INCOMPRESSIBLE

DERIVATION OF THE U-ω EULER EQUATION FROM THE U-P FORM (BLACKBOARD)

Euler equations in velocity-pressure form

① $\frac{Du}{Dt} = \frac{\partial u}{\partial t} + (u\cdot\nabla)u = -\frac{1}{\rho}\nabla p$ (Momentum equation)

② $\nabla\cdot u = 0$ (Continuity equation — incompressibility)

$\nabla\times$①:

$$\nabla\times\frac{\partial u}{\partial t} + \nabla\times\left[(u\cdot\nabla)u\right] = \nabla\times\left(-\frac{1}{\rho}\nabla p\right)$$

$\nabla\times\left(-\frac{1}{\rho}\nabla p\right) = 0$ (i) (curl of gradient of a scalar field)

$$\frac{\partial\omega}{\partial t} + \nabla\times\left[\frac{1}{2}\nabla(u\cdot u) - u\times(\nabla\times u)\right] =$$

$\frac{1}{2}\nabla(u\cdot u)$: 0 (i)

$\nabla\times u = \omega$ (ii)

ω (ii)

(ii) $\nabla\times u = \omega$

$\frac{1}{2}\nabla(u\cdot u) = (u\cdot\nabla)u + u\times(\nabla\times u)$

$$= \frac{\partial\omega}{\partial t} + (u\cdot\nabla)\omega - (\omega\cdot\nabla)u + \omega(\nabla\cdot u) - u(\nabla\cdot\omega) = 0$$

$\omega(\nabla\cdot u)$: ②

$\nabla\cdot(\nabla\times\omega) = 0$

$$\Rightarrow \boxed{\frac{\partial\omega}{\partial t} + (u\cdot\nabla)\omega = (\omega\cdot\nabla)u}$$

Further simplification in 2D: $(\omega\cdot\nabla)u = 0$

$$\Rightarrow \boxed{\frac{\partial\omega}{\partial t} + (u\cdot\nabla)\omega = 0}$$ 2D

RECOVERING OF VELOCITIES FROM VORTICITIES

$\nabla\times\left(\omega = \nabla\times u\right)$

$$\nabla\times\omega = \nabla\times(\nabla\times u) = \nabla(\nabla\cdot u) - \nabla^2 u$$

$\nabla(\nabla\cdot u)$: 0 ②

$$\Rightarrow \boxed{\Delta u = -\nabla\times\omega}$$

Poisson Equation

OR

$$\omega = \nabla\times u = \nabla\times(\nabla\times\psi)$$

$$= \nabla(\nabla\cdot\psi) - \nabla^2\psi$$

$\nabla(\nabla\cdot\psi)$: 0 (2D)

$$\Rightarrow \boxed{\Delta\psi = -\omega}$$

Poisson Equation

(scalar)

$$\rightarrow u = \nabla\times\psi$$

Green's Function Solution for the Diffusion Equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \qquad (1D)$$

the Green's function solution satisfies

$$\left[D\frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial t}\right] G = -\delta(x)\delta(t)$$

the Fourier Transform $\hat{G} = \int_{-\infty}^{\infty} G e^{-ikx} dx$

yields:

$$\left[Dk^2 + \frac{\partial}{\partial t}\right] \hat{G} = \delta(t)$$

this is now an ODE which has solution

$$\hat{G} = H(t) e^{-tDk^2} \qquad \left[\begin{array}{l} H: \text{Heaviside function} \\ \frac{\partial H(t)}{\partial t} = \delta(t) \end{array}\right]$$

test:

$$\frac{\partial \hat{G}}{\partial t} = \delta(t) - Dk^2 e^{-tDk^2}$$

Taking the inverse FT of $\hat{G}$, we obtain

$$G = \frac{1}{2\pi}\int_{-\infty}^{\infty} H(t) e^{-tDk^2} e^{ikx} dk =$$

$$= \frac{H(t)}{2\pi}\int_{-\infty}^{\infty} e^{-tD\left(k^2 - \frac{ikx}{tD}\right)} dk =$$

$$= \frac{H(t)}{2\pi}\int_{-\infty}^{\infty} e^{-tD\left(k - \frac{ix}{2tD}\right)^2 - \frac{x^2}{4tD}} dk =$$

$$= \frac{H(t)}{2\pi} e^{-\frac{x^2}{4tD}} \int_{-\infty}^{\infty} e^{-tD\left(k - \frac{ix}{2tD}\right)^2} dk =$$

$$\int_{-\infty}^{\infty} e^{-ak^2} dk = \sqrt{\frac{\pi}{a}}$$

$$= \frac{H(t)}{\sqrt{4\pi tD}} e^{-\frac{x^2}{4Dt}} \Longrightarrow \text{Gaussian!}$$

→ we are interested in $t > 0$, thus

$$G = \frac{1}{\sqrt{4\pi tD}} e^{-\frac{x^2}{4Dt}}$$

This is a short range interaction!

Cell-Lists

High Performance Computing for Science and Engineering

CSE**lab**
Computational Science & Engineering Laboratory
http://www.cse-lab.ethz.ch

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Diffusion as N-Body Problem

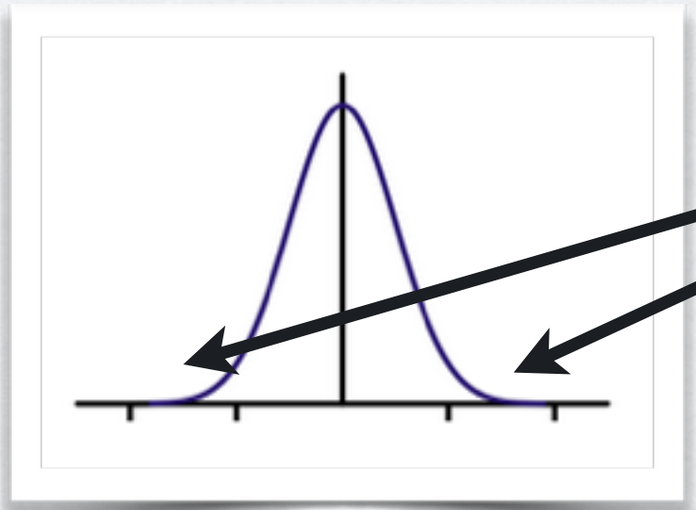
The fundamental solution to the diffusion equation

$$\frac{\partial u}{\partial t} = D\Delta u$$

is given by the Green's function

$$G(\mathbf{x}, t) = \left(\frac{1}{4\pi Dt}\right)^{d/2} e^{-\frac{\mathbf{x}\cdot\mathbf{x}}{4Dt}}$$

which is a *d*-dimensional Gaussian function



fast decay

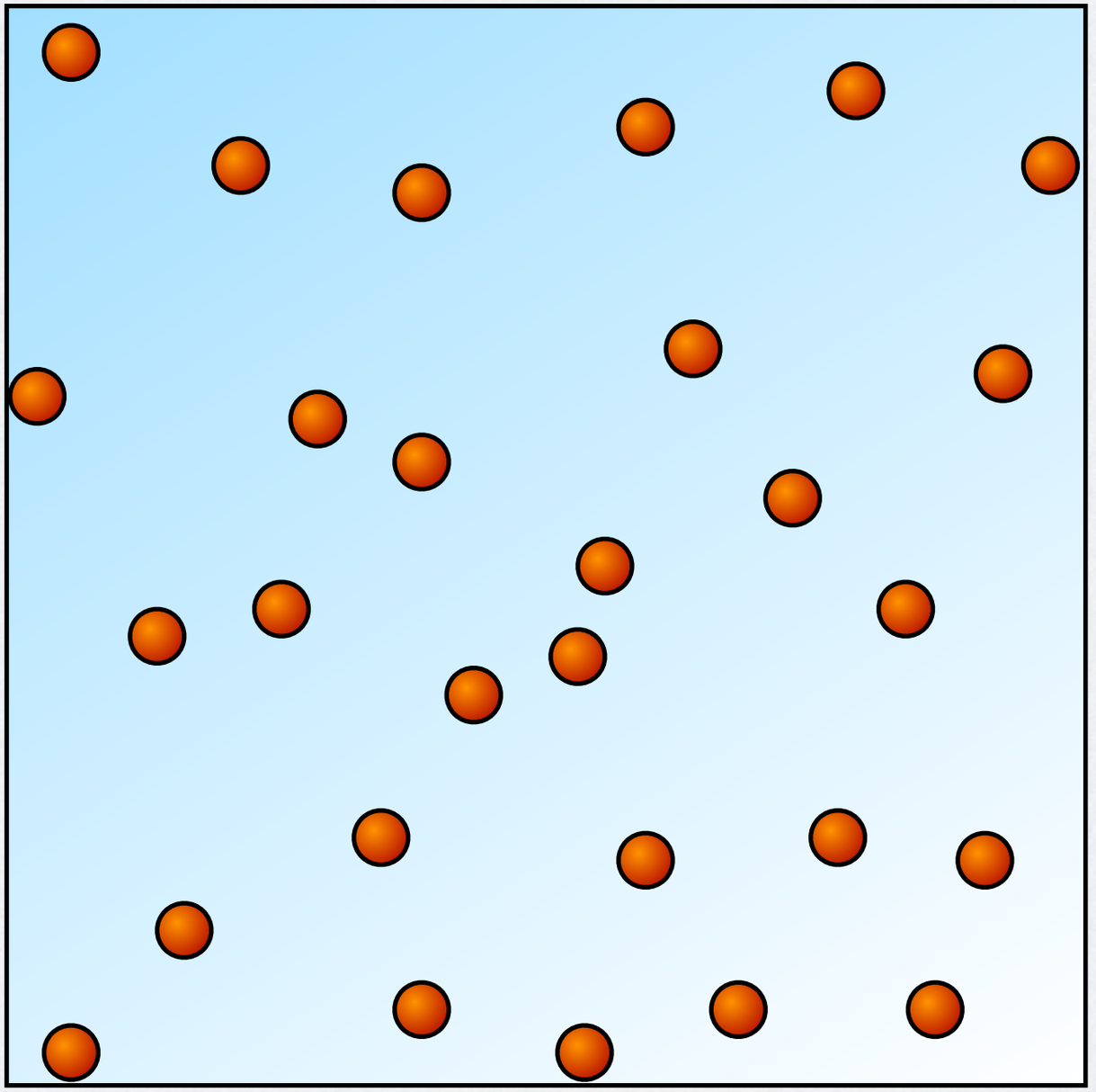
short-range interactions

N-Body Problem in MD

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i$$

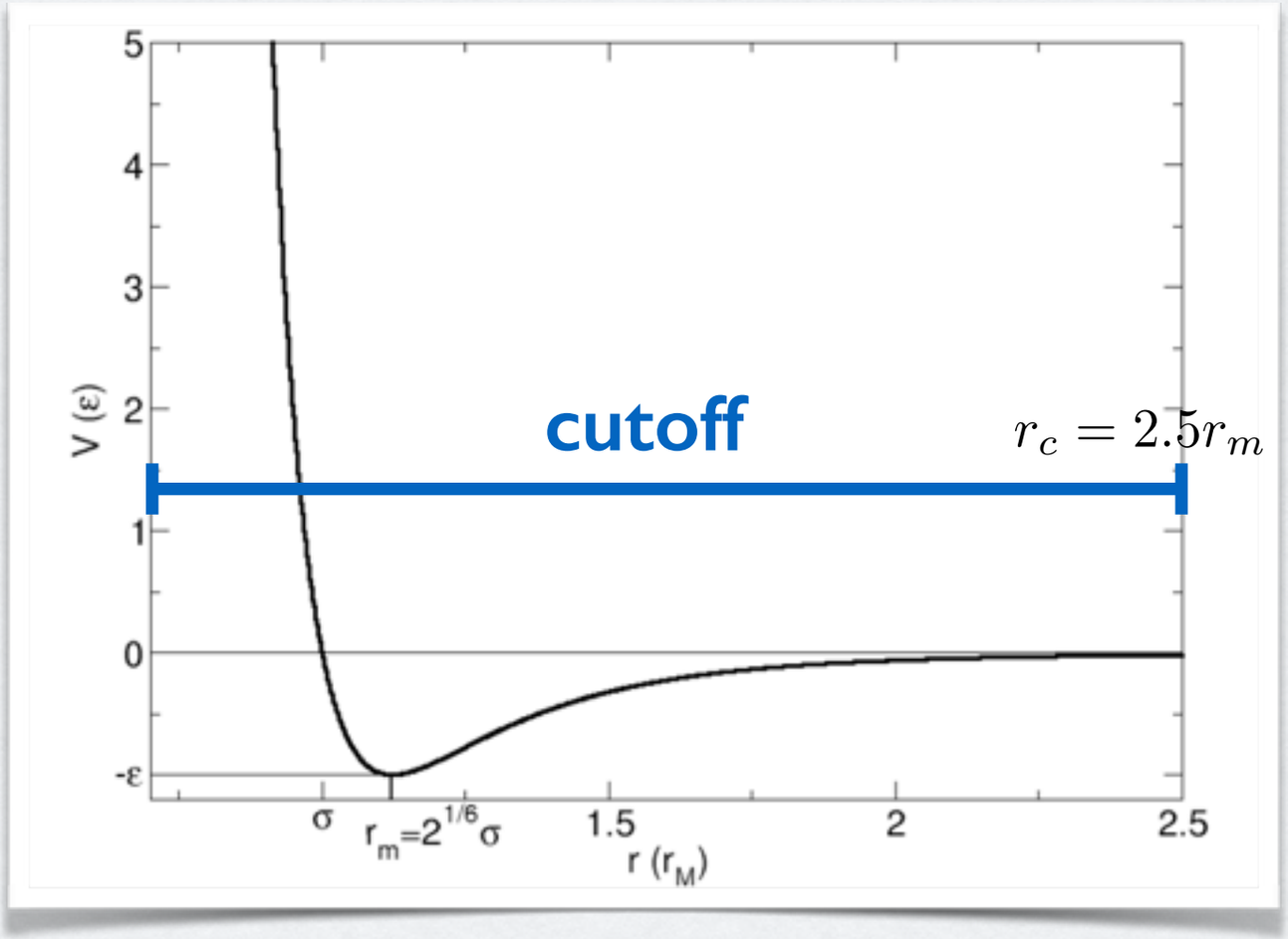
$$m_i \frac{d\mathbf{u}_i}{dt} = \sum_{j=1;j\neq i}^{N} \mathbf{F}_{ij}$$

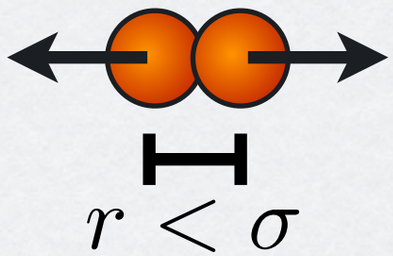
$$\mathbf{F}_{ij} = -\frac{\mathbf{x}_i - \mathbf{x}_j}{||\mathbf{x}_i - \mathbf{x}_j||}\frac{dV}{dr}$$



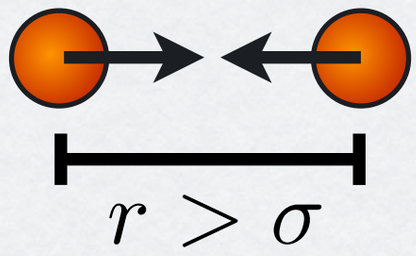
The Lennard-Jones Potential

$$V_c(r) = \begin{cases} 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] - V(r_c) & \text{for } r < r_c, \\ 0 & \text{else,} \end{cases}$$



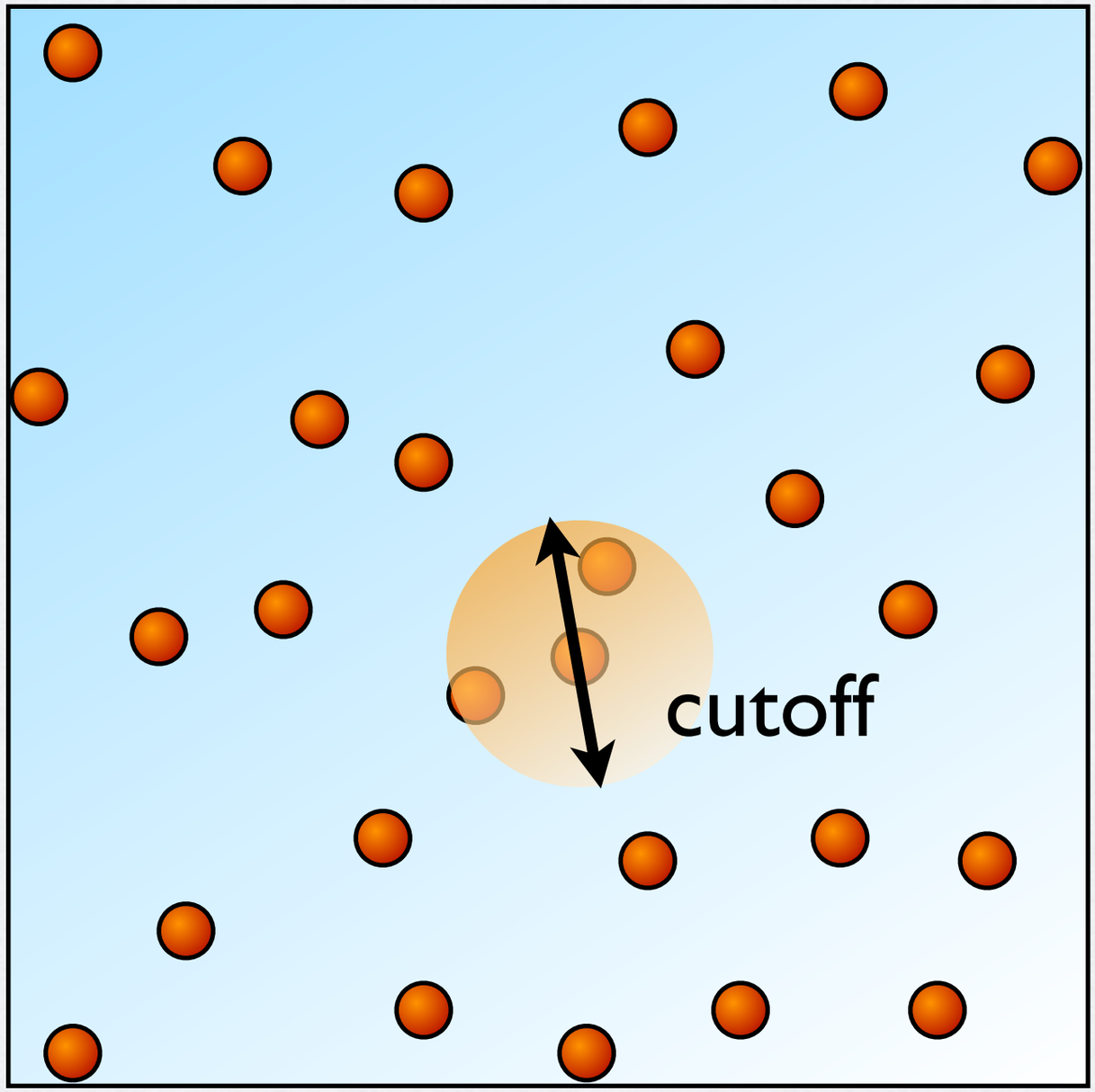


$r < \sigma$



$r > \sigma$

Local Interactions



Can we take advantage of this to avoid $\mathcal{O}(N^2)$ operations?

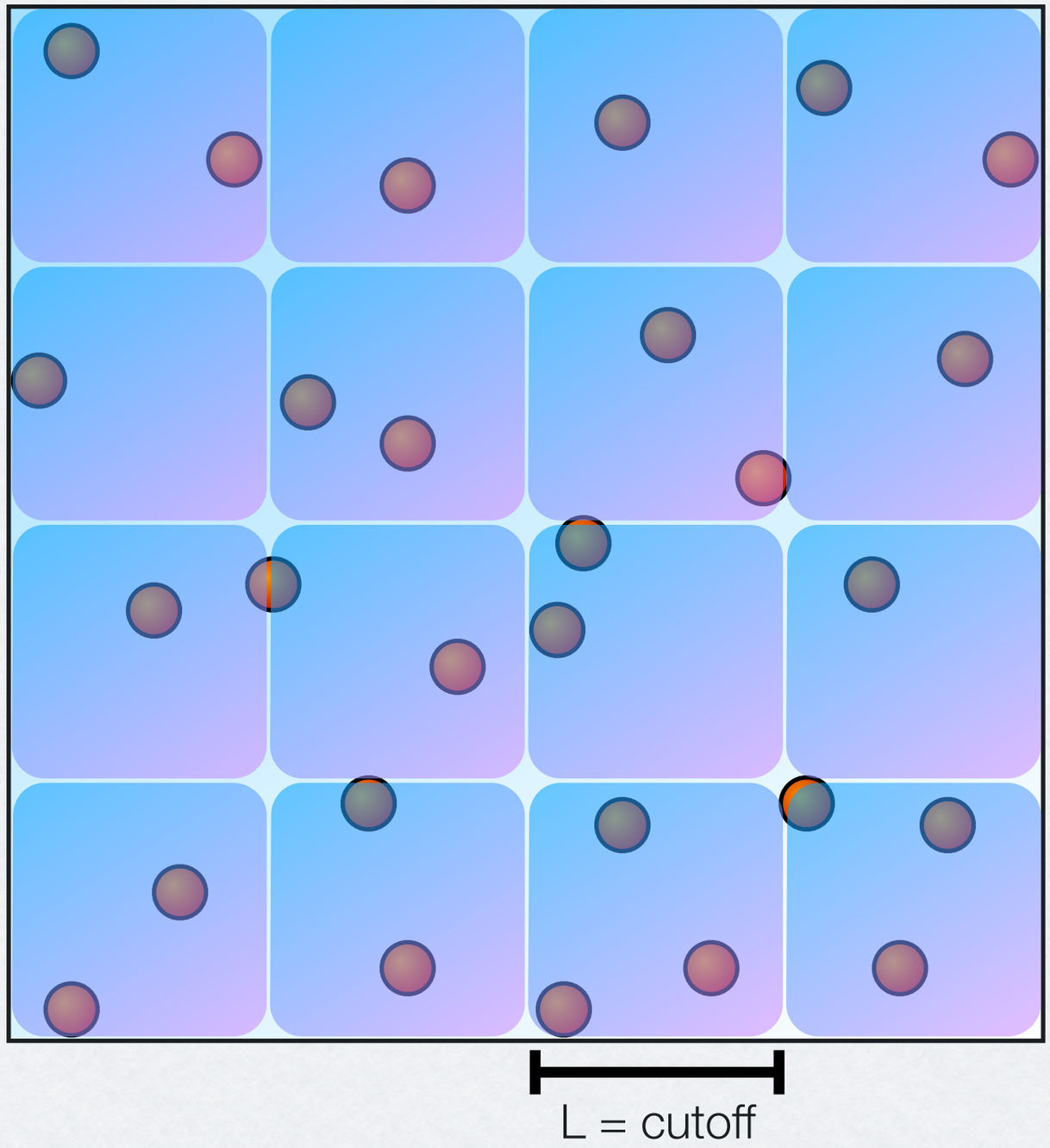
Idea - Subdivide Domain

Domain subdivision in *cells:*

- Cell size is the cutoff
- Cells contain particles

Particles:

- Spread into the cells according to their position



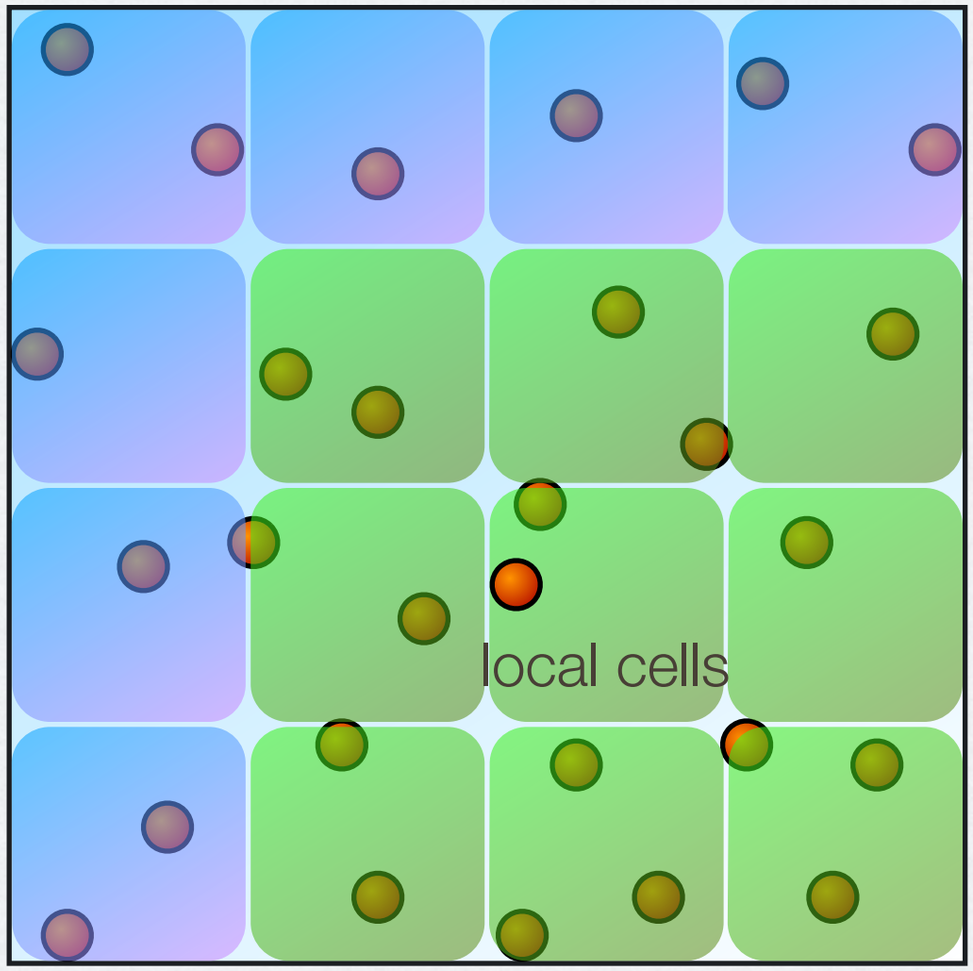
Computing Interactions

Interactions: only local cells contribute

Cost of N interactions (2D):

- c=N/m (average #particles/cell)
- assume constant c w.r.t. N
- cost for one particle: 9c
- total: 9cN ➡ $\mathcal{O}$(N)
- algorithmic improvement:

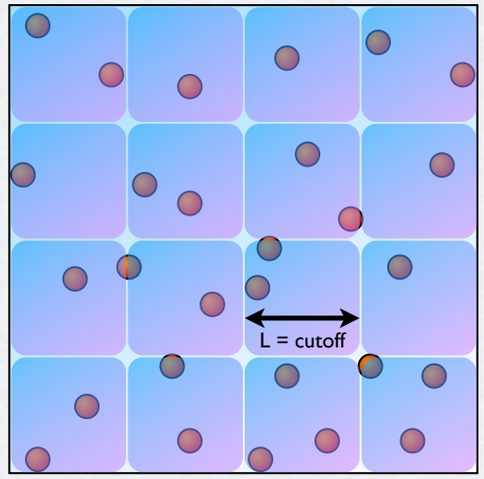
$$\frac{N^2}{9cN} = \frac{N}{9c}$$



m cells

Cell List Construction

HOW TO FIND THE PARTICLE NEAREST NEIGHBORS?



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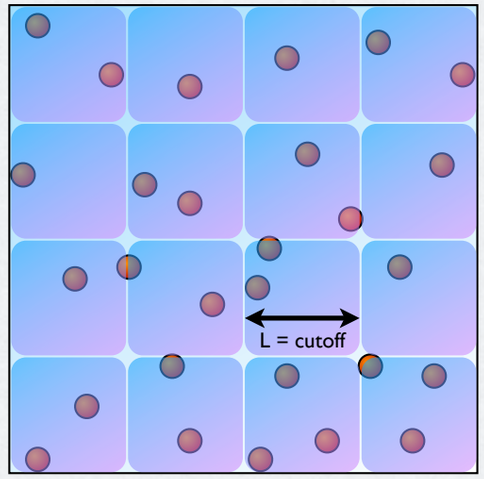
- Group particles according to the “address” of their cell



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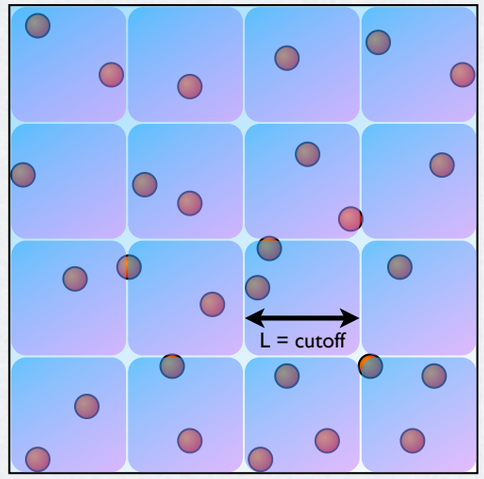

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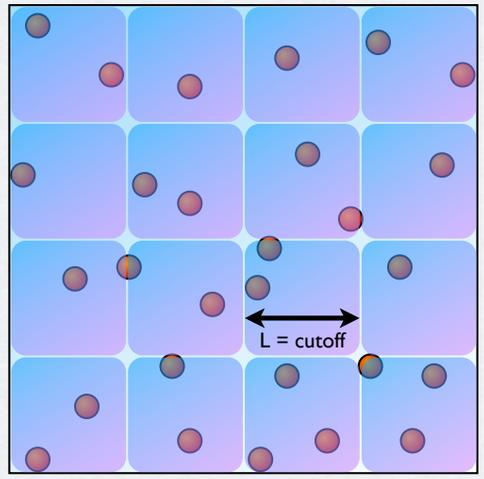

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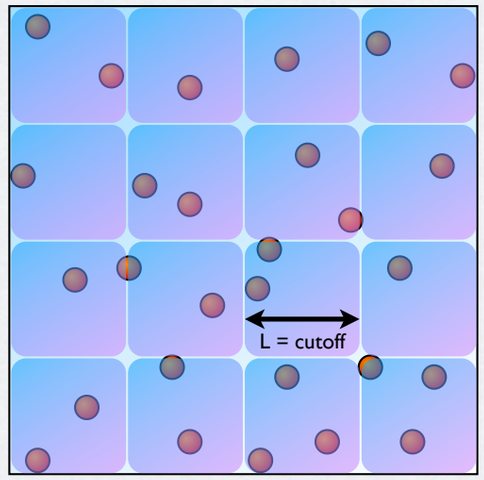

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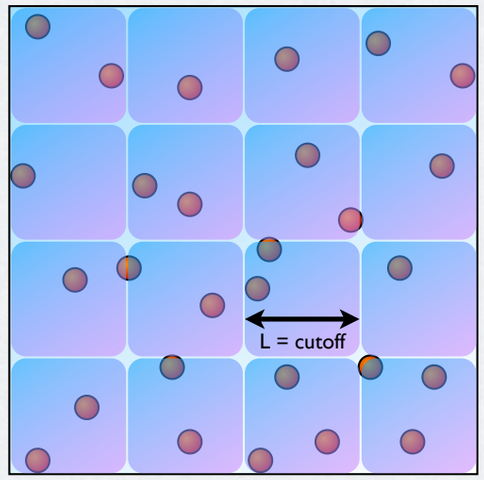

STL-based implementation with M^3 cells (3D, domain $[0,1)^3$)

Cell List Construction

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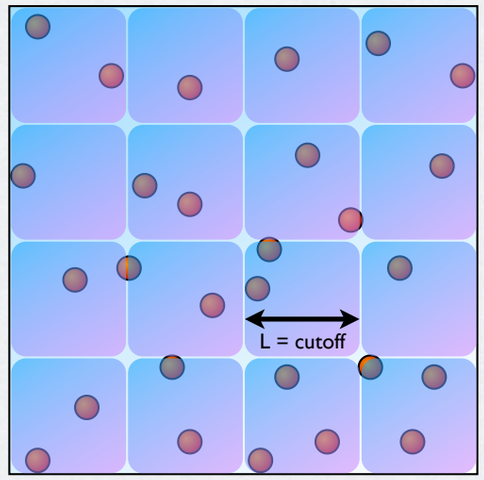

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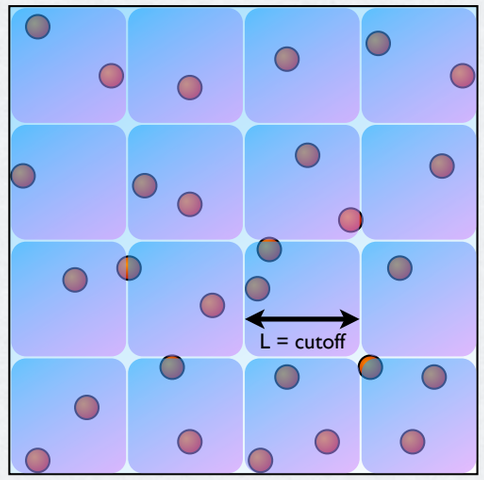

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Cell List Construction

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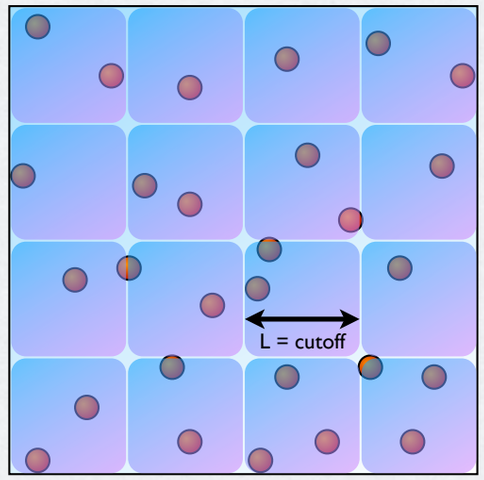

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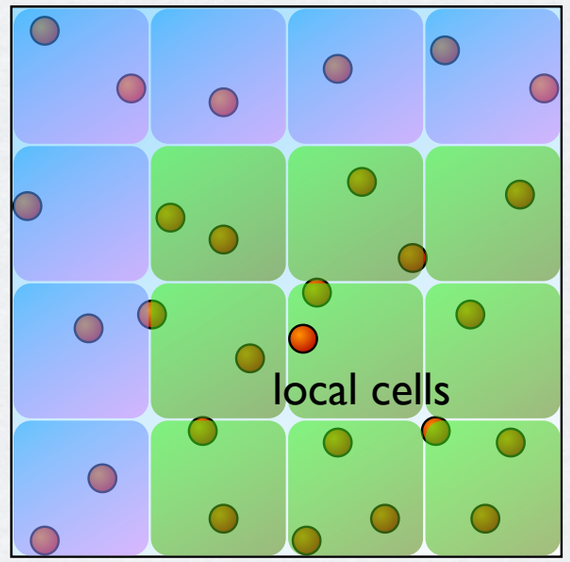
- cell address for particle at (x,y,z): (ix,iy,iz) = (floor(x/L)), floor(y/L), floor(z/L)), L = 1/M
  - 1D address into `cells`: `idx = ix + iy*M + iz*M*M = ix + M*(iy + M*iz)`

Cell List Traversal



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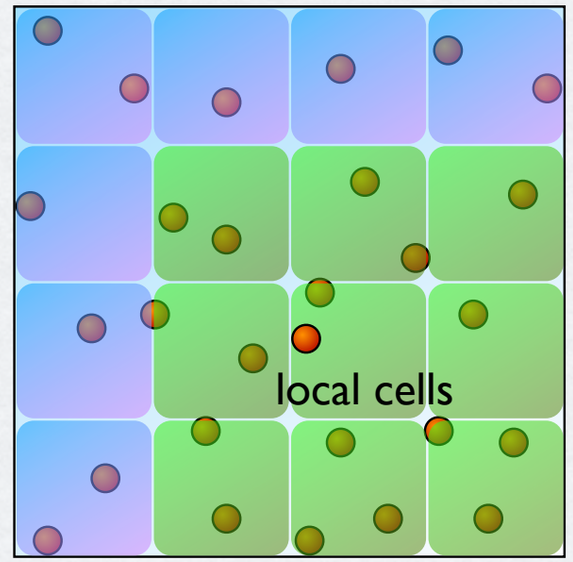

Cell List Traversal

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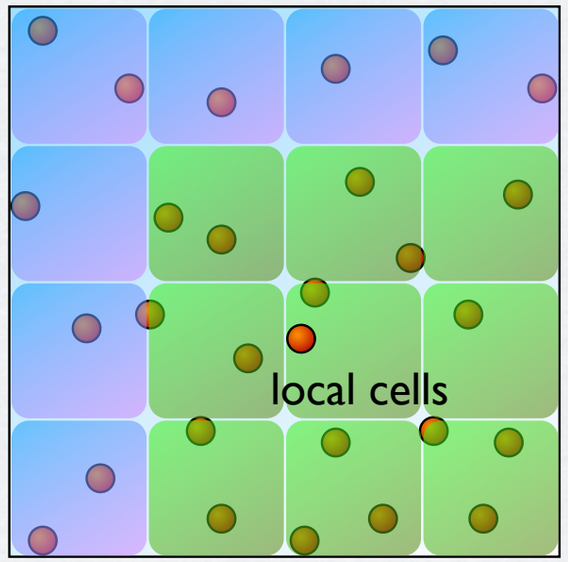
- **Algorithm**:

  Loop over all cells[i]



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- Given an initialized
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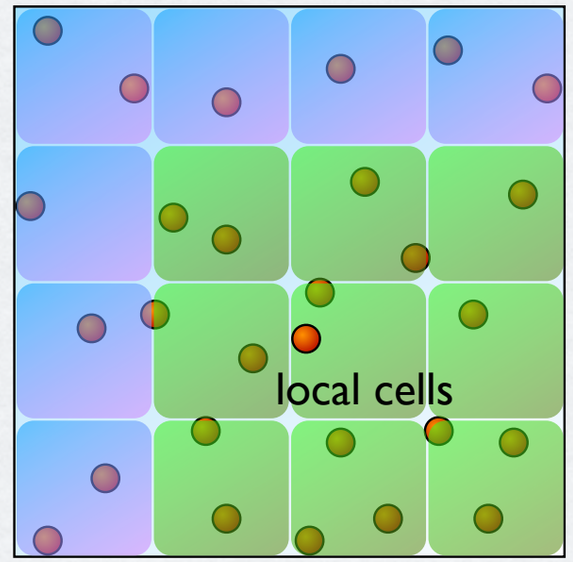

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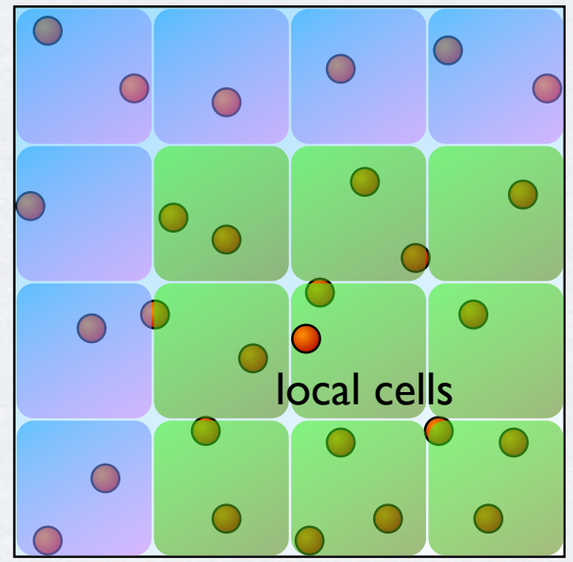

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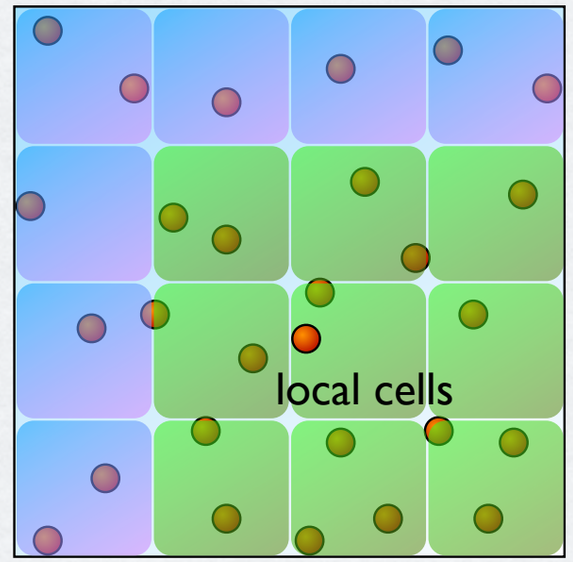

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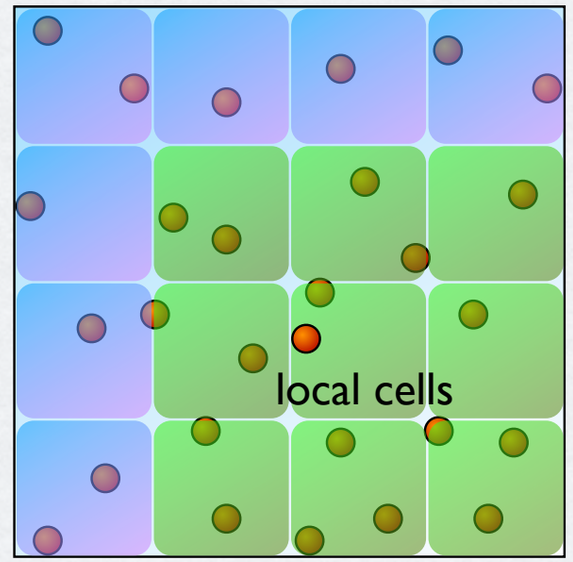

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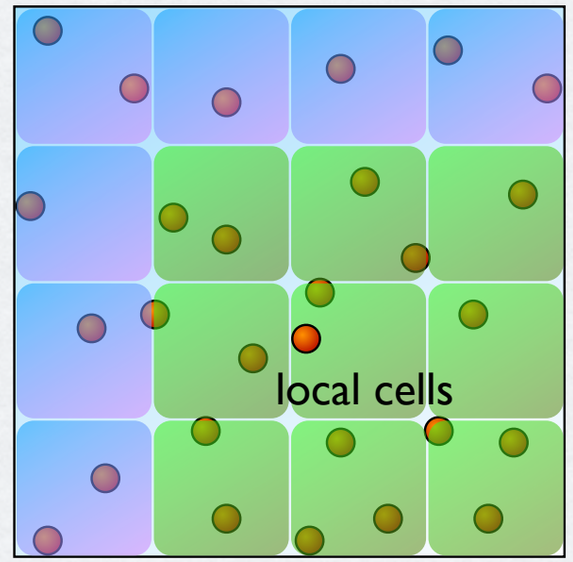
      - Careful to skip interaction with own particle (i.e. p[k] == p[l])
      - Always check the cutoff distance: Cell list guarantees that all particles within the cutoff are in neighboring cells, not the other way around!

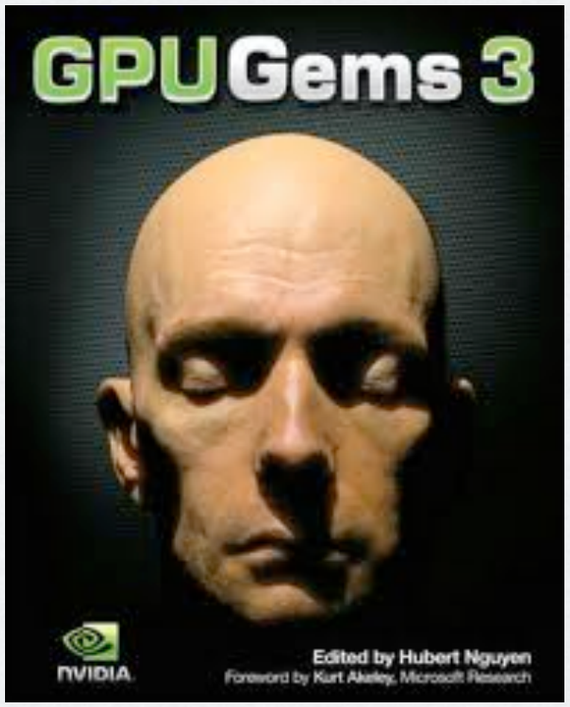


Using Cell List

- Cell list is created at each time-step
- Cell list creation is $\mathcal{O}$(N), it does not mean cheap!
- Particle position coherence can be exploited
  - Keep previous cell list
  - Refresh cell list:
    - Look for particles that moved into another cell
    - Erase the particle from the old cell
    - Insert the particle in the new cell

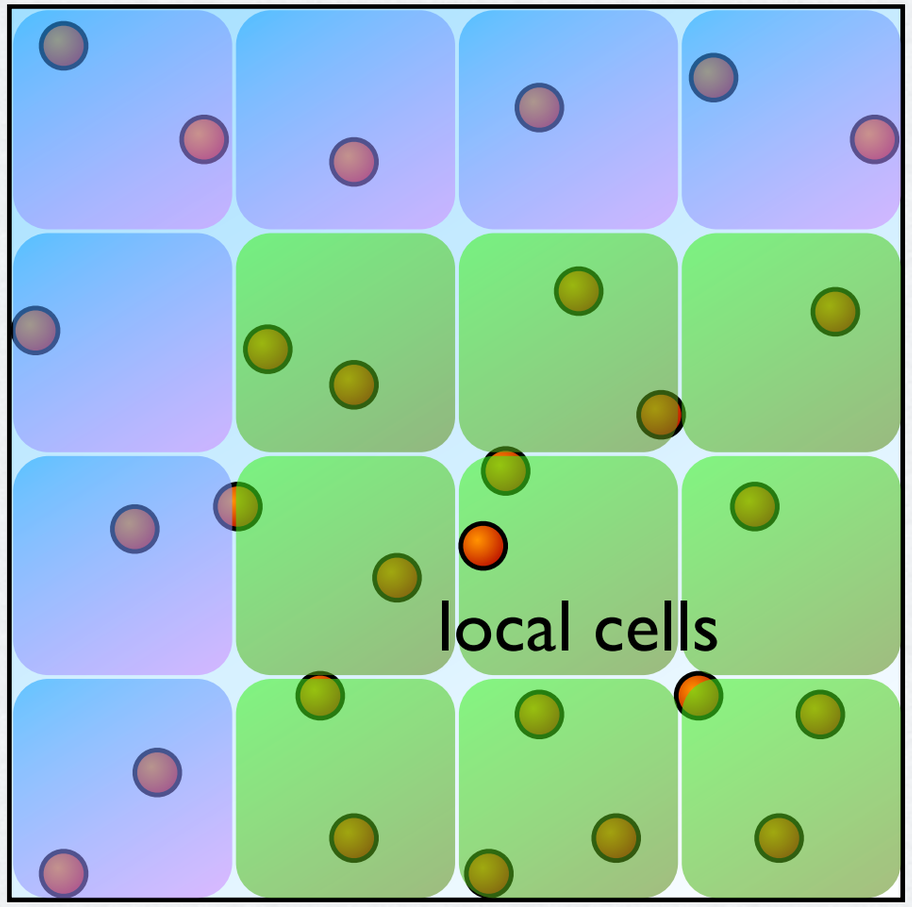
Cell List Implementation

- Information taken from GPU Gems 3
  - GPU Gems 3 is a collection of state-of-the-art GPU programming examples
  - available online: http.developer.nvidia.com/GPUGems3/gpugems3_ch32.html



- Broad-phase collision detection with CUDA
  - called “**Spatial Subdivision**” algorithm
- Analogous to cell-lists in MD

Sequential Implementation



Sequential Implementation

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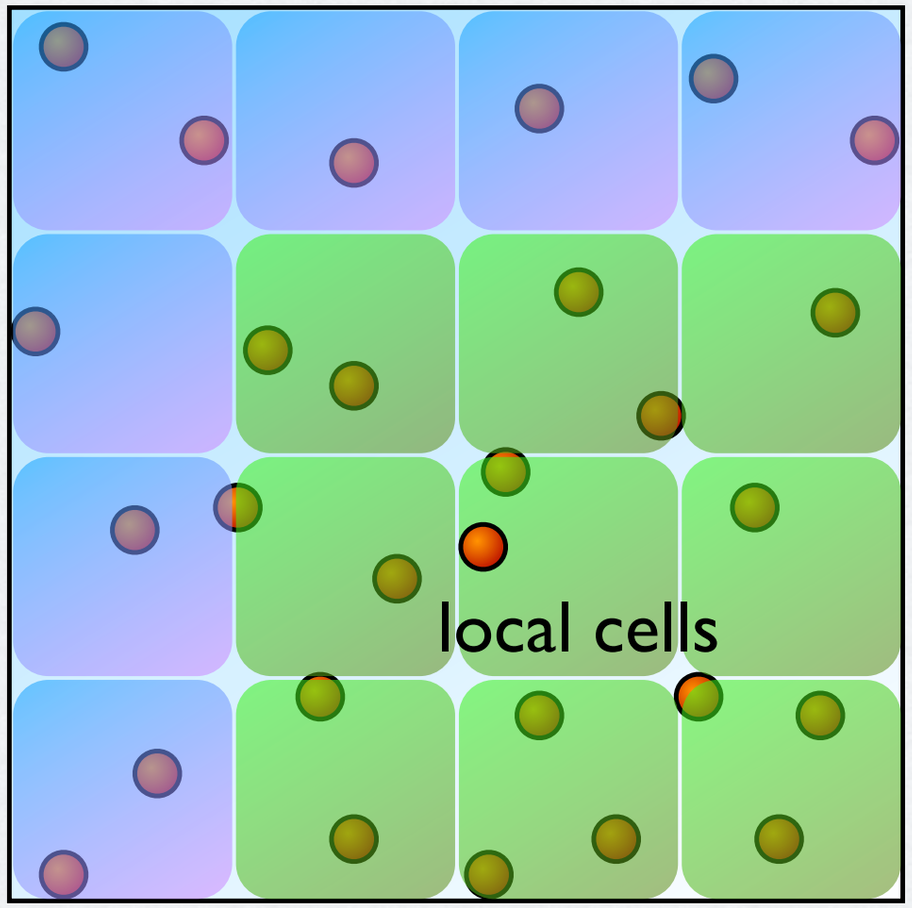
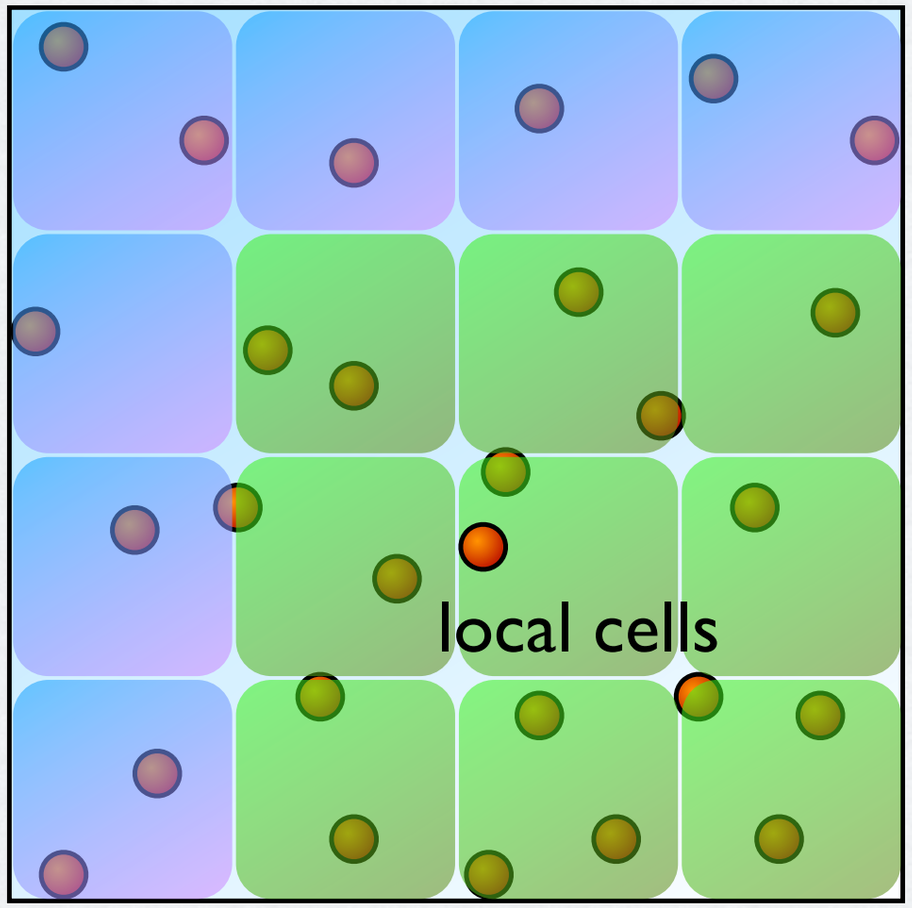


Sequential Implementation

1. For each particle find the ID of its container cell

2. Form list of particle IDs and corresponding cell IDs



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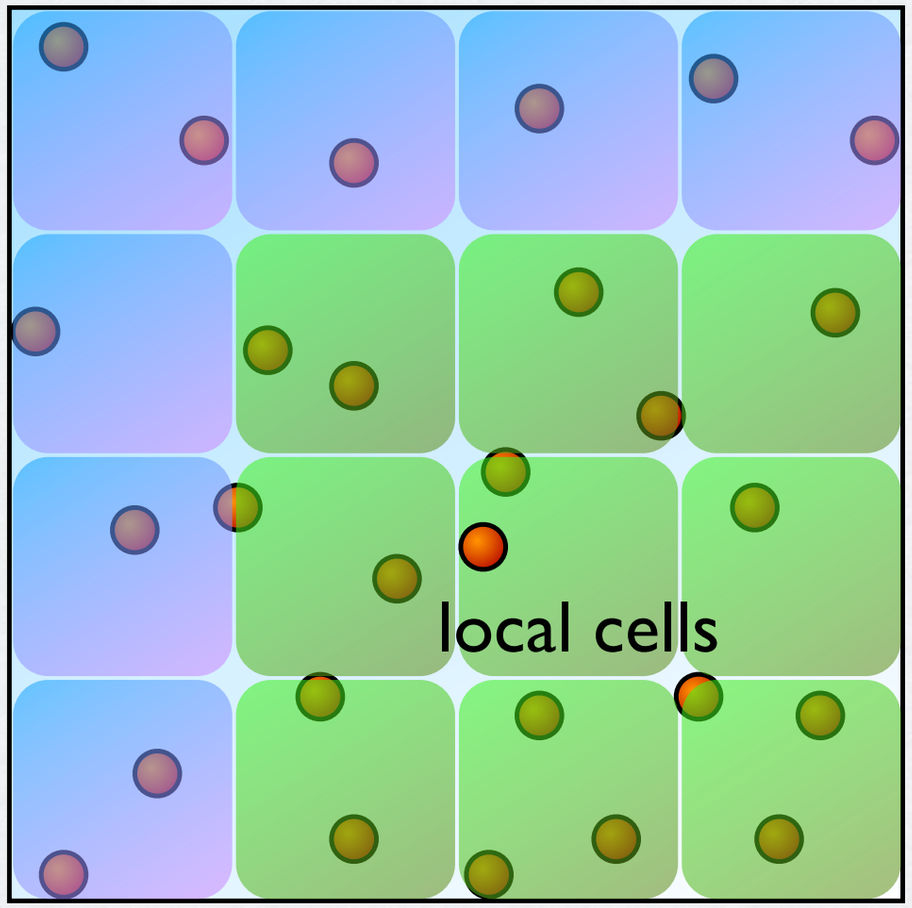

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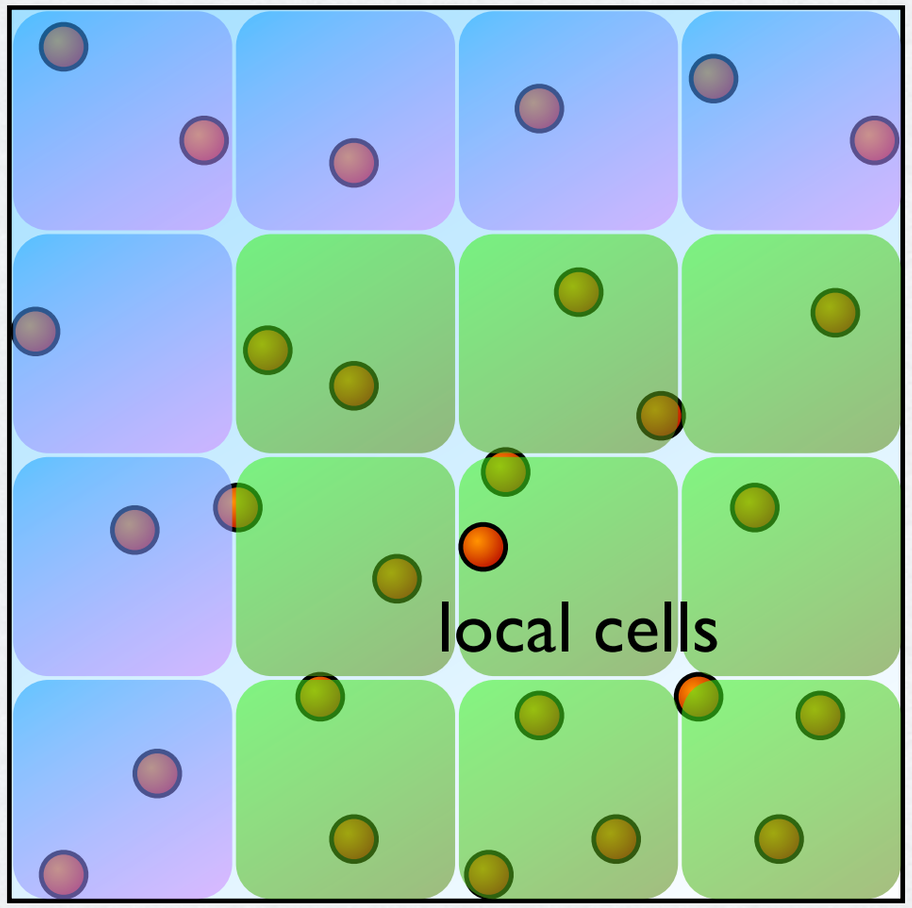

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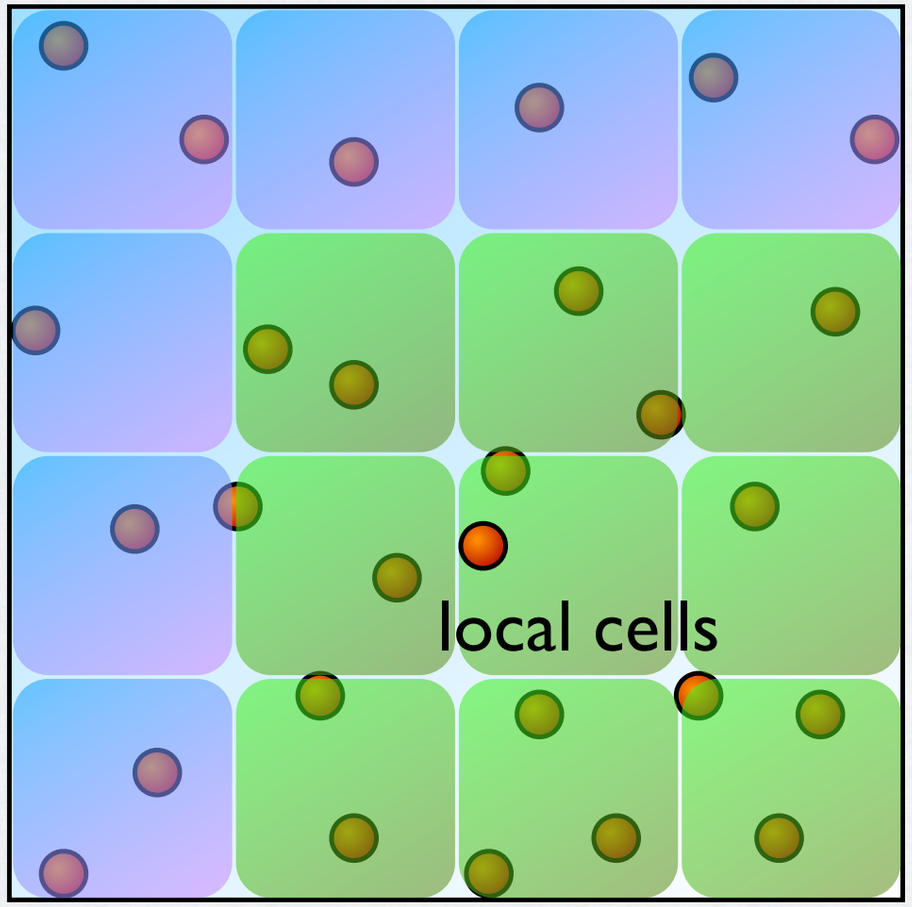

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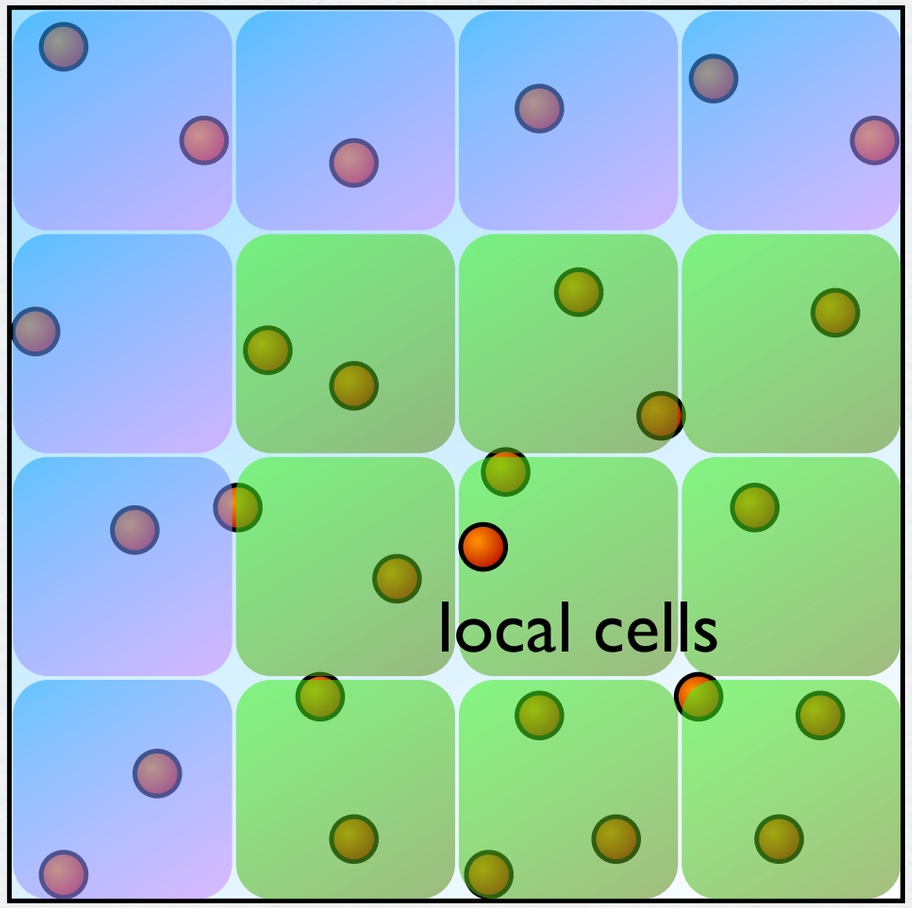
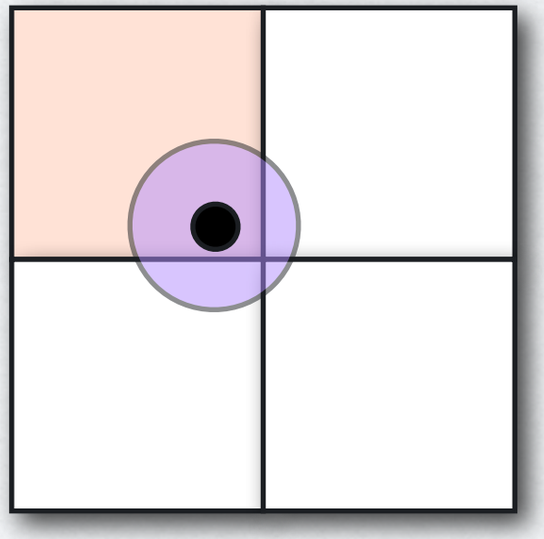


➡ **How to parallelize ?**

Data Structures

For each particle

particle ID
container cell ID



particle-ID	0	1	2	3	4	5	6	7	8	9	10
cell-ID	6	5	8	6	3	4	4	9	7	10	1

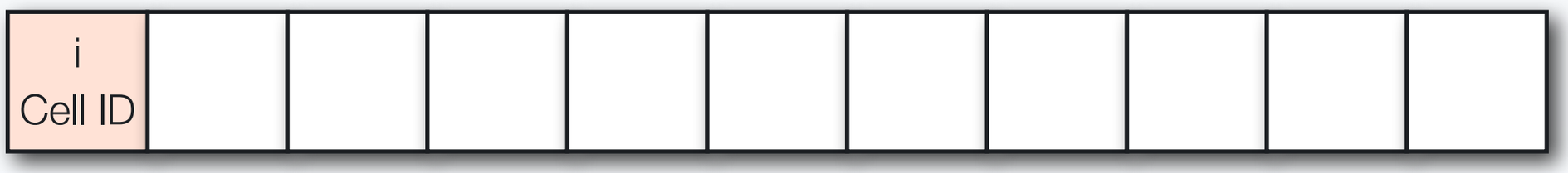
The array contains pairs of (particle-ID, cell-ID)

Constructing the 1D Cell-ID Array

Container cell ID H (hash) for particle i
with position (x_i,y_i,z_i) in]-1,1[^{3}

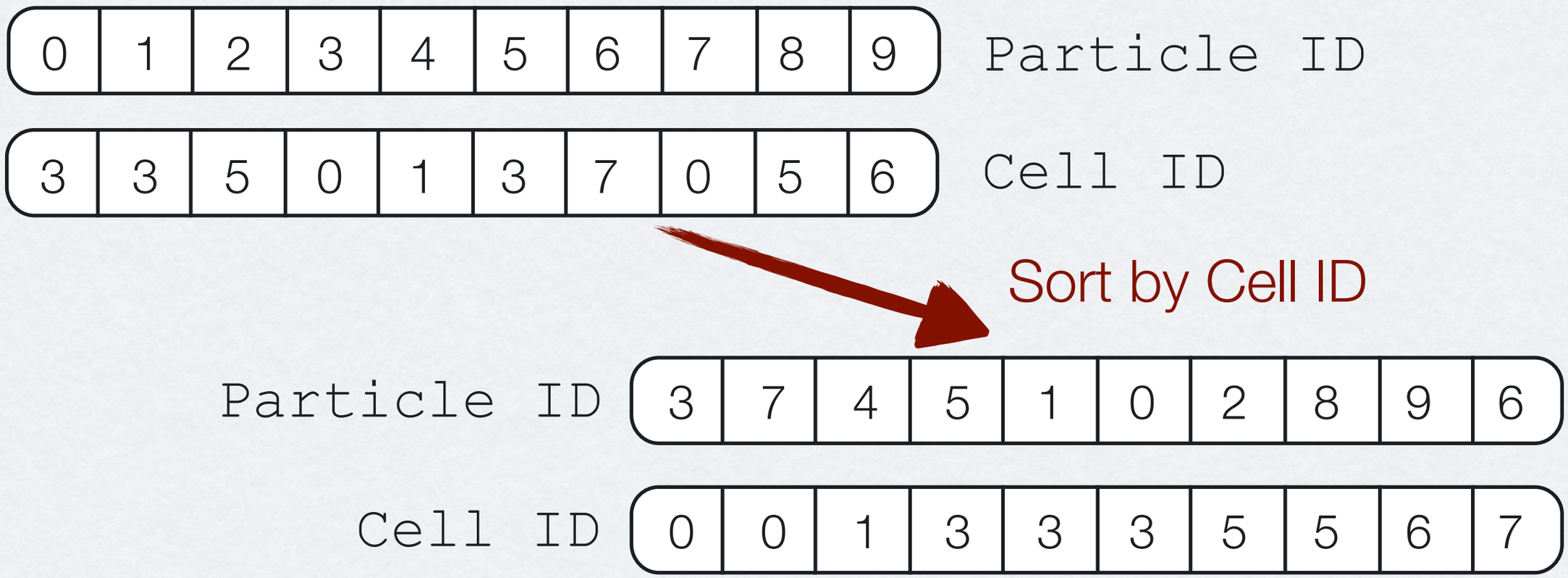
$$\text{cell ID} = \left\lfloor M \frac{x_i + 1}{2} \right\rfloor + M \left\lfloor M \frac{y_i + 1}{2} \right\rfloor + M^2 \left\lfloor M \frac{z_i + 1}{2} \right\rfloor$$

M: number of cells in a given direction



Sorting the Cell ID Array

- Cell ID array is sorted by cell ID
- Particle ID array is also sorted by cell ID
- Cell IDs may appear multiple times
- Radix sort: $\mathcal{O}$(N) sorting



Sorting with C++ - std::sort()

simple:

```
#include <algorithm>
#include <utility>
#include <vector>


//  Custom comparator for pair,
// compares only by the first field
struct compare_first
{
    template <typename T>
    bool operator() (const T& a, const T& b)
    {
     return a.first < b.first;
    }
};

//  Vector storing cellids as first member of pair
// and particleids as second member
std::vector<std::pair<unsigned int, unsigned int> > cellid_particleid(n_particles);


//  Fill the vector with cellids
// x, y, z - arrays storing coordinates of particles
// get_cell_index() returns the index of enclosing cell
for (int i=0; i<n_particles; i++)
    cellid_particleid[i] = std::make_pair(get_cell_index(x[i], y[i], z[i]), i);

std::sort(cellid_particleid.begin(), cellid_particleid.end(), compare_first());
```

BUT: this sorting is $\mathcal{O}$(N logN)!

Creating the Interaction Cell List

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- ***Interaction cell*** *(non-empty cell)*: contains 1 or more particles

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  - created from the sorted cell ID array
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  - the sorted cell ID array is scanned for **changes of cell ID**
  - **changes** mark the end of one cell and the beginning of another.
- ***Parallelization***: each thread is assigned a (roughly equal) segment of the cell ID array to scan for changes

Creating the Interaction Cell List

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Creating the Interaction Cell List

- ***Parallelization***: threads assigned to portions of the 1D array.
- *HOW TO*:
  - each thread scans past the end point of its pre-assigned segment and stops when it finds a change in cell-ID (except for the last thread)
  - each thread skips its first change as it has been found by a thread assigned to the preceding segment(except for the first thread)

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  - `First scan`
    - count the number of particles within each interaction cell
    - convert them into offsets in the 1D array (through a parallel prefix sum in several passes)

Creating the Interaction Cell List

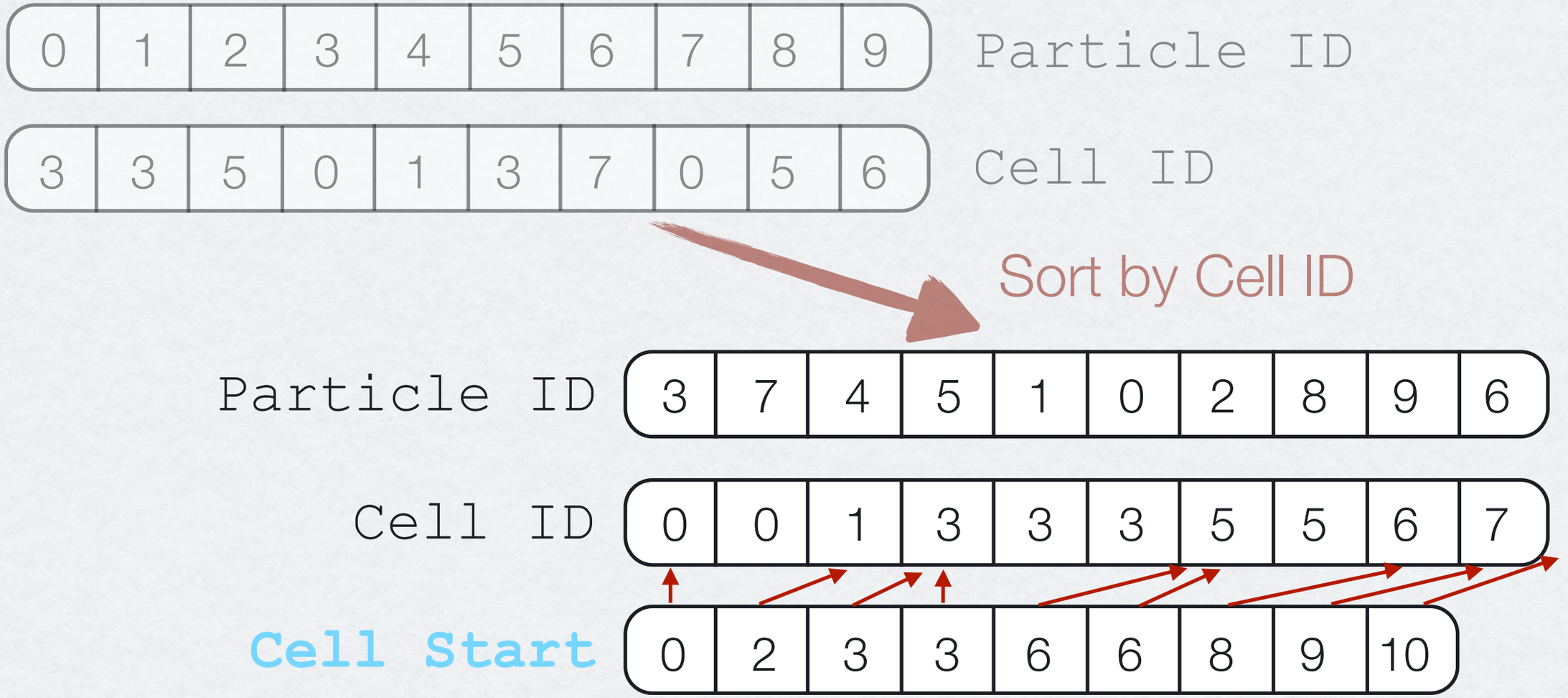
- The sorted 1D cell ID array is scanned **twice**

  - First scan
    - count the number of particles within each interaction cell
    - convert them into offsets in the 1D array (through a parallel prefix sum in several passes)

  - Second scan
    - create entries for each interaction cell in a **new array (“Cell Start”):**
    - **This array tells at which index in the 1D cell-ID array starts each cell**

Sorting the Cell ID Array

- Cell Start array marks the first particle in Particle ID array that is contained by the cell
- The size of Cell Start array is the number of cells plus one
- The last element always marks the end of Particle ID array



Cell Start Array

In C++ Cell Start calculation is straightforward

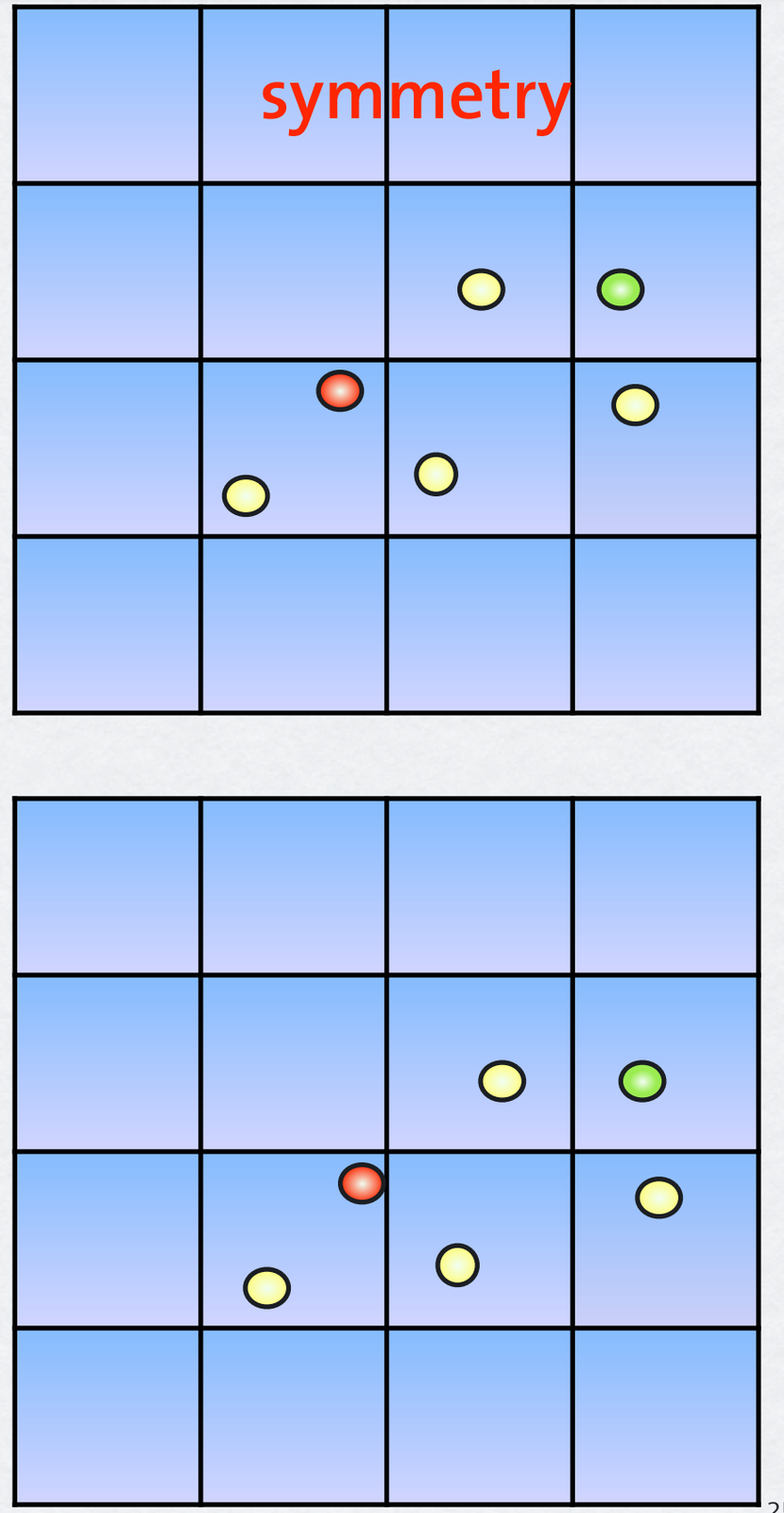
```
int current_cell = -1;
for (int i = 0; i < n_particles; i++)
{
    for (int j = current_cell; j < cellids[i]; j++)
    {
        start[j+1] = i;
    }
    current_cell = cellids[i];
}

for (int j = current_cell; j <= n_cells; j++)
    start[j+1] = n_particles;
```

Traversing the list

- After the creation of the list all the **particle neighbors are found** by:
  - **visiting all the cells that are adjacent to the cell containing the target particle**
- This make up a total of 9/27 (2D/3D) cells to look up
- Additional care has to be taken for the cells on the border of domain.
  Special case : Periodic Boundary Conditions.

Parallelization over Particles

- one thread processes one particle
  - particle of thread 1
  - particle of thread 2
  - other particles



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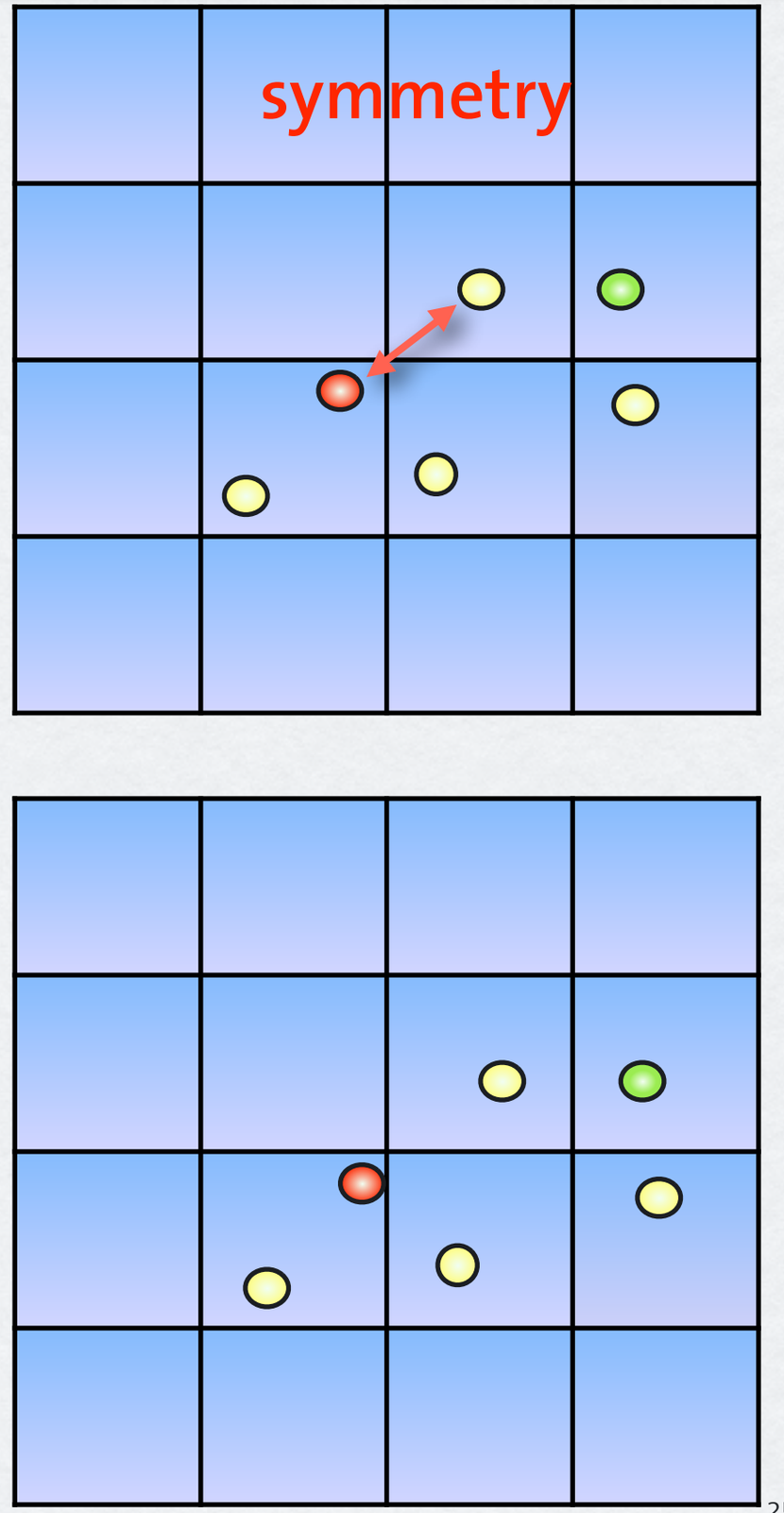

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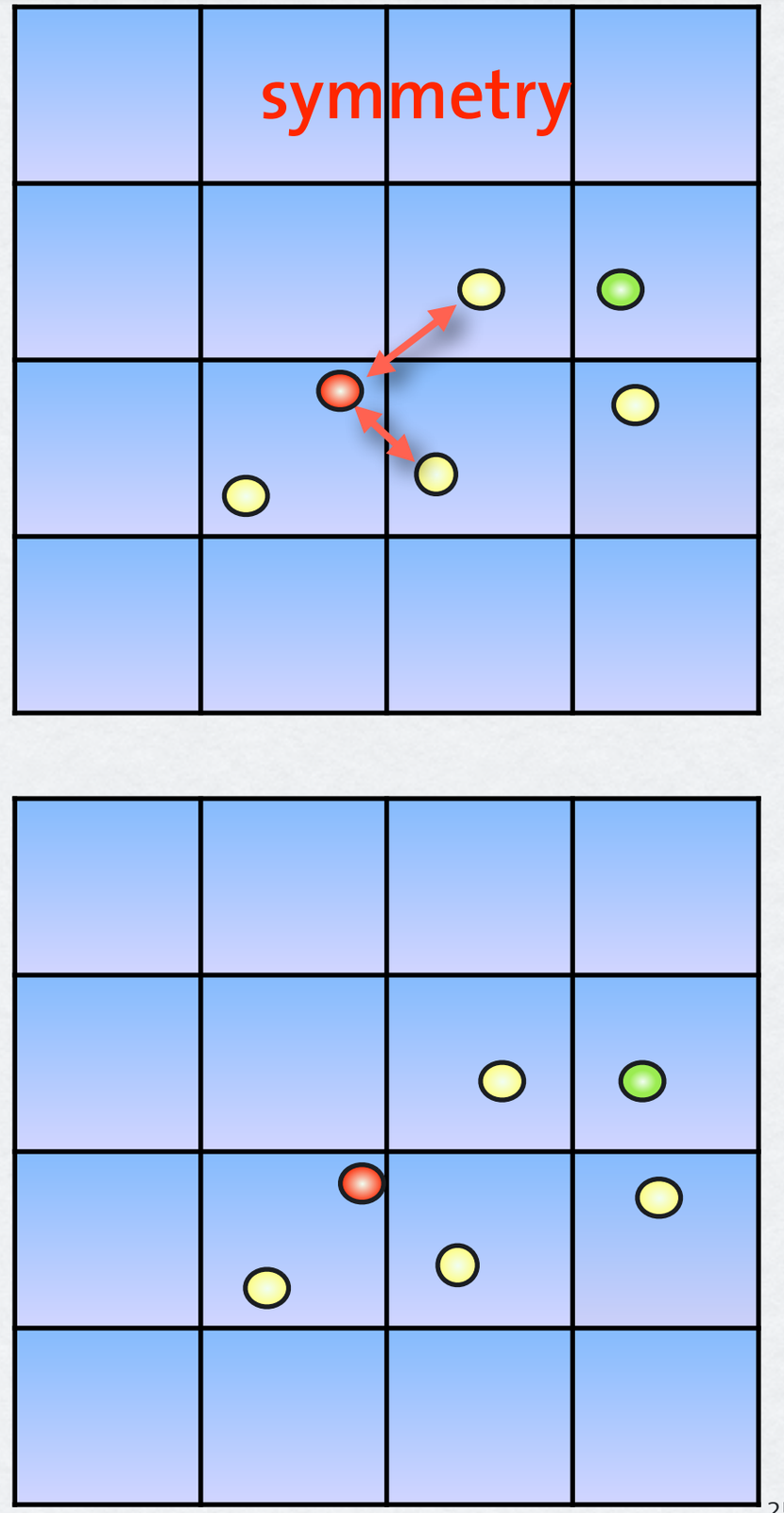

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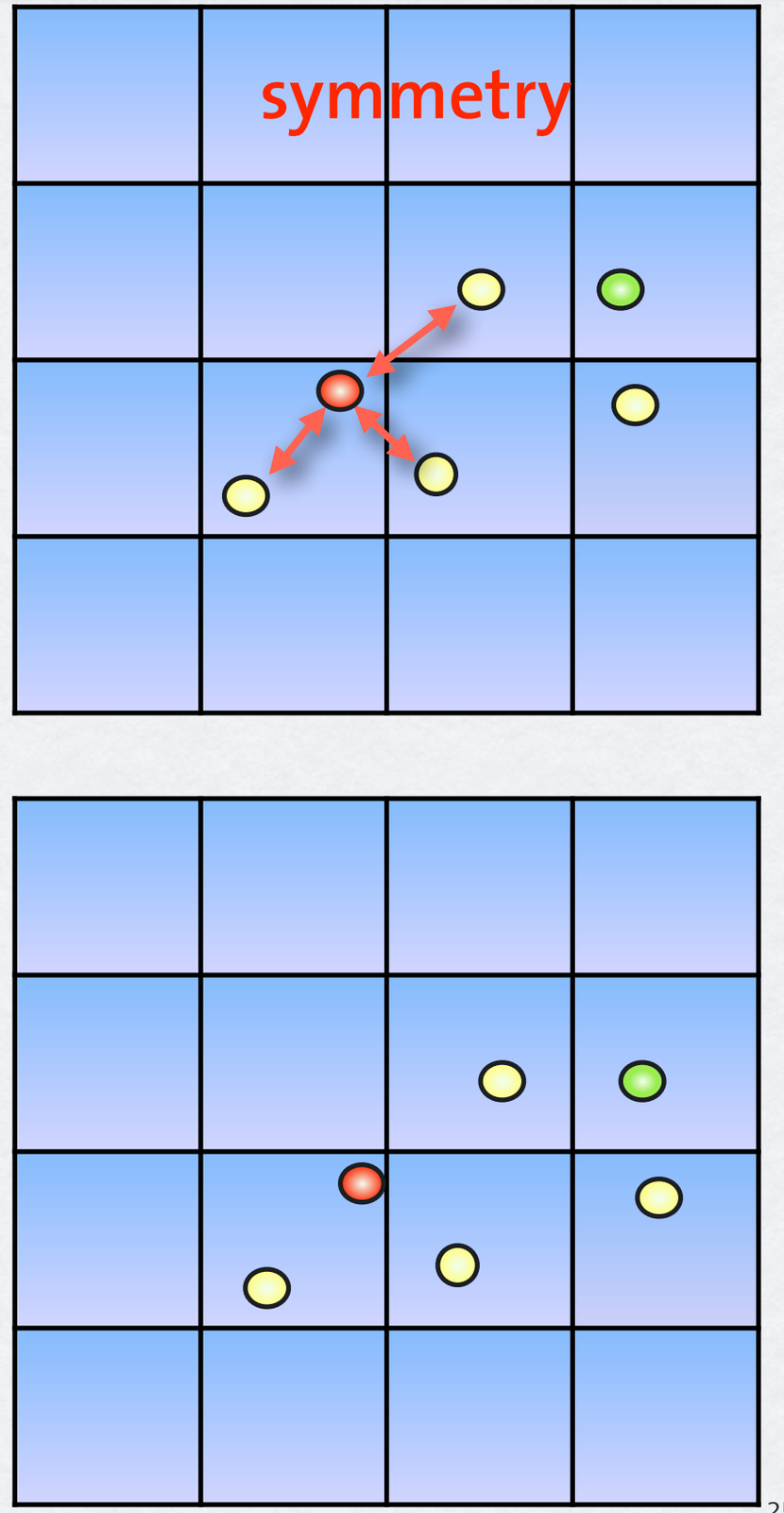

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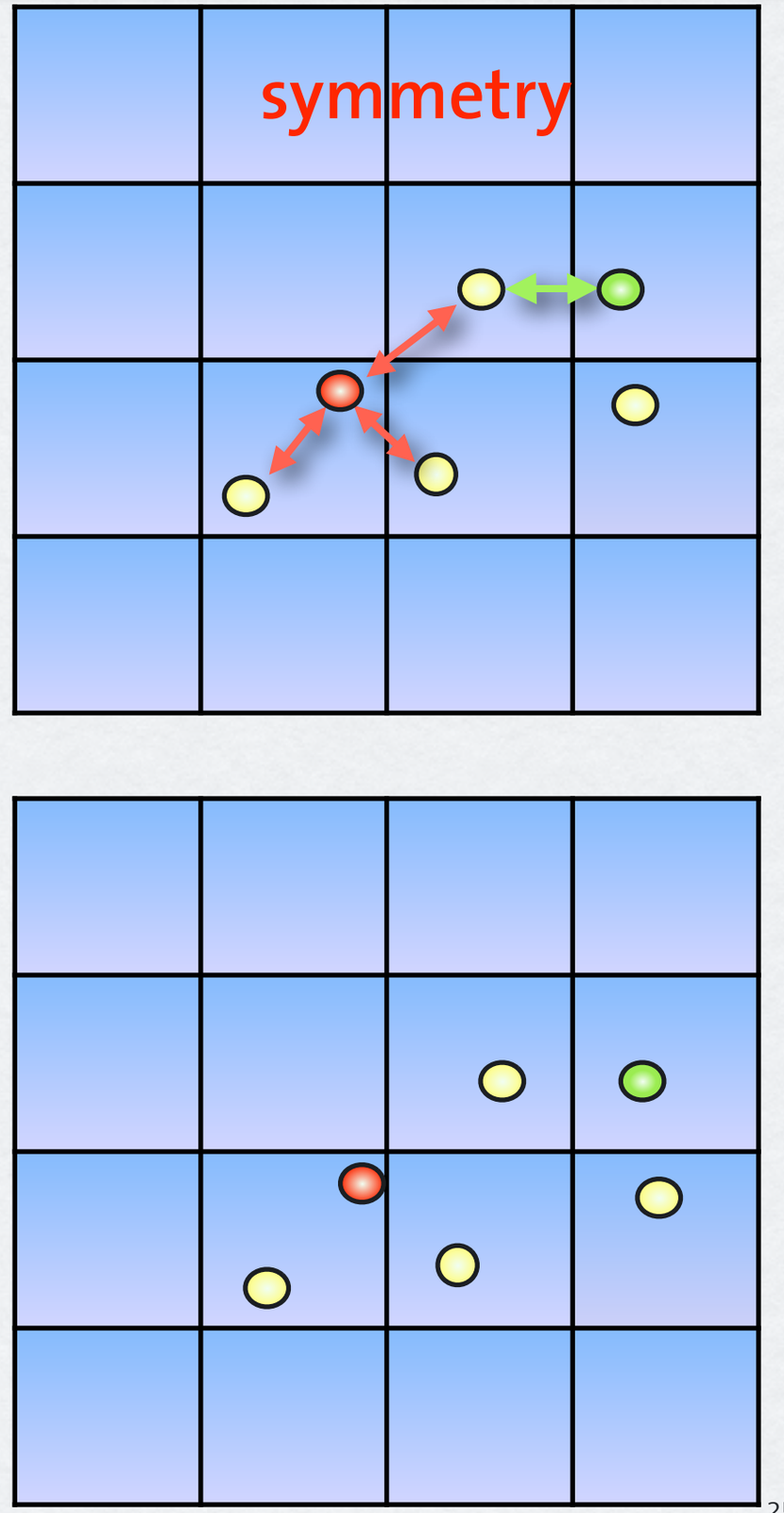

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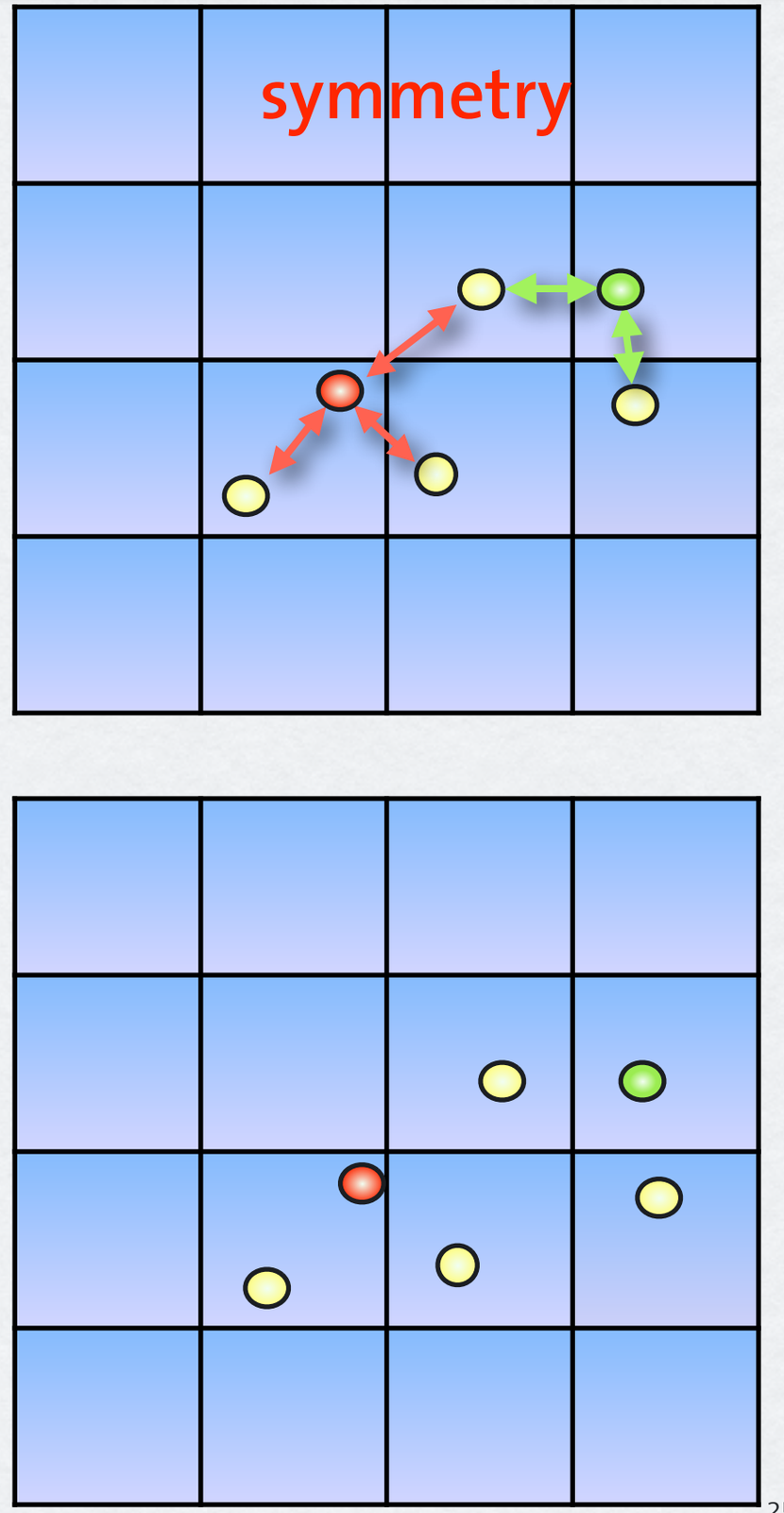

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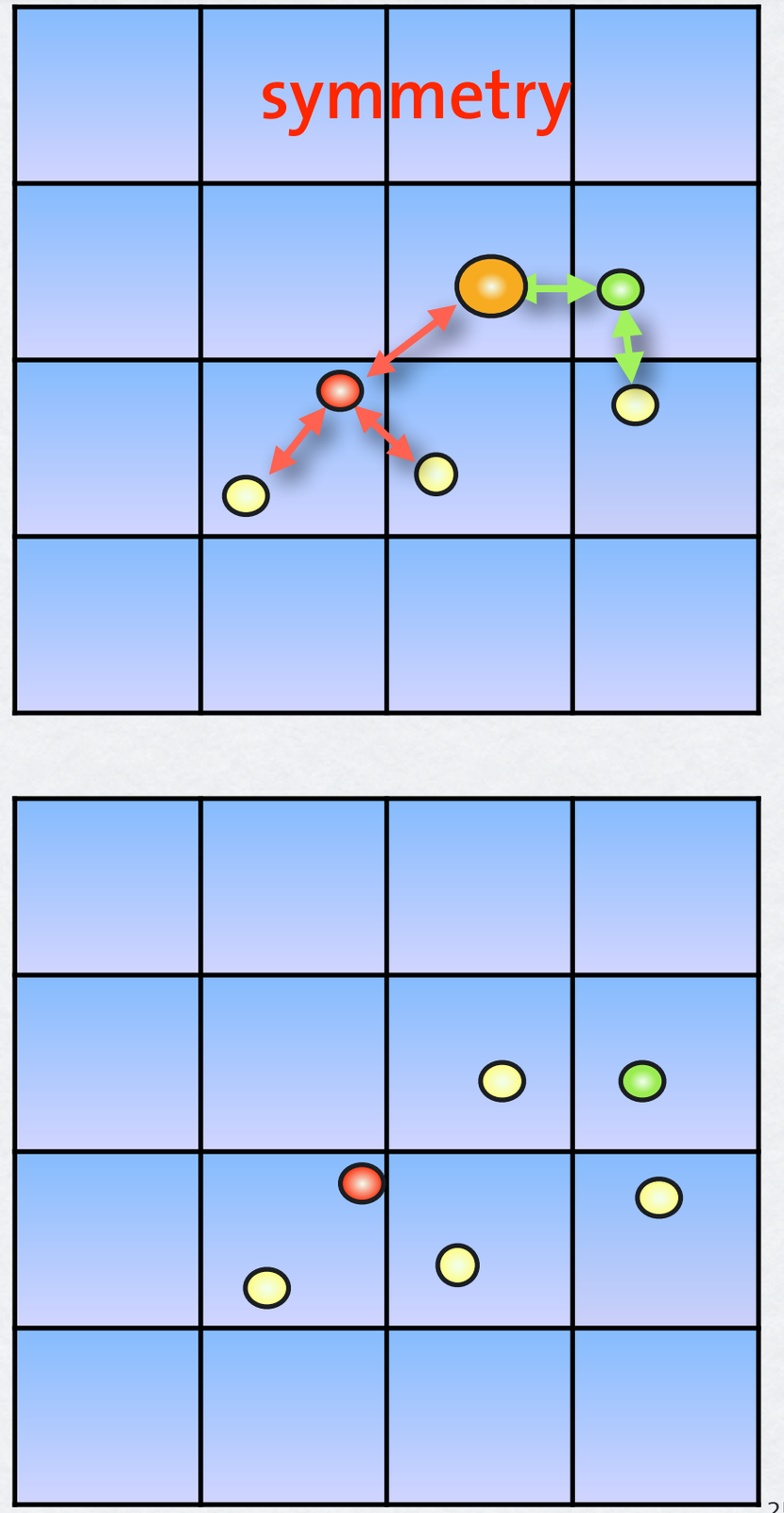

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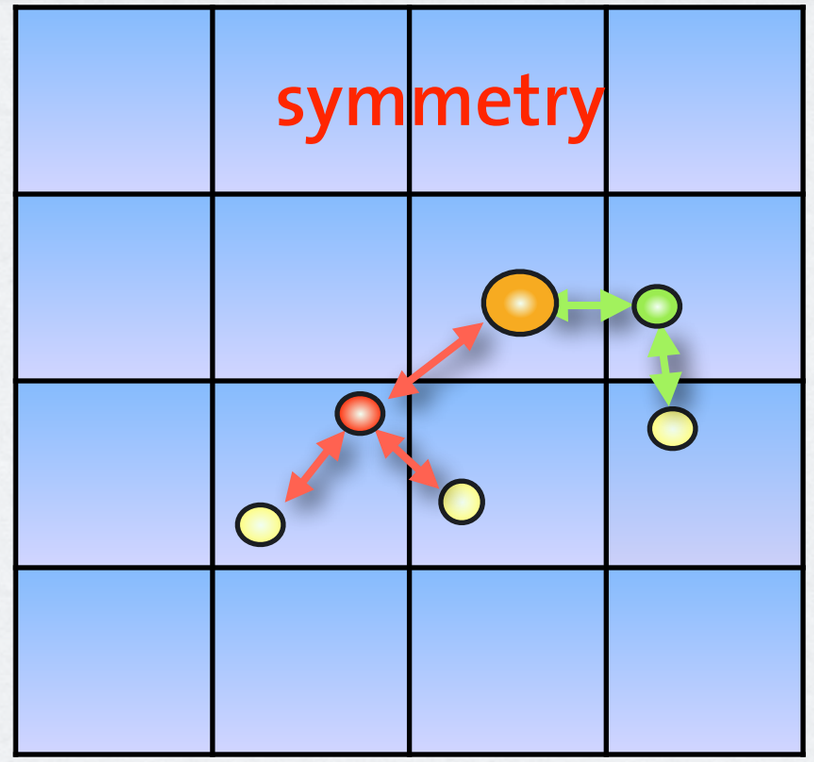

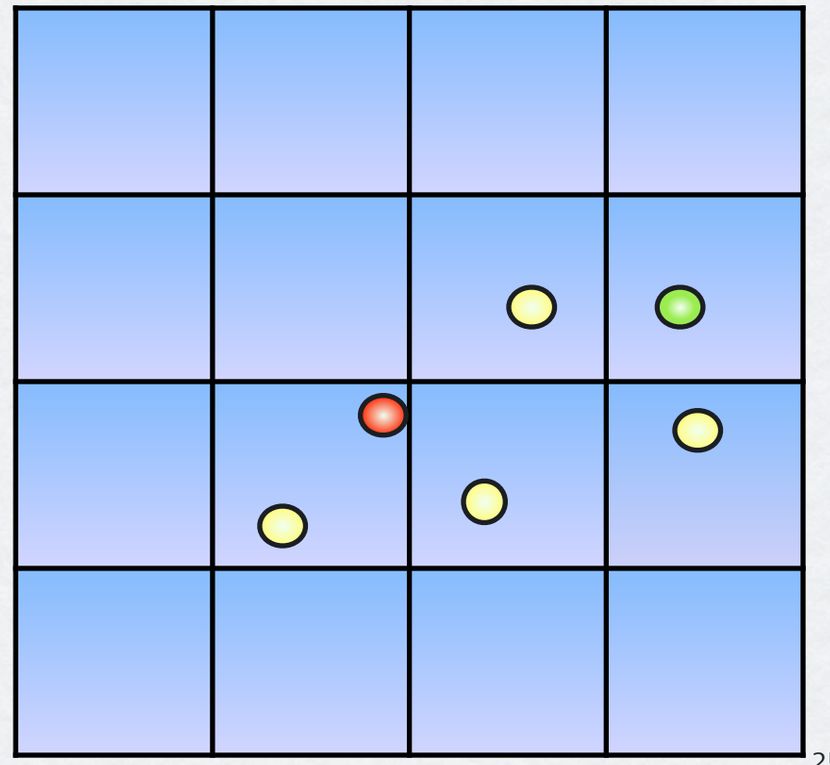

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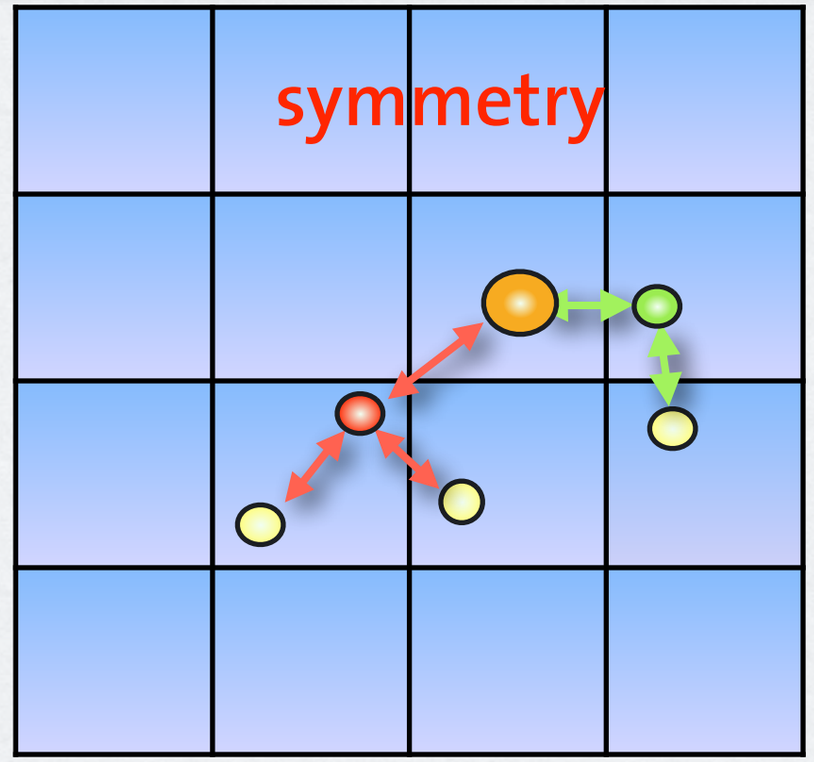

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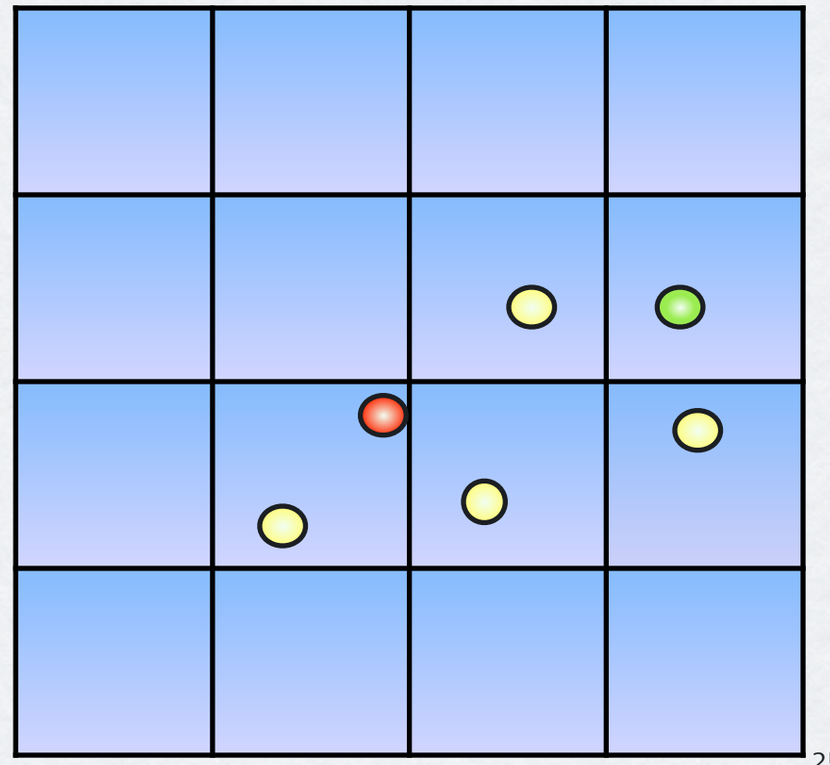

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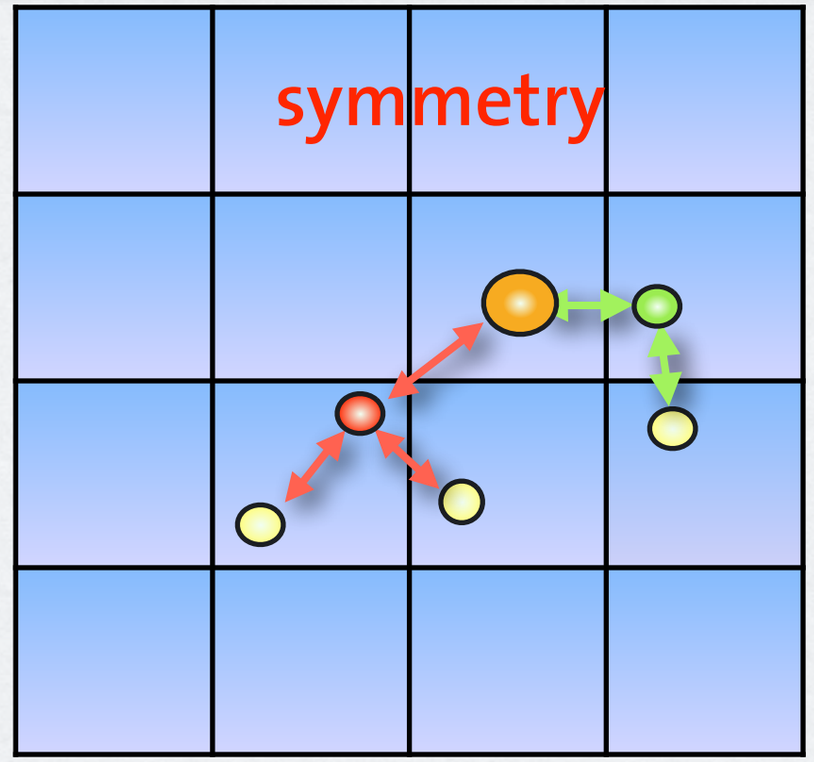

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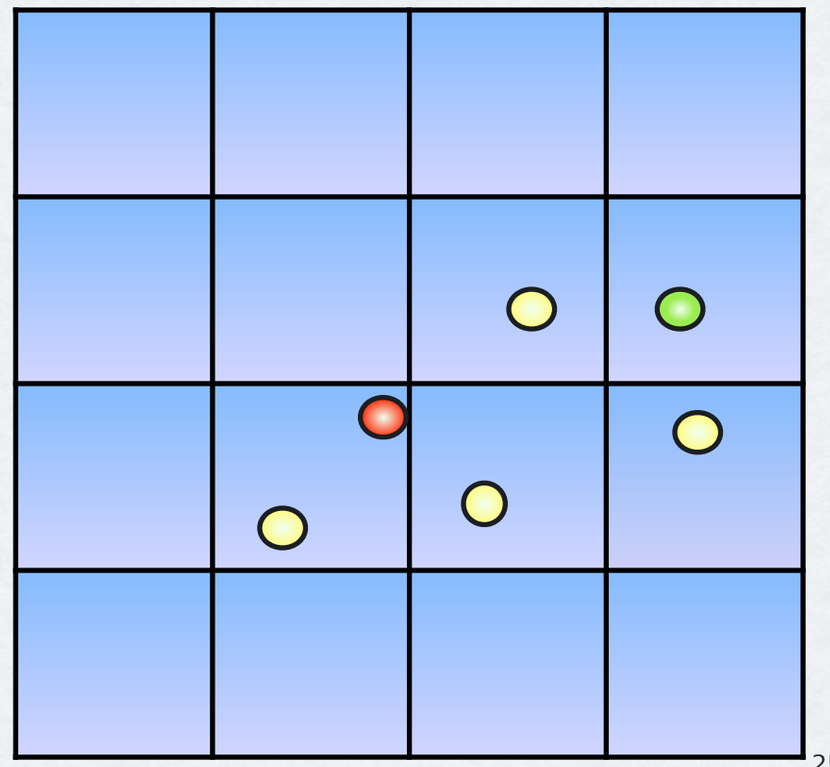

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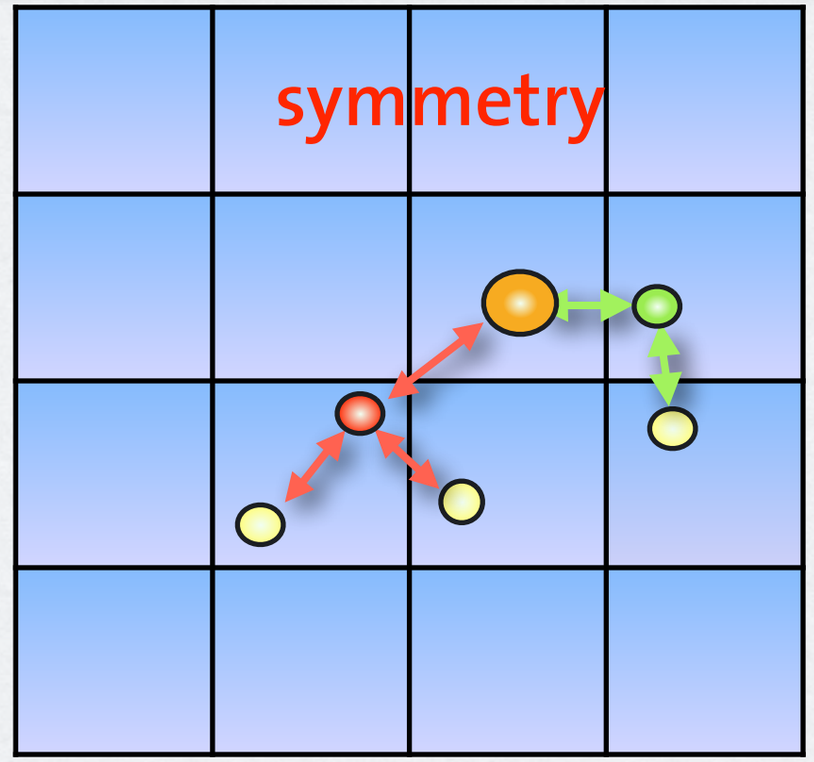

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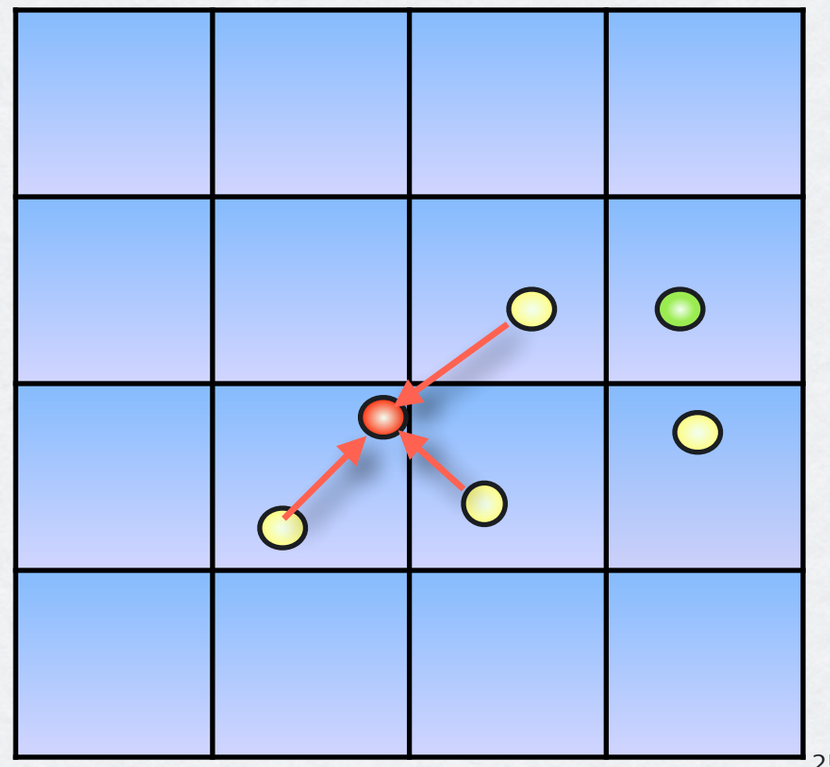

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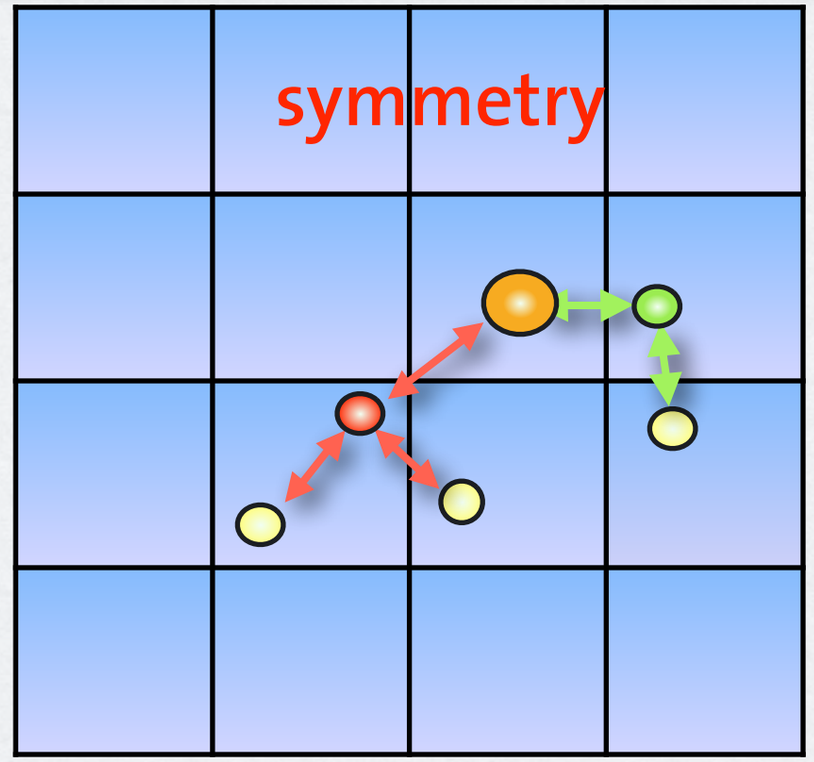

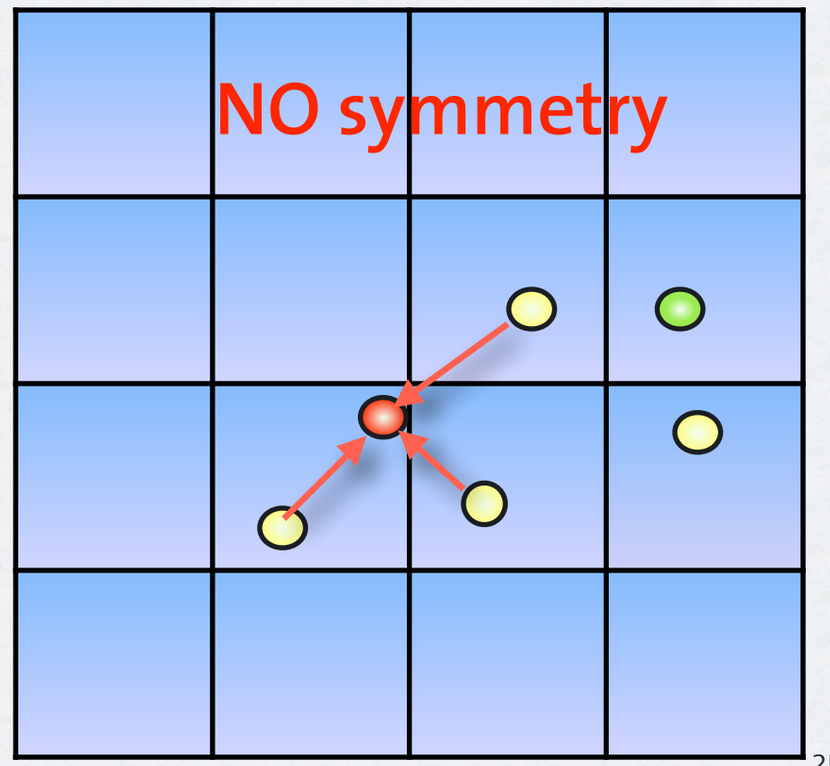

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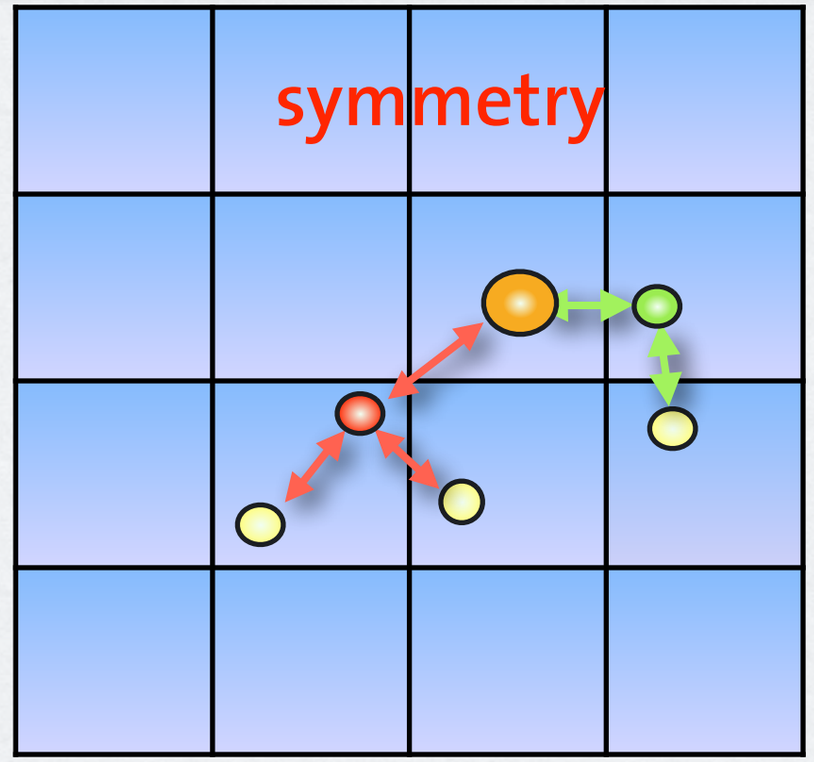

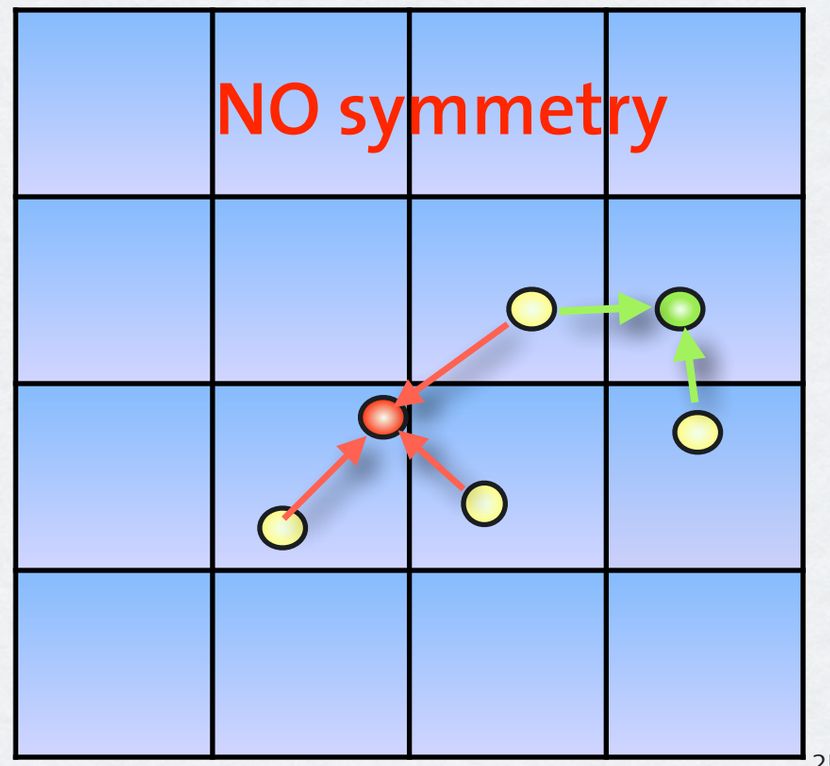

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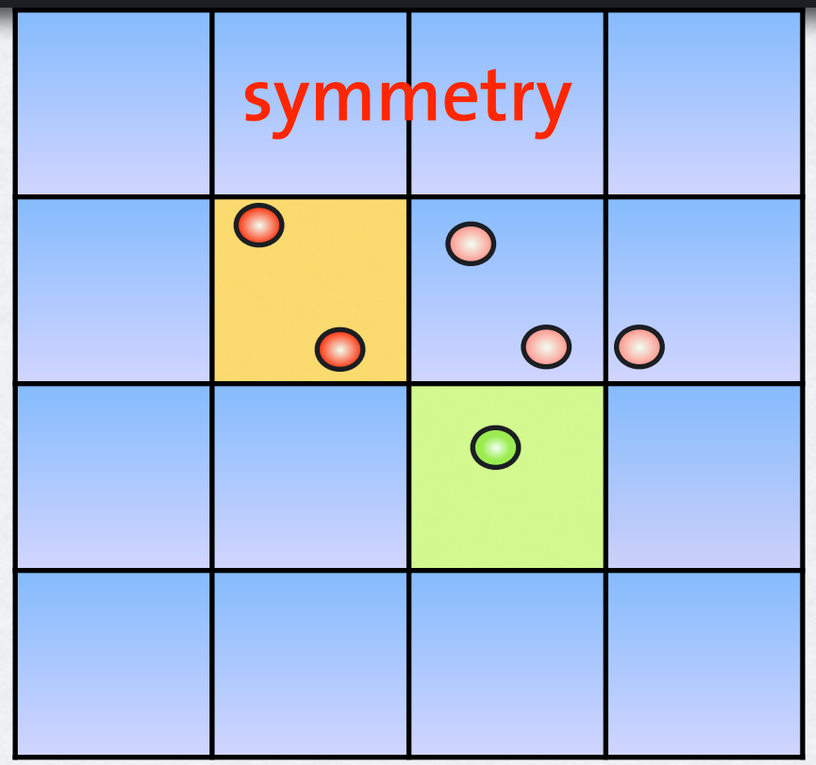

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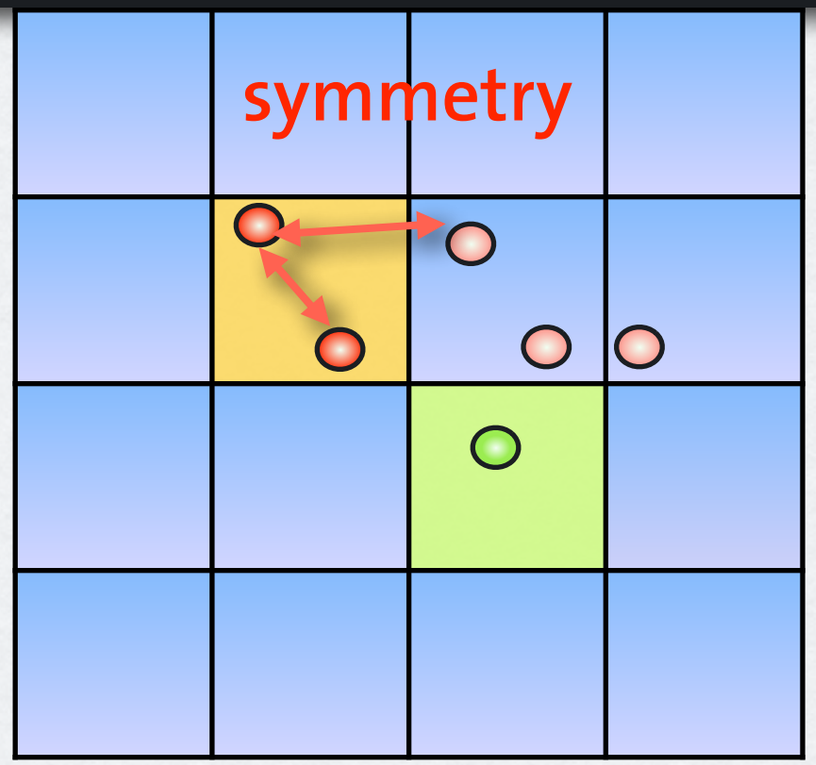

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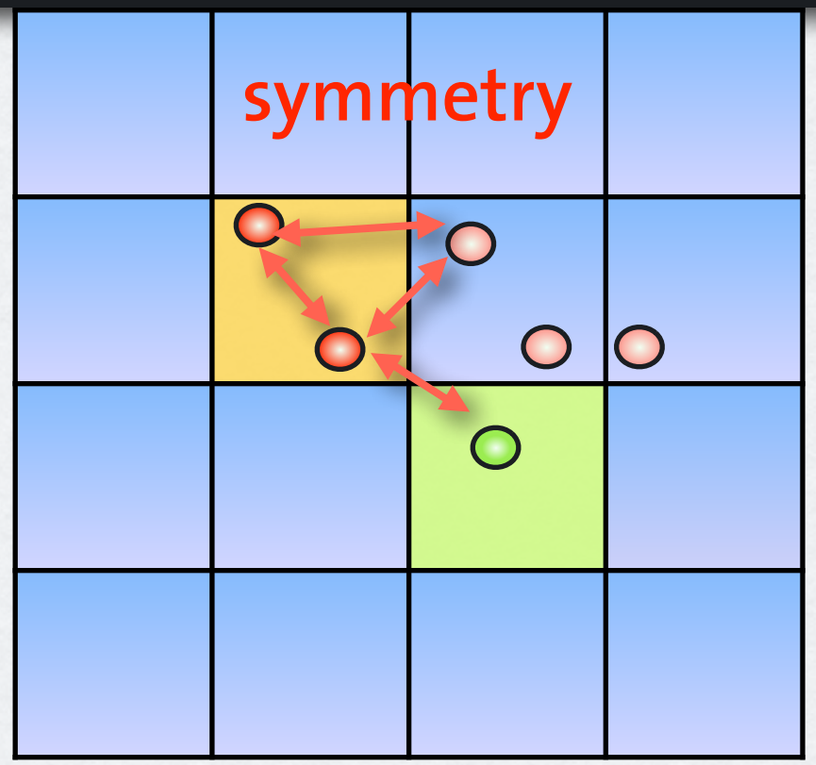

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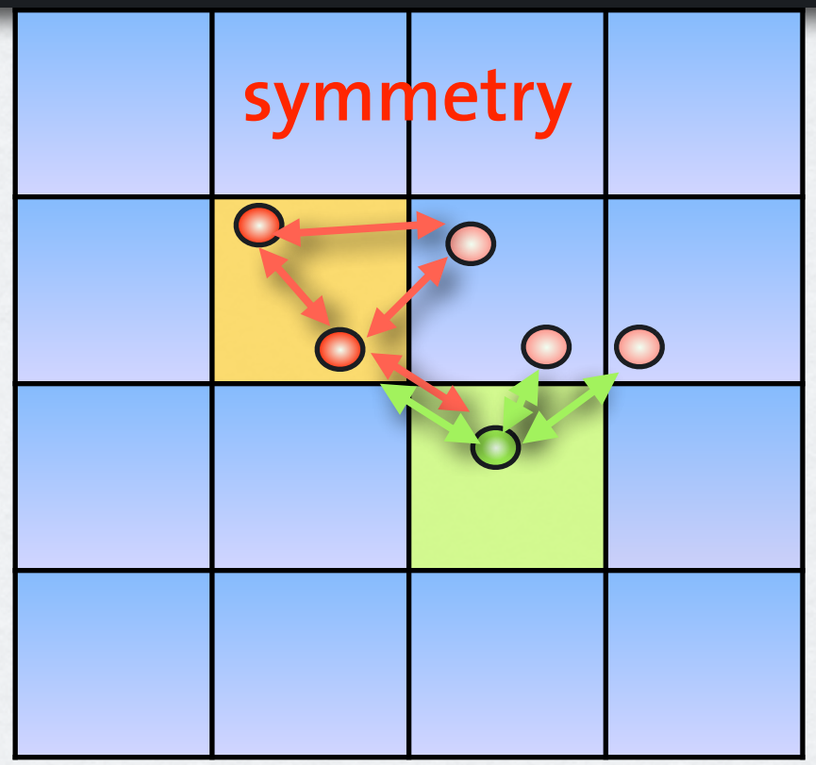

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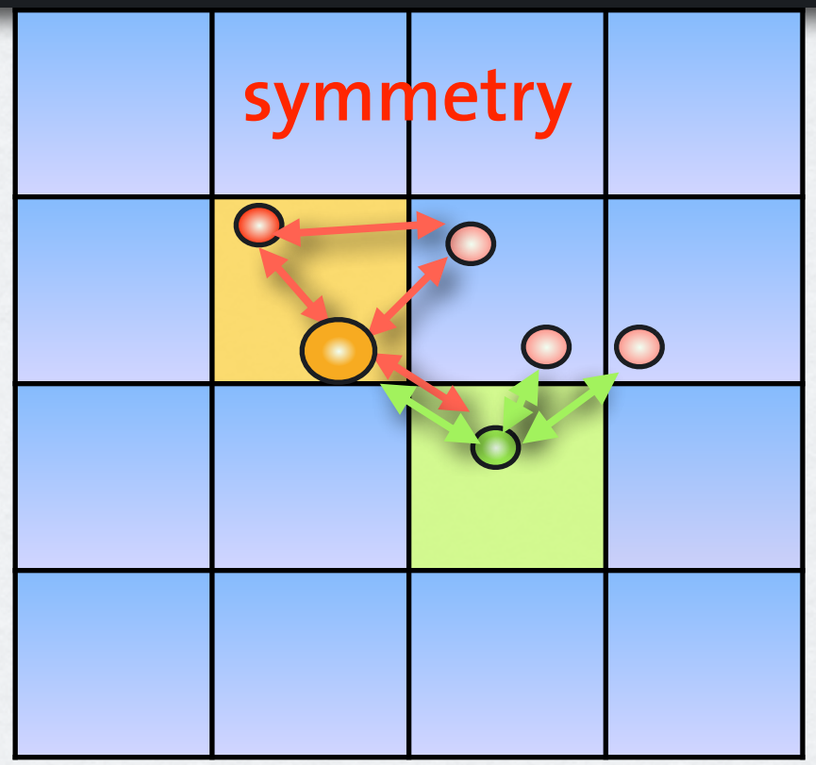

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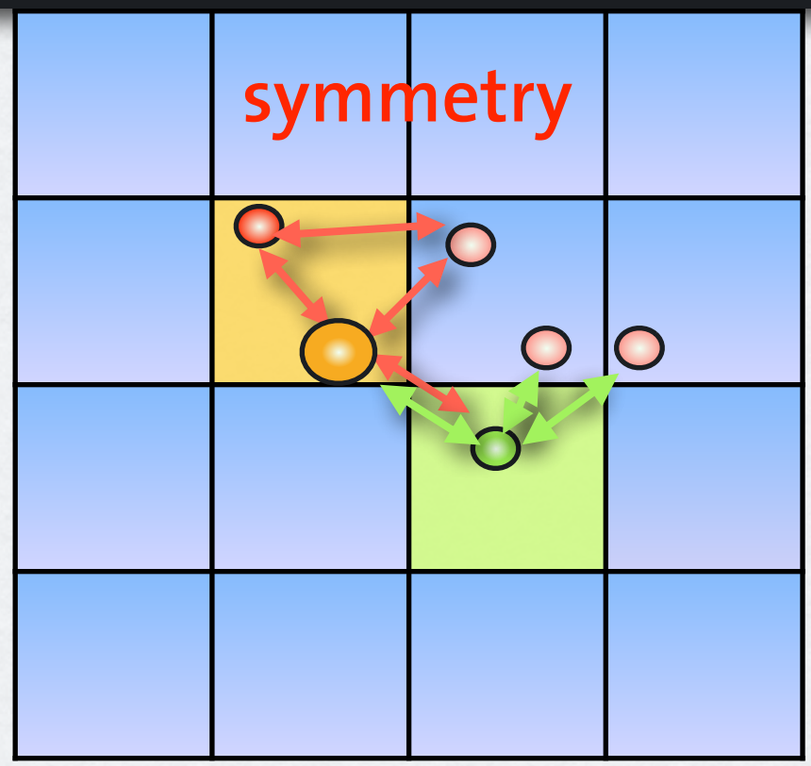
- load imbalance (e.g. if some cell is empty)



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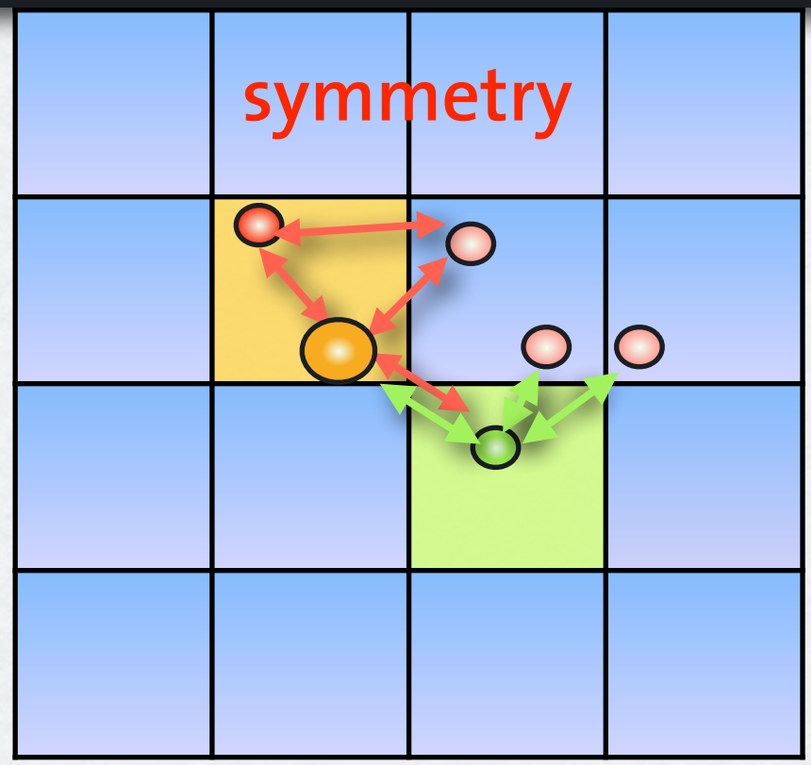

How to reduce load imbalance:

- ☑ skip empty cells
- ☑ TASKING : handling each cell is a task

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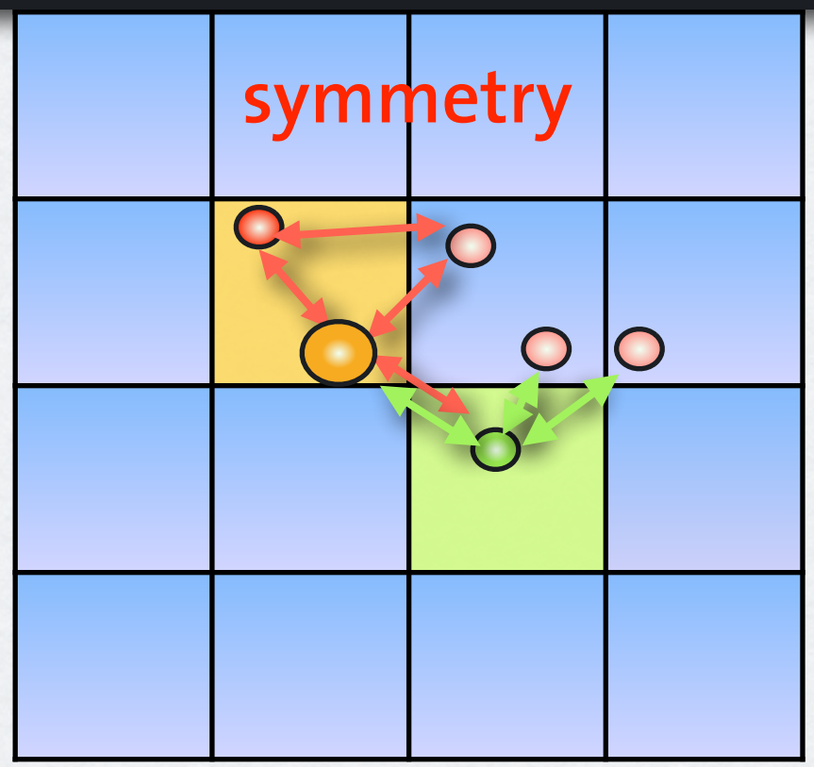

How to reduce load imbalance:

- ☑ skip empty cells
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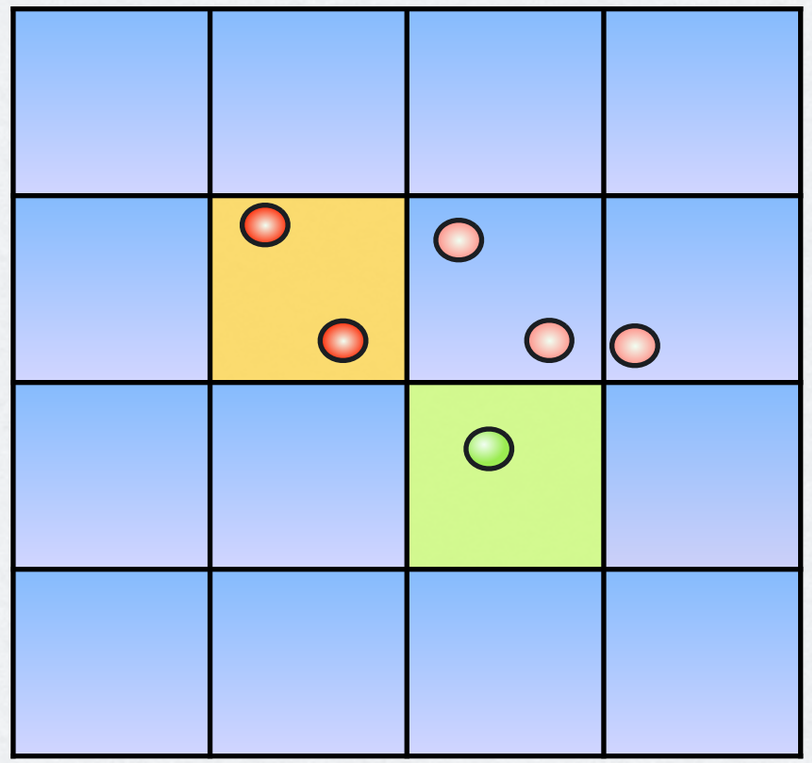

How to fix race condition:

- ☑ each particle updates just itself

Parallelization over Cells

➡ one thread processes one cell

- particles in cell of thread 1
- particles in cell of thread 2
- particles in other cells

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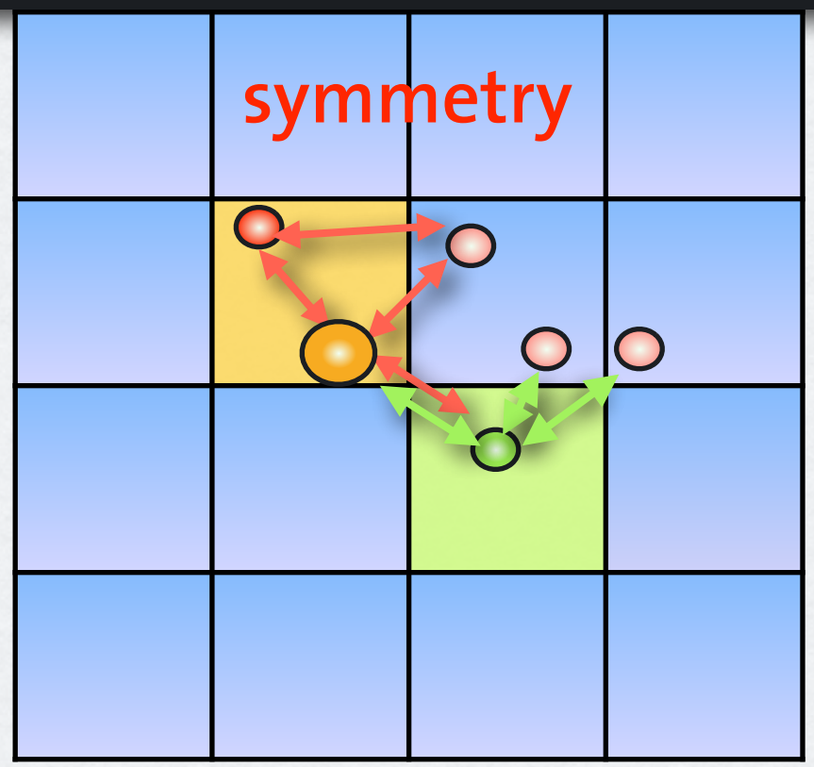

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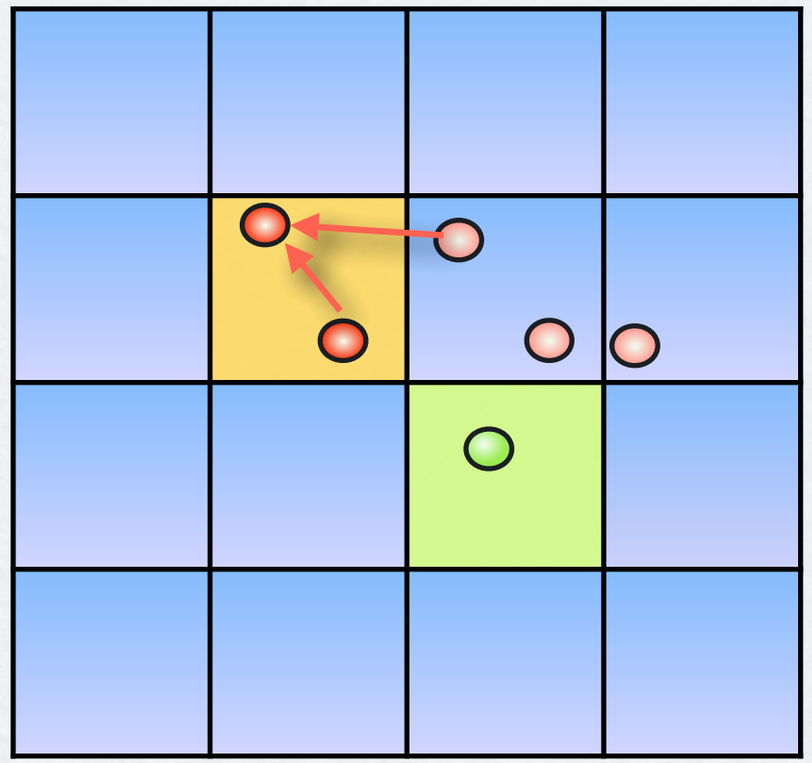

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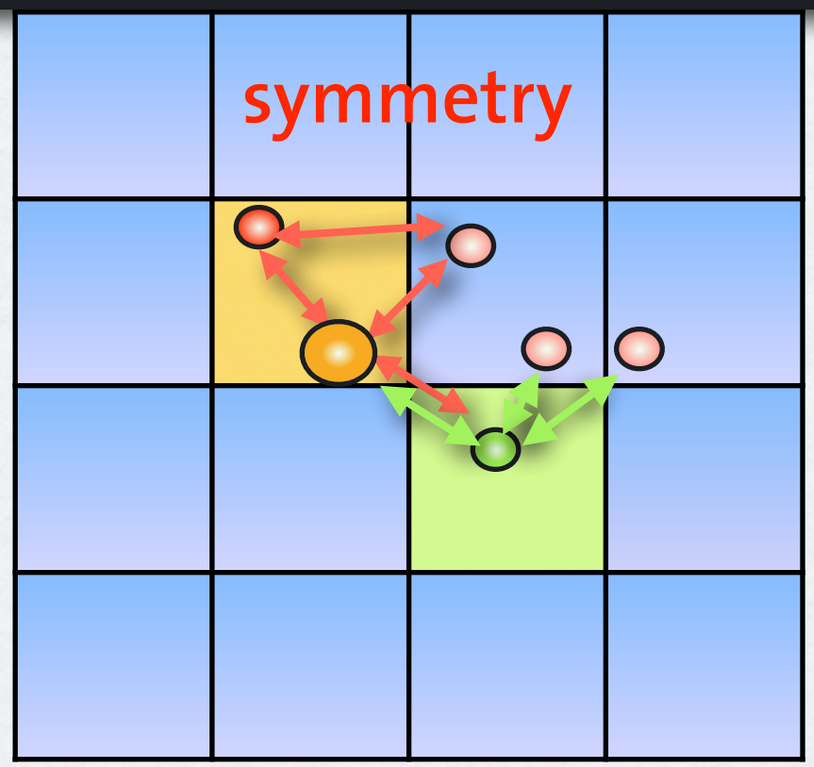

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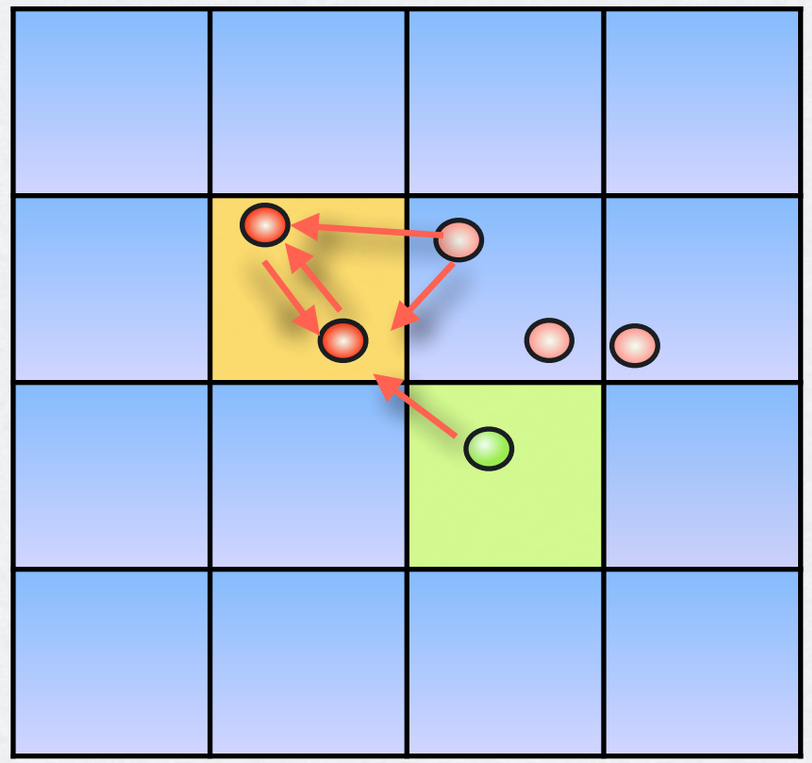

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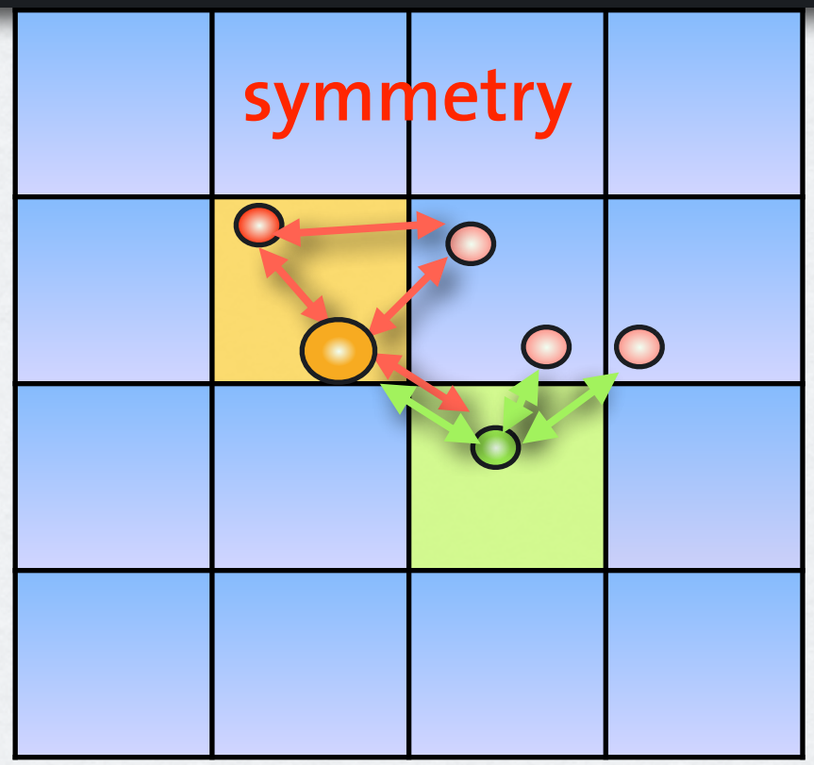

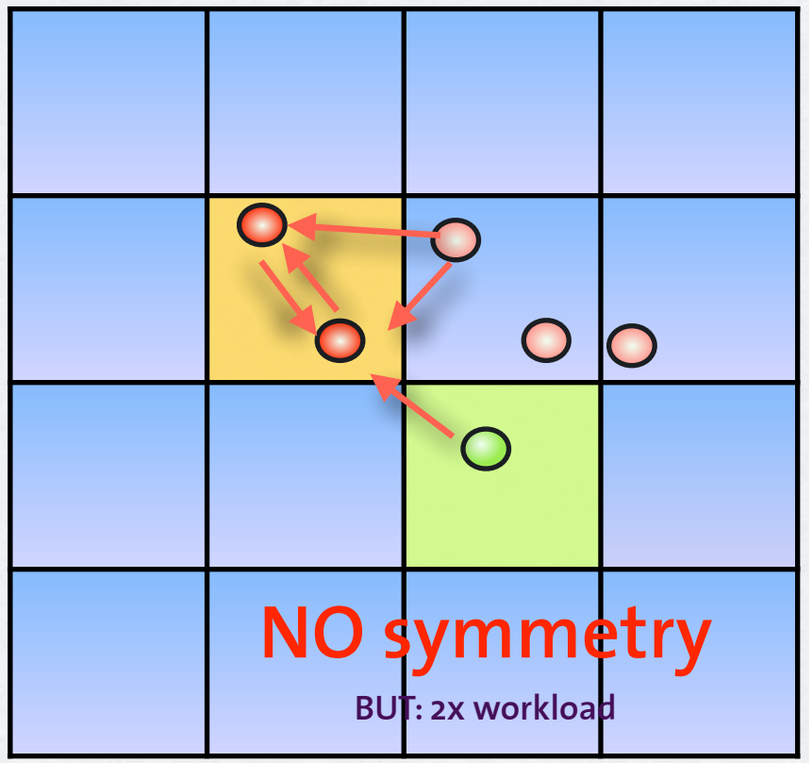

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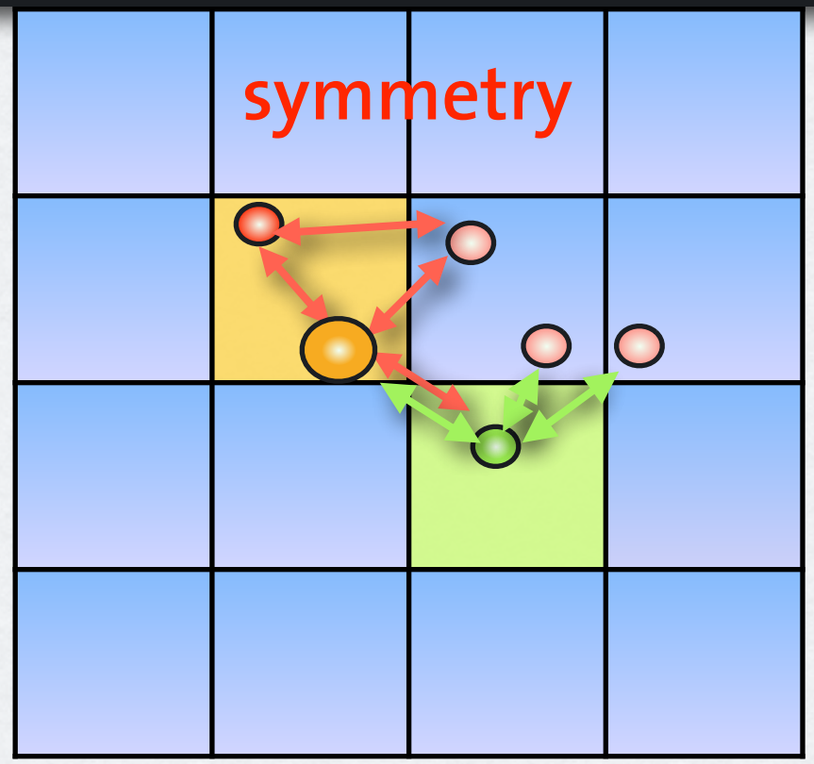

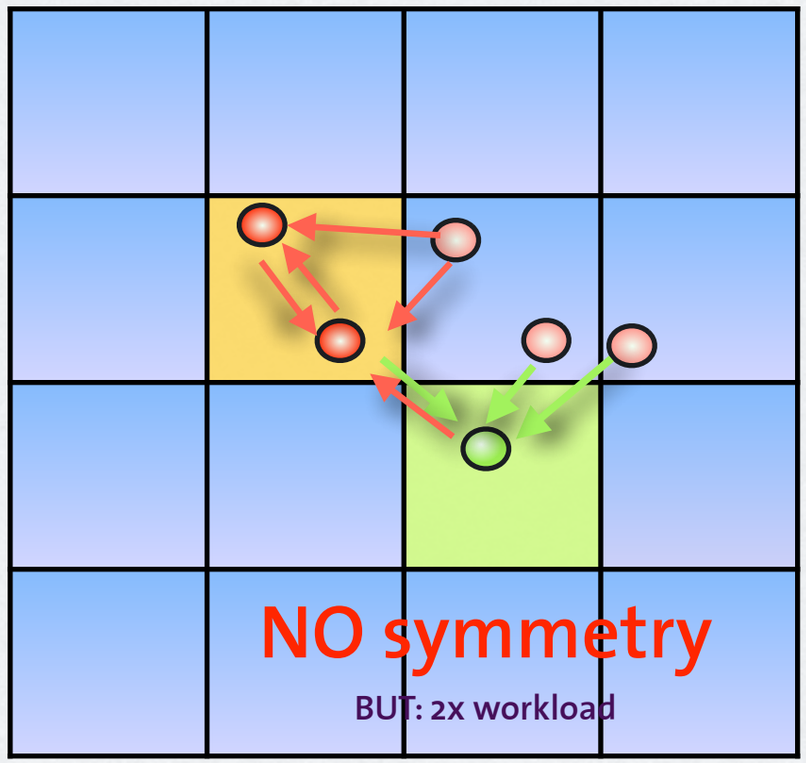

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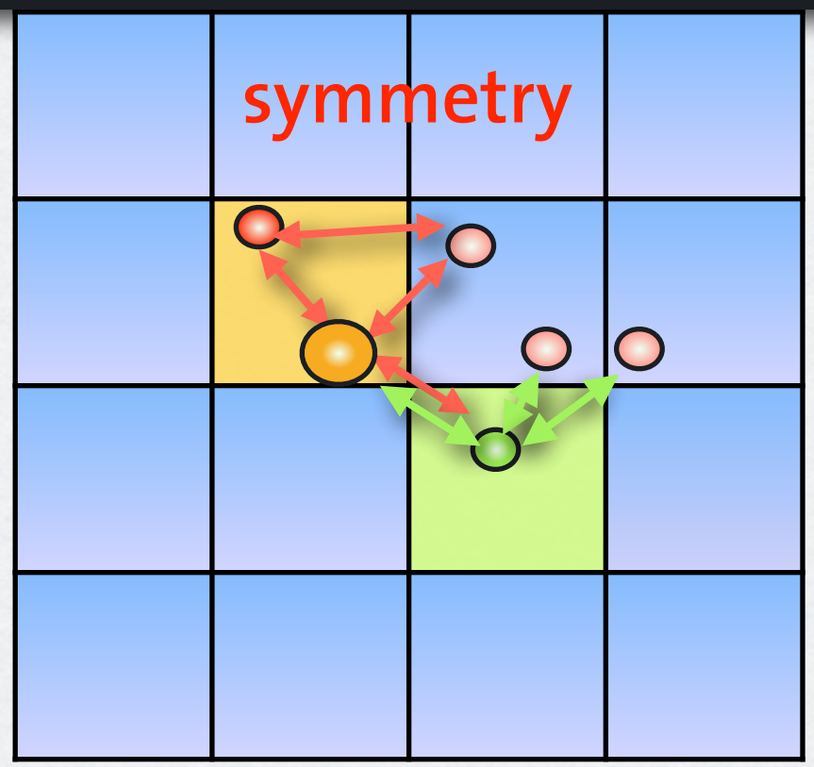

How to reduce load imbalance:

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How to fix race condition:

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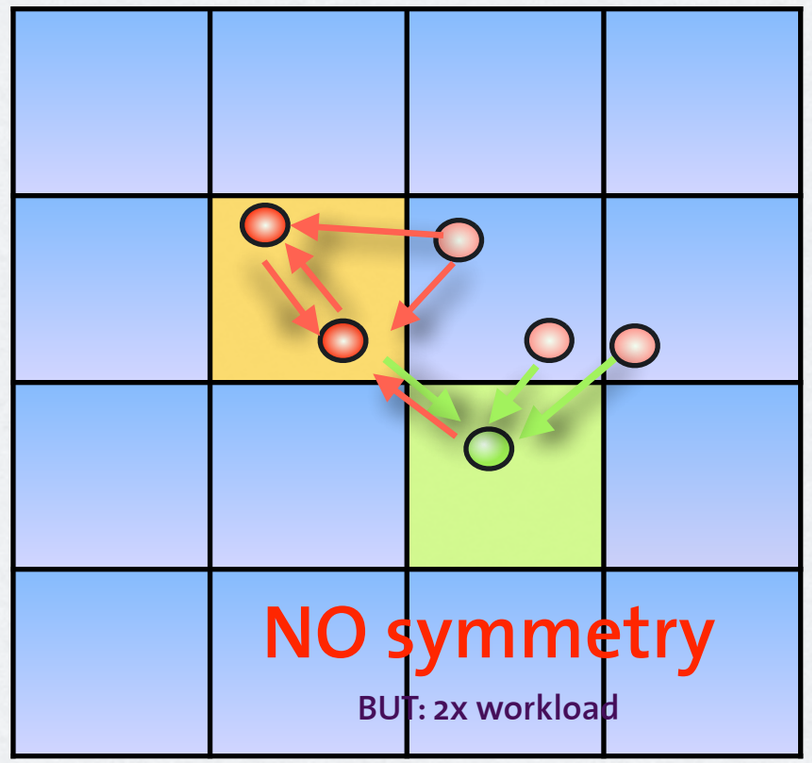
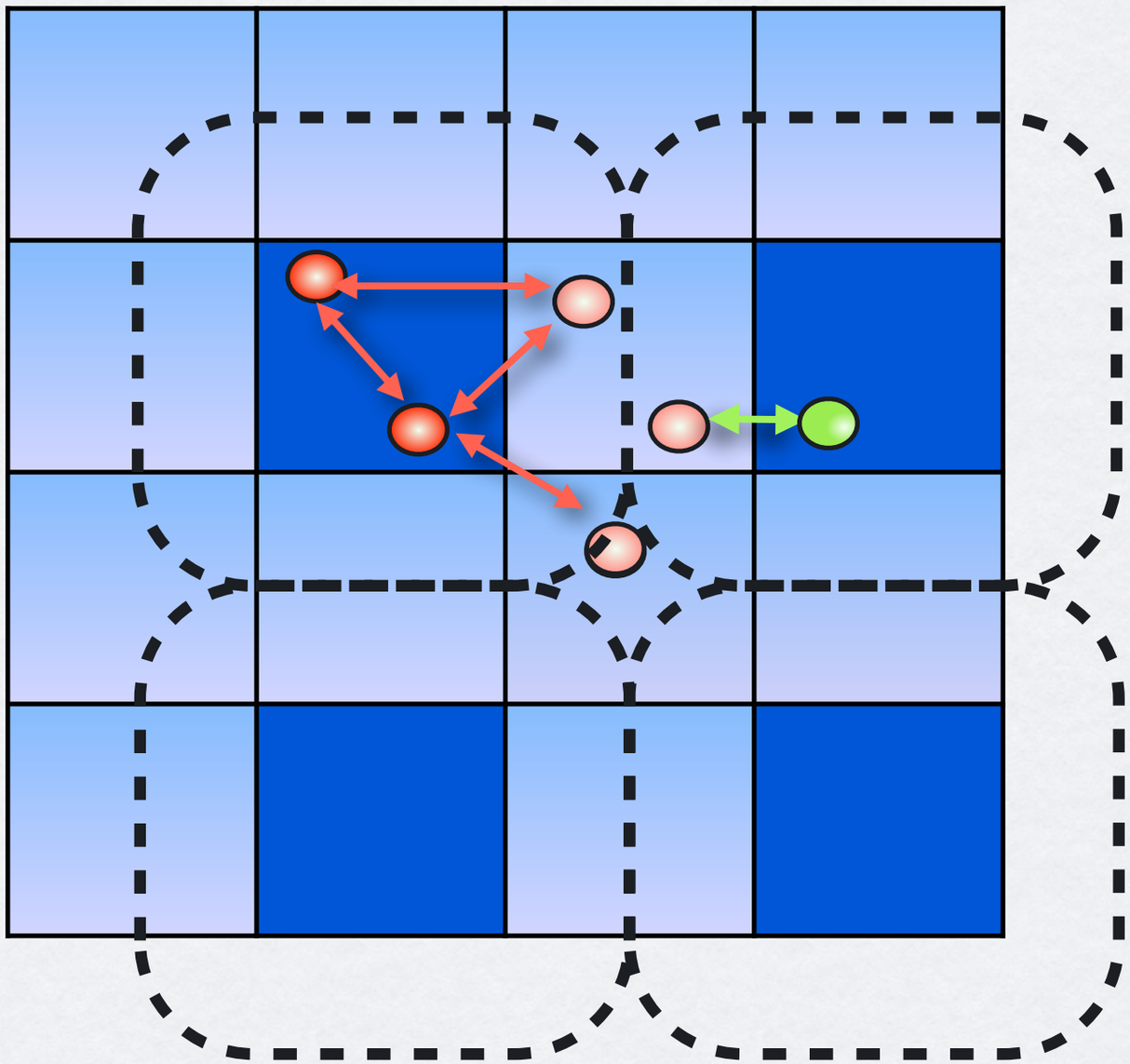
- ☑ multipass (next slide)



Divide and Conquer - Multipass

Define Cell size ≧ interaction *diameter* of particles

“Pass” : Process non-neighboring cells simultaneously



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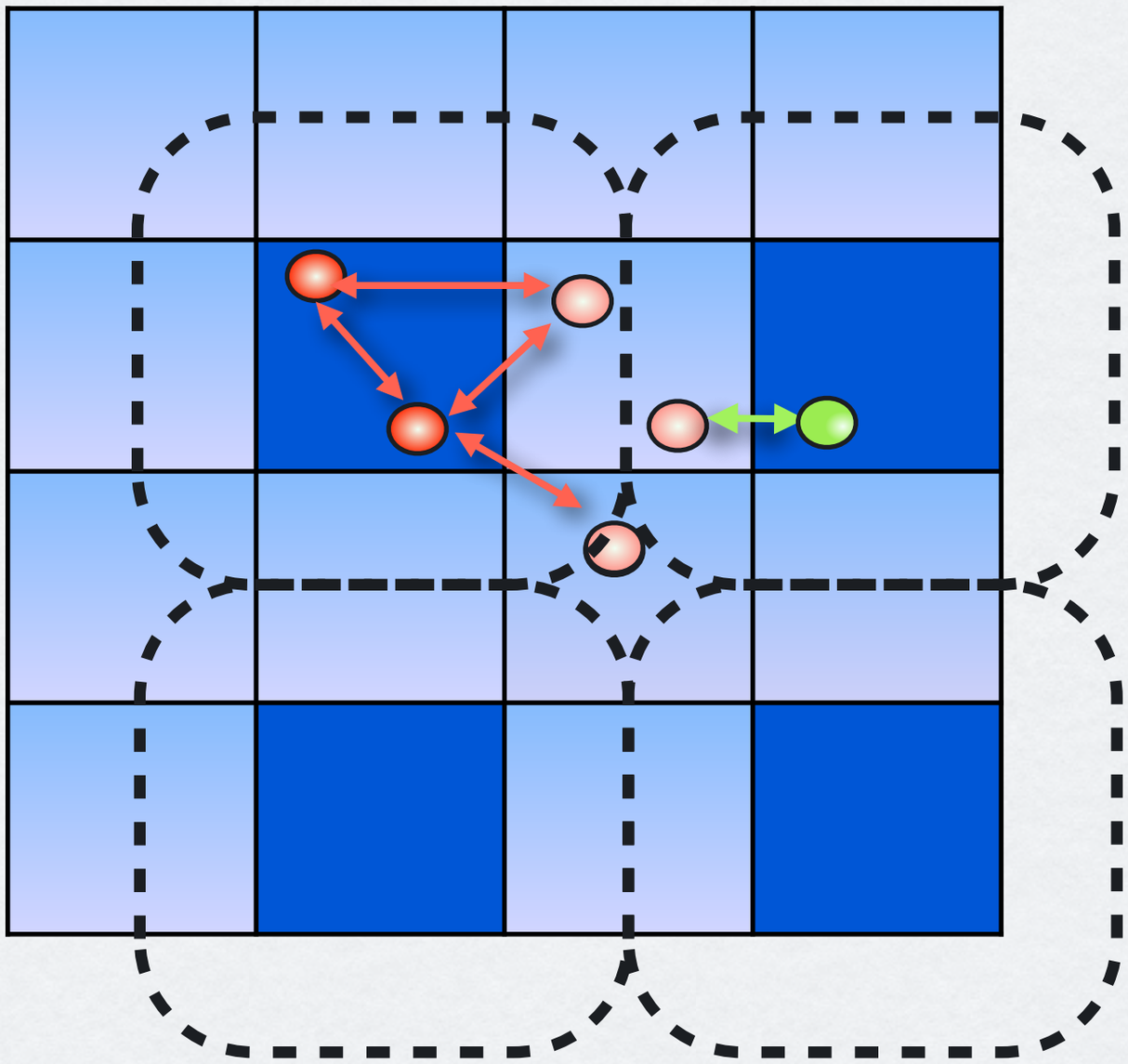


☑ **NO race condition**

Divide and Conquer - Multipass

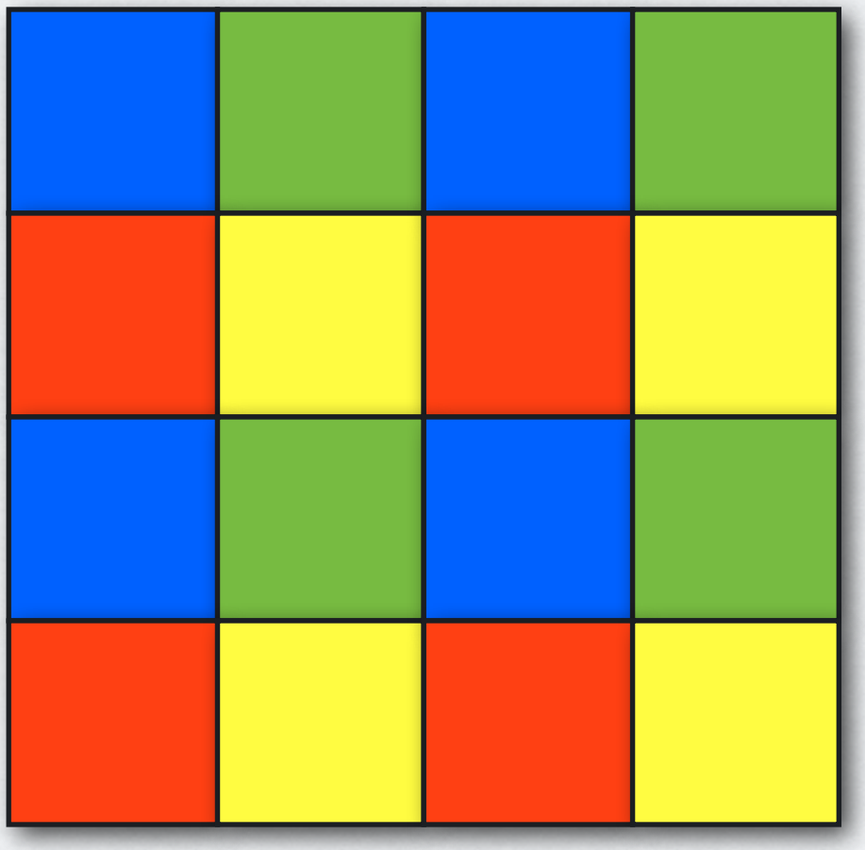
➡ in 2D there must be 4 passes to cover all possible cells

cells of pass 1

cells of pass 2

cells of pass 3

cells of pass 4



cells of the same color can be processed at the same time

➡ in 3D: 8 passes are needed

Issues with Cell Lists

- Curse of dimensionality:
  - 2D - 35% of the particles checked are within the cutoff
  - 3D - 16% of the particles checked are within the cutoff
- Building cell lists every timestep might be expensive