PSE Molekulardynamik

Short range interaction, Linked Cell algorithm

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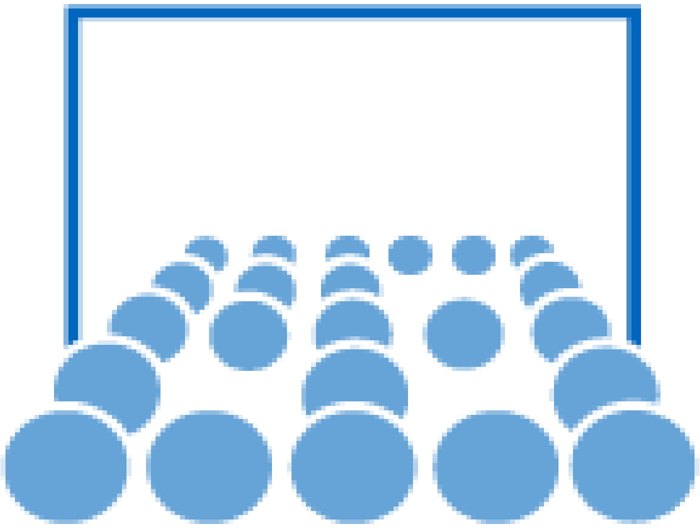
07.11.2014



Outline

- Schedule
- Presentations: Worksheet 2
- Short range interaction
- Linked-cell algorithm
- Preparation: Worksheet 3

Schedule

10.10.2014	Intro 1 WS
24.10.2014	Review 1 WS / Intro 2 WS
07.11.2014	Review 2 WS / Intro 3 WS
28.11.2014	Review 3 WS / Intro 4 WS
12.12.2014	Review 4 WS / Intro 5 WS
16.01.2015	Review 5 WS

Presentations: Worksheet 2

Revision: Lennard-Jones potential

- Interaction between molecules or atoms

$$U(x_i, x_j) = 4\epsilon \left(\left(\frac{\sigma}{\|x_i - x_j\|_2} \right)^{12} - \left(\frac{\sigma}{\|x_i - x_j\|_2} \right)^{6} \right)$$

- Resulting force calculation

$$F_i = \sum_{\substack{j=1 \\ j \neq i}}^{\#\text{particles}} F_{ij}, \quad F_{ij} = \frac{24\epsilon}{(\|x_i - x_j\|_2)^2} \left(\left(\frac{\sigma}{\|x_i - x_j\|_2} \right)^{6} - 2 \left(\frac{\sigma}{\|x_i - x_j\|_2} \right)^{12} \right) (x_j - x_i)$$

Revision: Lennard-Jones potential

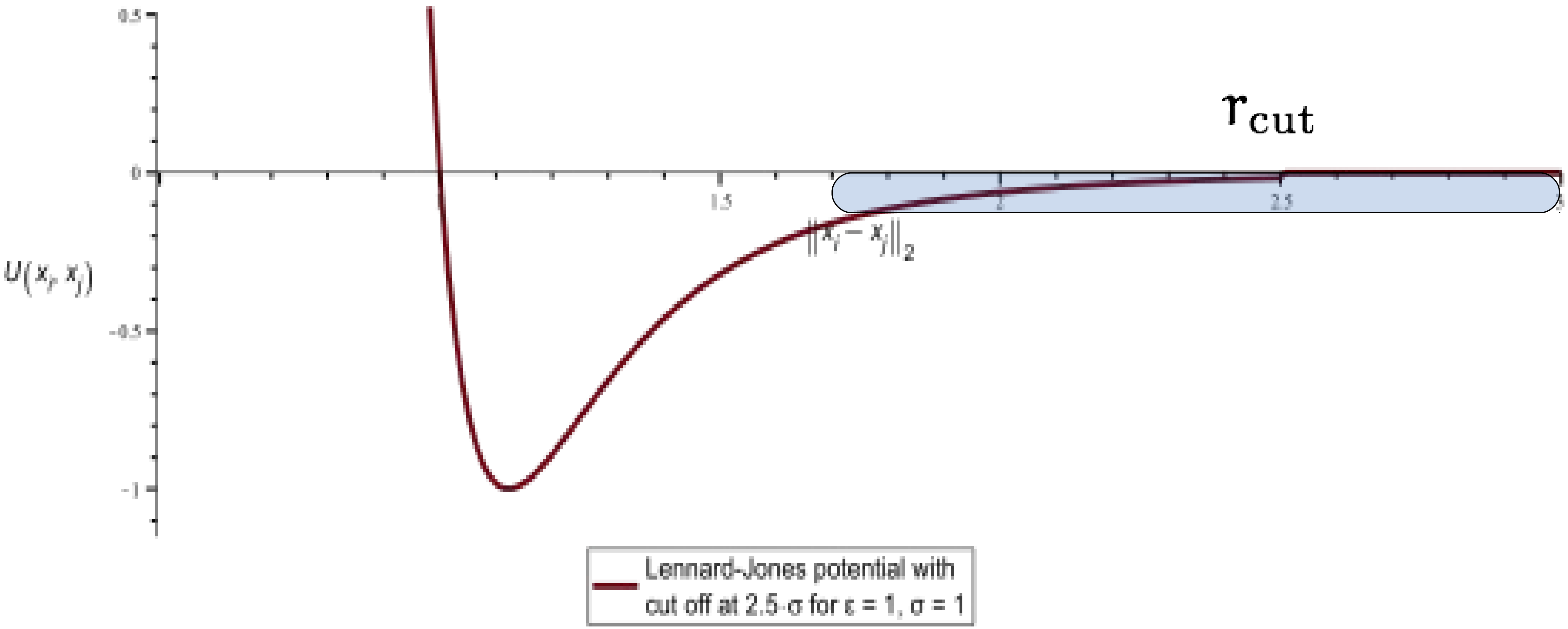
- Dense force matrix

$$\begin{pmatrix} 0 & F_{1,2} & F_{1,3} & \cdots & F_{1,\#particles} \\ F_{2,1} & 0 & F_{2,3} & \cdots & F_{2,\#particles} \\ F_{3,1} & F_{3,2} & 0 & \cdots & F_{2,\#particles} \\ \vdots & \vdots & \vdots & & \vdots \\ F_{\#particles,1} & F_{\#particles,2} & F_{\#particles,3} & \cdots & 0 \end{pmatrix}$$

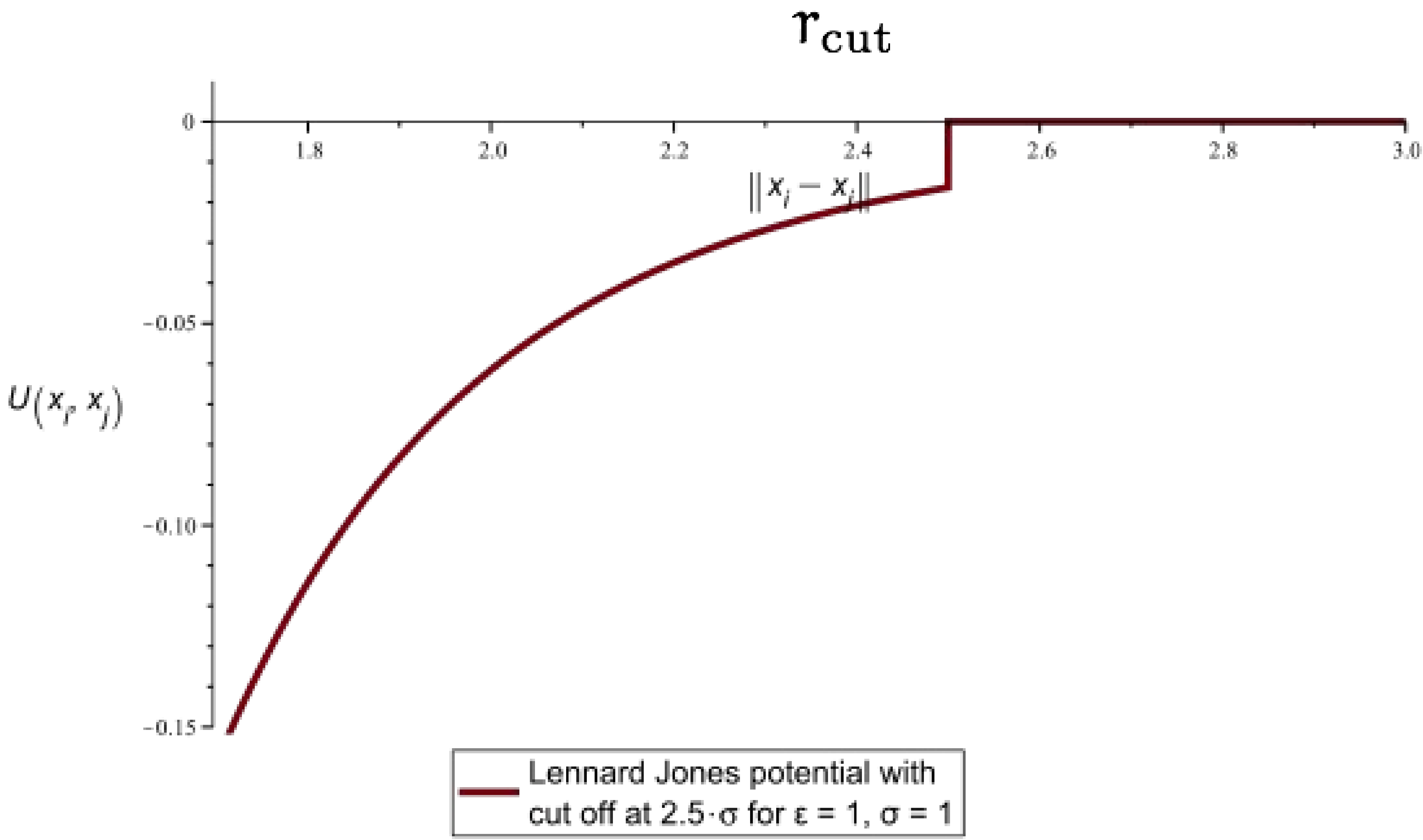
⇒ complexity: $\mathcal{O}(\#particles^2)$

Idea: Neglect near zero forces

Short range interaction

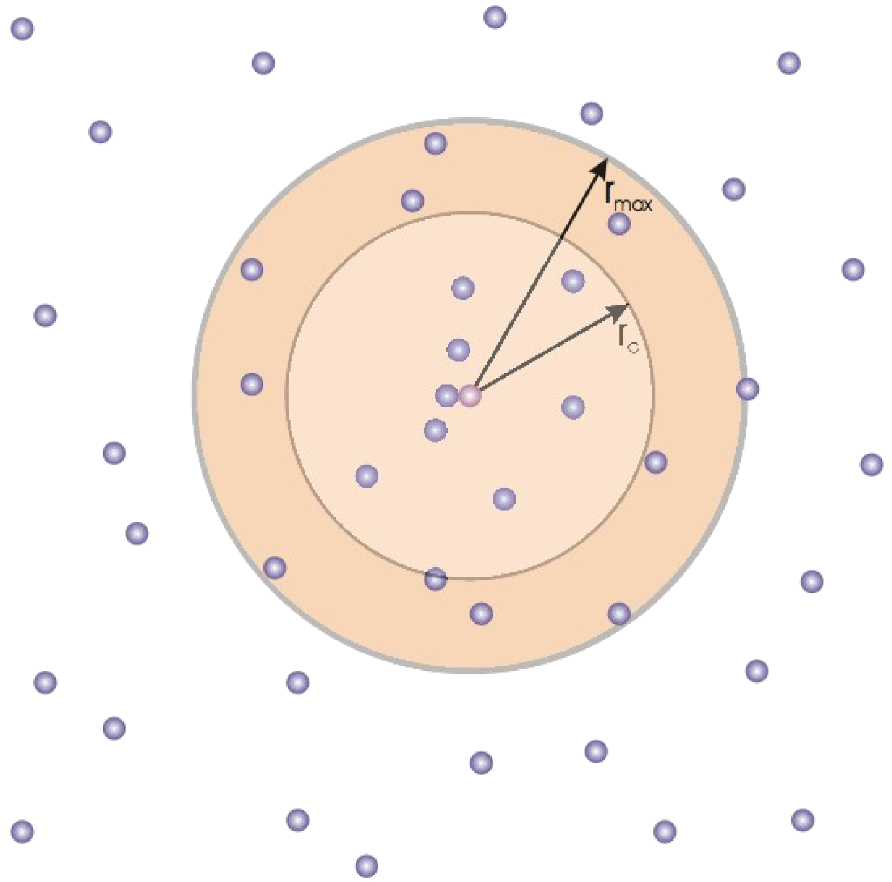


Short range interaction



Short range interaction

$\mathcal{O}(\#\text{particles})$

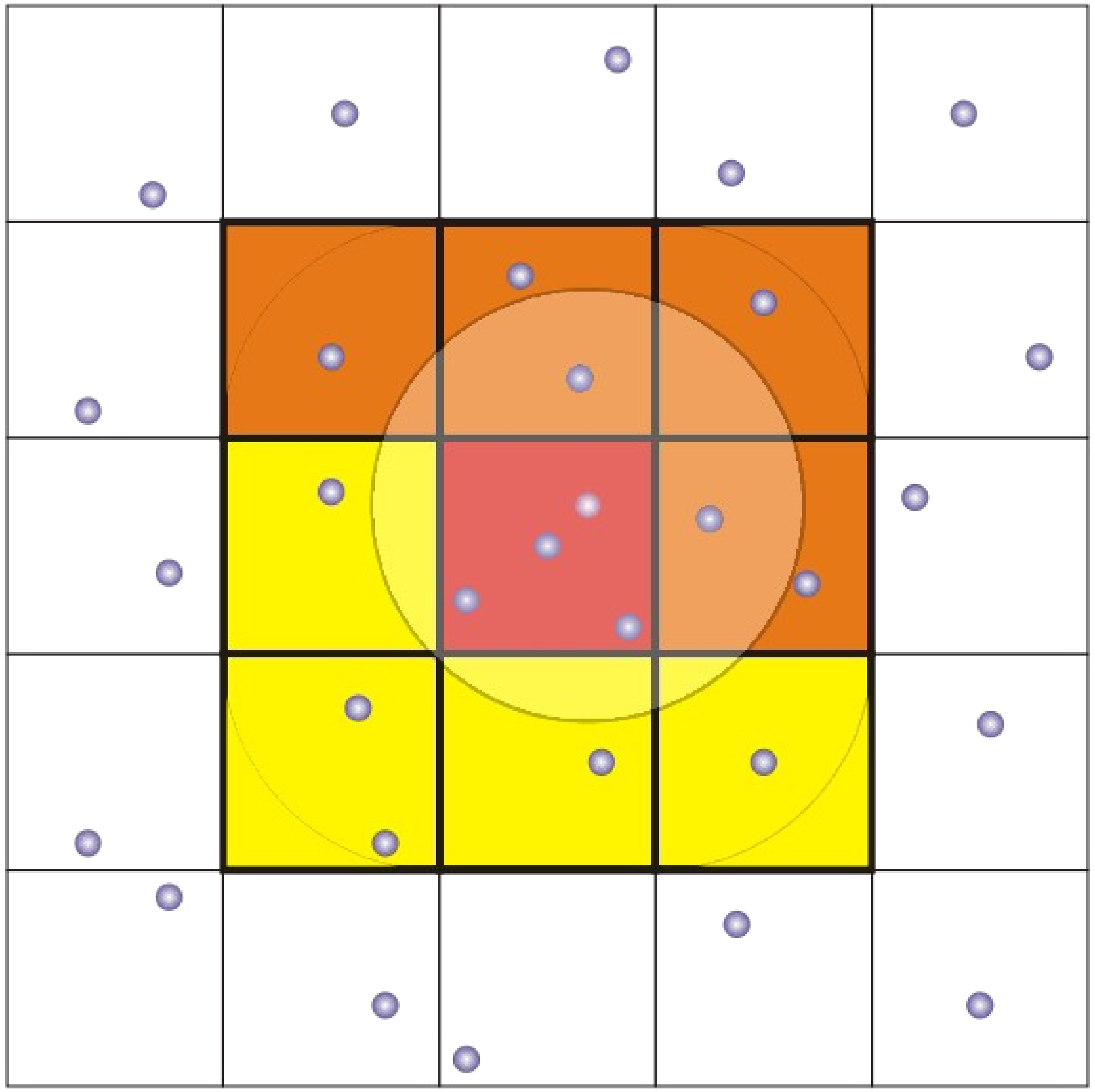


- Each molecule → list of neighboring molecules depending on r_{max}
- List update every $n_{update}(r_{max})$ time steps

⇒ buffer with:

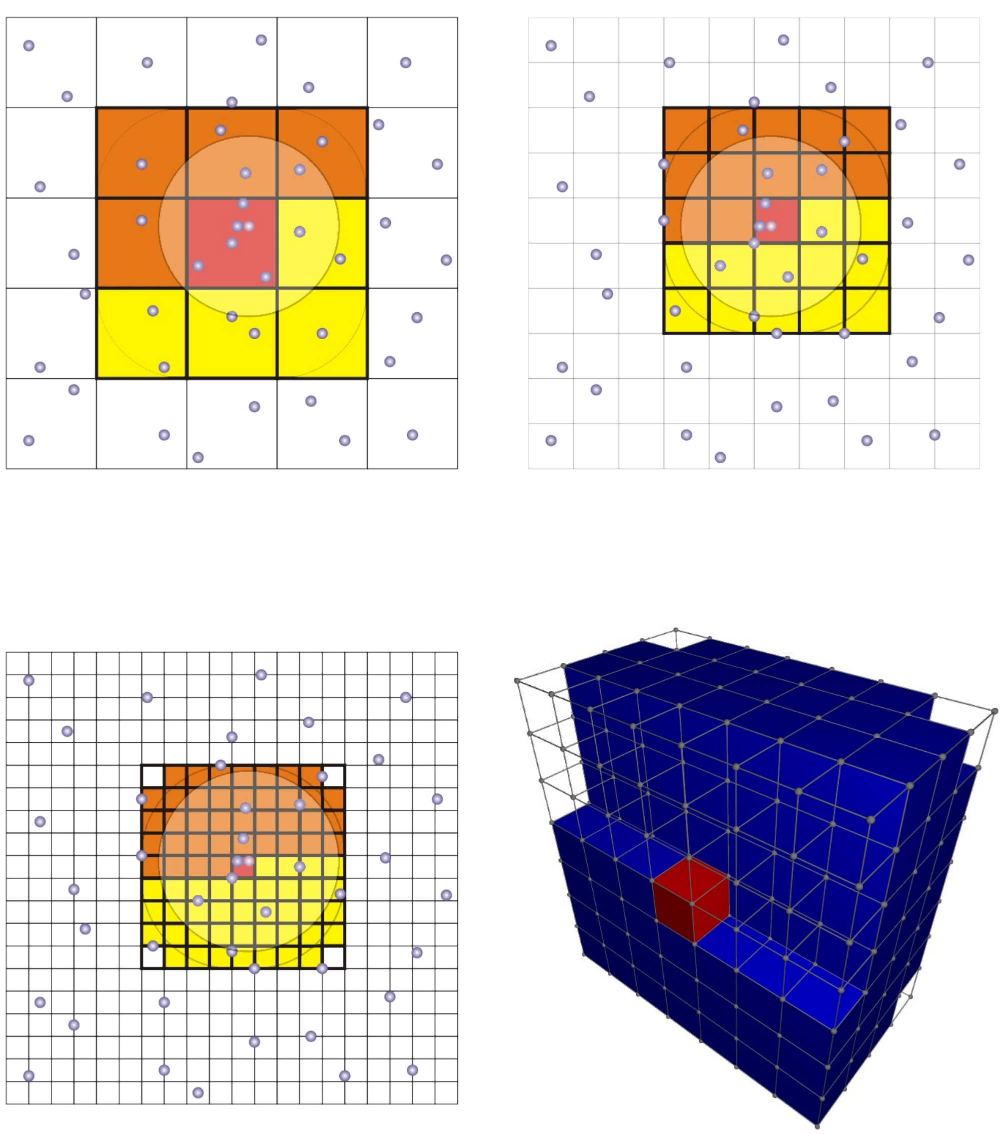
$$r_{max} - r_c > n_{update}(r_{max}) \cdot \Delta t \cdot v_k$$

Linked-cell algorithm (classic)



- Introduction of a cubic spatial mesh
- Side length given by cut-off radius
- Newton's third law: Iterate only over neighbor cells
- natural application of existing particle containers (sheet 3)
- Domain decomposition
  ⇒ parallelization? (sheet 5)

Linked-cell algorithm (outlook)



- cubic mesh with side length:

$$\frac{r_c}{\lambda}, \quad \lambda \in \mathbb{R}^+ \vee \lambda \in \mathbb{N}^+$$

- Converges against cut-off sphere for $\lambda \to \infty$

Linked-cell algorithm: Data structure

- linearized array (2D/3D → 1D)
- mesh: 1D vector of cells
- cells: list of molecules

- Halo region: boundary conditions/ghost layer
  - outflow: delete molecules after time step (sheet 3)
  - reflecting boundaries (sheet 3)
  - periodic? (sheet 4)
  - distributed memory parallelization?

Preparation: Worksheet 3