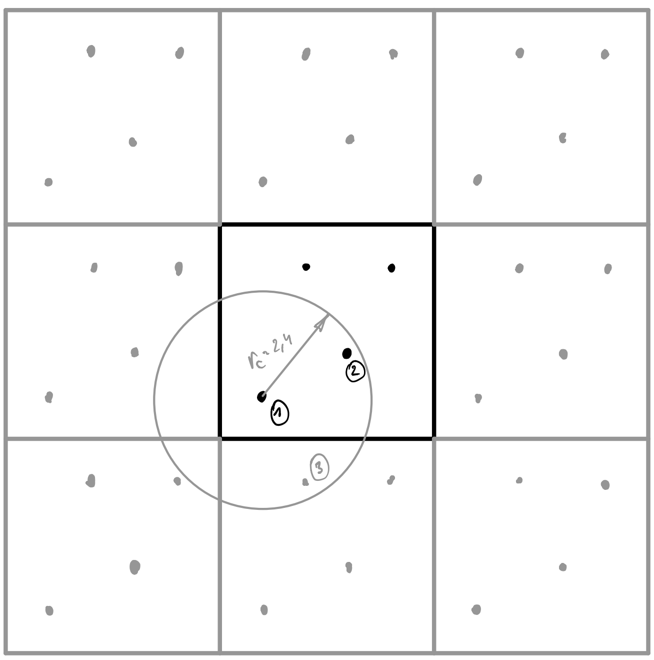
$$\underline{d}_{14} = \begin{Bmatrix} 4 \\ 4 \\ 0 \end{Bmatrix} - \begin{Bmatrix} 1 \\ 1 \\ 0 \end{Bmatrix} = \begin{Bmatrix} 3 \\ 3 \\ 0 \end{Bmatrix}, \quad |\underline{d}_{14}| = \sqrt{9+9+0} = 4{,}243 \checkmark$$

$$\underline{d}_{23} = \begin{Bmatrix} 2 \\ 4 \\ 0 \end{Bmatrix} - \begin{Bmatrix} 3 \\ 2 \\ 0 \end{Bmatrix} = \begin{Bmatrix} -1 \\ 2 \\ 0 \end{Bmatrix}, \quad |\underline{d}_{23}| = \sqrt{1+4+0} = 2{,}236 \checkmark$$

$$\underline{d}_{24} = \begin{Bmatrix} 4 \\ 4 \\ 0 \end{Bmatrix} - \begin{Bmatrix} 3 \\ 2 \\ 0 \end{Bmatrix} = \begin{Bmatrix} 1 \\ 2 \\ 0 \end{Bmatrix}, \quad |\underline{d}_{24}| = \sqrt{1+4+0} = 2{,}236 \checkmark$$

$$\underline{d}_{34} = \begin{pmatrix}4\\4\\0\end{pmatrix} - \begin{pmatrix}2\\4\\0\end{pmatrix} = \begin{pmatrix}2\\0\\0\end{pmatrix}, \quad |\underline{d}_{34}| = \sqrt{4+0+0} = 2{,}000 \checkmark$$

Including periodic boundary conditions



Atom list cutoff radius without periodic boundary conditions: $r_c = 2{,}4$ ($r_c < l/2$) ✓

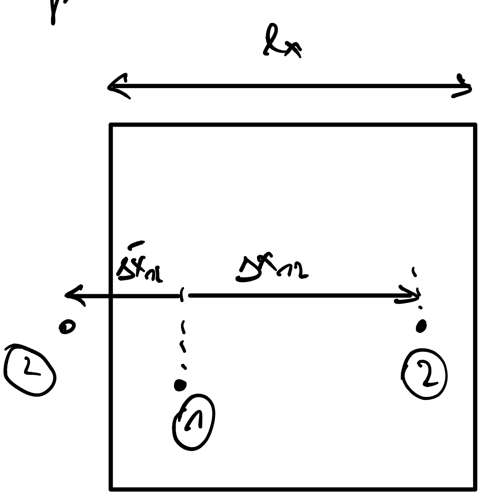
atom	neighbors
1	2 ✓
2	(1), 3, 4 ✓
3	(2), 4 ✓
4	(2), (3) ✓

Atom list cutoff radius with periodic boundary conditions: $r_c = 2{,}4$

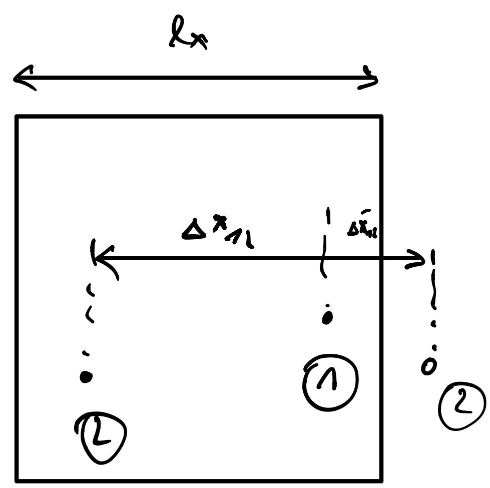
atom	neighbors
1	2, 3 ✓
2	(1), 3, 4 ✓
3	(1), (2), 4 ✓
4	(2), (3) ✓

Minimum image criterion

"positive distance"



"negative distance"



if $\Delta x_{12} > \frac{l_x}{2} \Rightarrow \Delta\bar{x}_{12} = \Delta x_{12} - l_x$; if $\Delta x_{12} < -\frac{l_x}{2} \Rightarrow \Delta\bar{x}_{12} = \Delta x_{12} + l_x$

$\Rightarrow$ general formula:

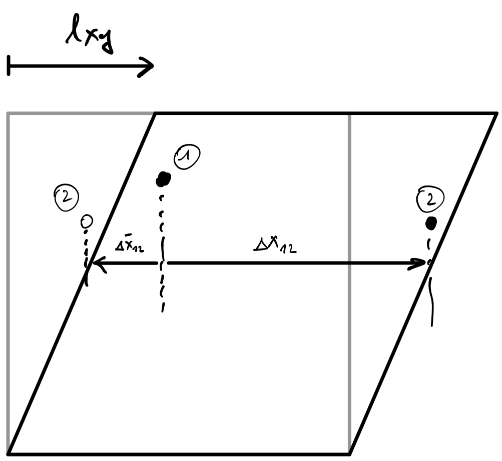
$$\boxed{\begin{array}{l} \text{if } \Delta x_{12} > \frac{l_x}{2} \Rightarrow \bar{\Delta x}_{12} = \Delta x_{12} - l_x \\ \text{if } \Delta x_{12} < \frac{l_x}{2} \Rightarrow \bar{\Delta x}_{12} = \Delta x_{12} + l_x \end{array}}$$

Periodic boundary conditions are applied step-by-step for every coordinate direction.

Lees-Edwards boundary conditions

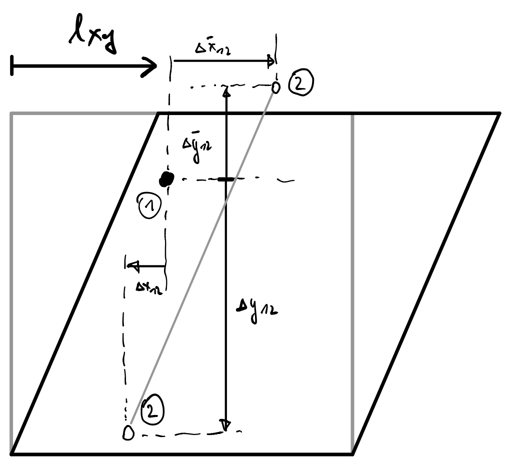
Case: only shearing in xy direction $\Rightarrow l_{xy} \neq 0$

x-direction:



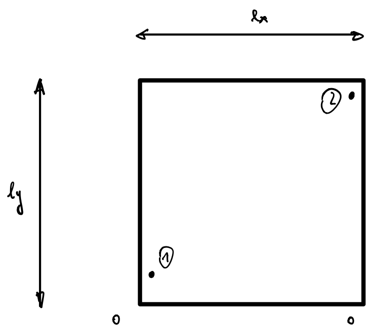
$$\boxed{\begin{array}{l} \text{if } \Delta x_{12} > \frac{l_x}{2} \Rightarrow \bar{\Delta x}_{12} = \Delta x_{12} - l_x \\ \text{if } \Delta x_{12} < \frac{l_x}{2} \Rightarrow \bar{\Delta x}_{12} = \Delta x_{12} + l_x \end{array}}$$

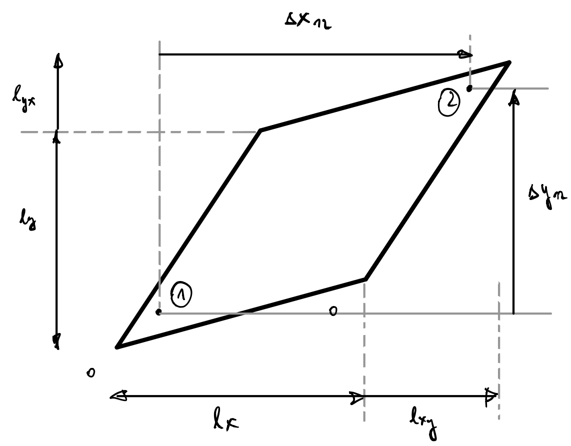
y-direction:

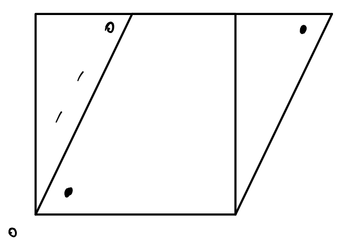


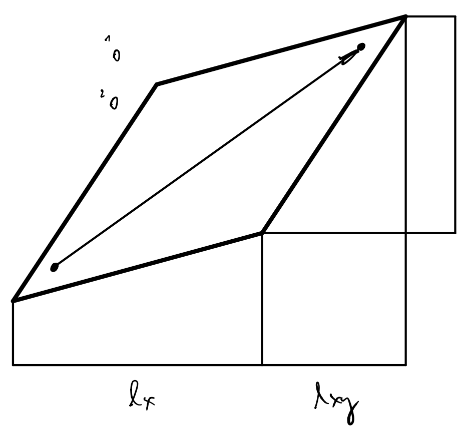
$$\boxed{\begin{array}{l} \text{if } \Delta y_{12} > \frac{l_y}{2} \Rightarrow \begin{cases} \bar{\Delta x}_{12} = \Delta x_{12} - l_{xy} \\ \bar{\Delta y}_{12} = \Delta y_{12} - l_y \end{cases} \\ \text{if } \Delta y_{12} < \frac{l_y}{2} \Rightarrow \begin{cases} \bar{\Delta x}_{12} = \Delta x_{12} + l_{xy} \\ \bar{\Delta y}_{12} = \Delta y_{12} + l_y \end{cases} \end{array}}$$

Applying Lee's Edwards boundary conditions in terms of "Lees-Edwards corrections"

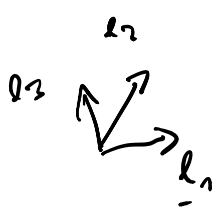


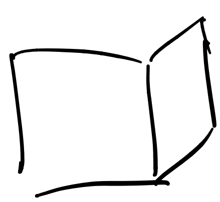


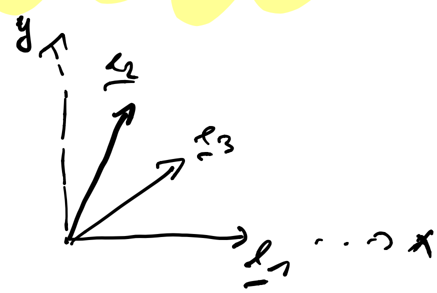




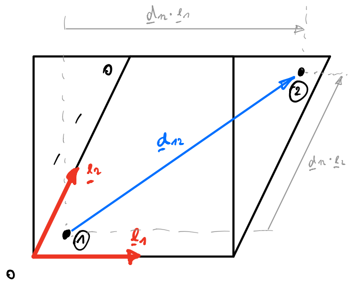
Conclusion: Evaluate distances via the box basis vectors

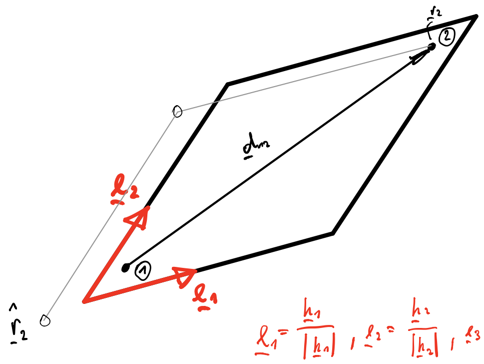






$$\underline{h}_1 = \begin{pmatrix} l_x \\ 0 \\ 0 \end{pmatrix}, \quad \underline{h}_2 = \begin{pmatrix} l_{xy} \\ l_y \\ 0 \end{pmatrix}, \quad \underline{h}_3 = \begin{pmatrix} l_{xz} \\ l_{yz} \\ l_z \end{pmatrix}$$





$e_1 = \frac{h_1}{|h_1|}$, $e_2 = \frac{h_2}{|h_2|}$, $e_3 = \frac{h_3}{|h_3|}$

Distance from atom 1 to atom 2

Creating a ghost atom with position $\hat{r}_2$ ⇒ start $\hat{r}_2 := r_2$

Basis direction e_1:

$$\boxed{\begin{array}{l} \text{if } d_{12}\cdot e_1 > \frac{|h_1|}{2} \Rightarrow \hat{r}_2 = \hat{r}_2 - h_1 \\ \text{if } d_{12}\cdot e_1 < -\frac{|h_1|}{2} \Rightarrow \hat{r}_2 = \hat{r}_2 + h_1 \end{array}}$$

Basis direction e_2:

$$\boxed{\begin{array}{l} \text{if } d_{12}\cdot e_2 > \frac{|e_2|}{2} \Rightarrow \hat{r}_2 = \hat{r}_2 - h_2 \\ \text{if } d_{12}\cdot e_2 < -\frac{|h_2|}{2} \Rightarrow \hat{r}_2 = \hat{r}_2 + h_2 \end{array}}$$

Basis direction e_3: equivalent