An efficient SIMD implementation of pseudo Verlet-lists for neighbour interactions in particle-based codes

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Team

This work is a collaboration between two departments at Durham University (UK):

- The Institute for Computational Cosmology,
- The School of Engineering and Computing Sciences,

with contributions from the astronomy group at the University of St. Andrews, University of Dublin, ETH Lausanne and the DiRAC software team.

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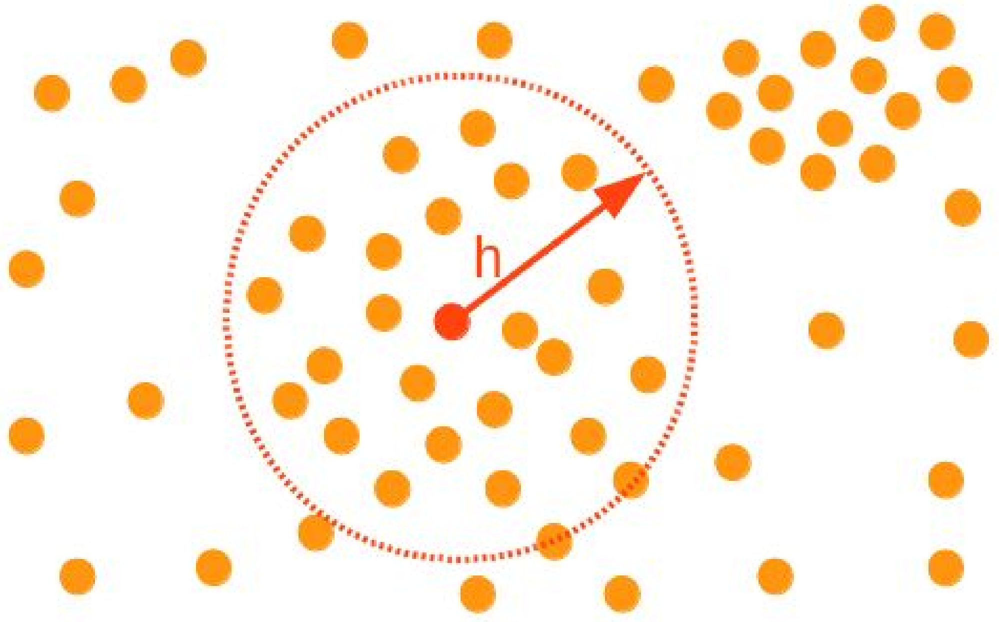
Overview

- Problem to solve
- Solution
  - Pseudo Verlet list
  - Particle sorting
- SIMD vectorisation strategy for particle based codes (MD, SPH, etc.)
  - Particle caches AoS to SoA
- Strategy applied to SWIFT
- Performance results
- Conclusions

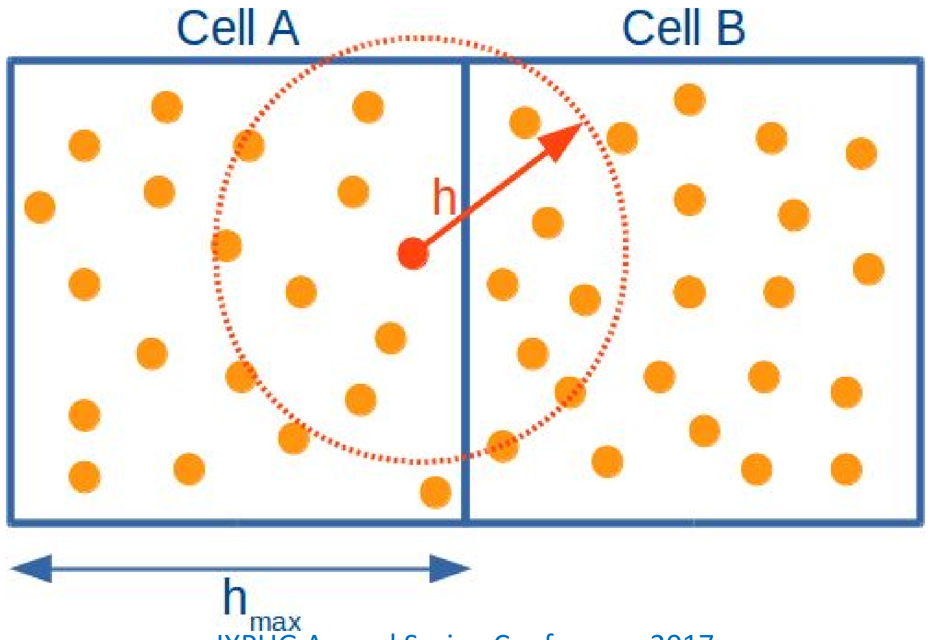
Problem

- We update each particle using SPH (Smoothed-Particle Hydrodynamics)
- Each particle interacts with its neighbours that are within a smoothing length, **h**
- The smoothing length varies depending on the particle density of the region
- Interaction cheap to compute



Problem

- The particles are divided up into cells of edge $\mathbf{h_{max}}$, where $\mathbf{h_{max}}$ is the maximum particle smoothing length in the simulation
- Computing the interactions of particles in two neighbouring cells would require a lot of unnecessary distance calculations
- The majority of particles will not be within range of each other



Naive Solution

<u>Brute Force</u>

- Perform a double for loop over all particles
- Interact particles that are within range of each other, $\mathbf{r^2 < h^2}$

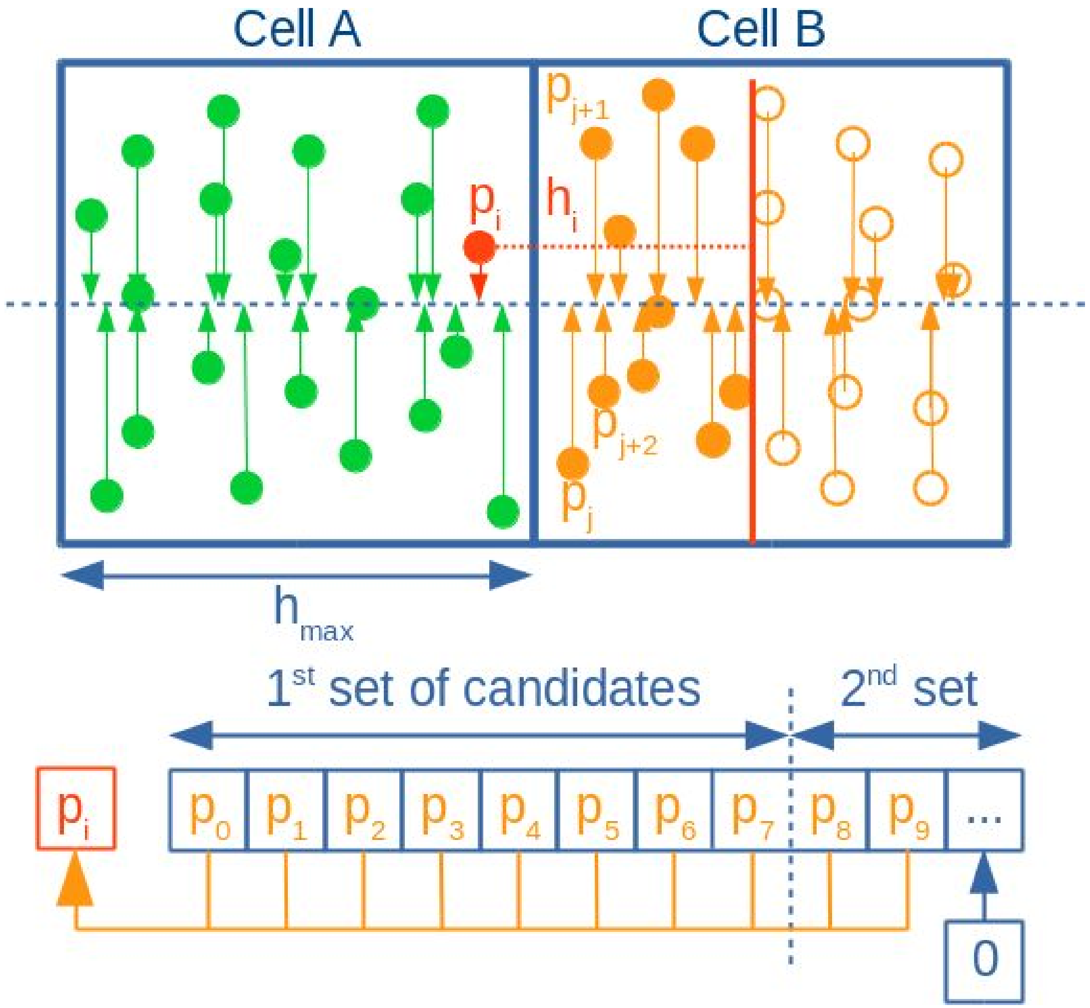
```
for(int i=0; i<count_i; i++) {
  struct part pi = parts_i[i];
  float hi = pi.h;

  for(int j=0; j<count_j; j++) {
    struct part pj = parts_j[j];

    float dist = calc_dist(pi,pj);

    if(dist*dist < h*h) interact(pi,pj);
  }
}
```

Smart Solution

Particle Sorting

- Place particles into a pseudo Verlet list:
  - Project particles onto the axis joining the center of the two cells
  - Sort the particles on the axis based upon their position on the axis
  - Sorting performed using a merge sort
  - Only occurs when the particles have moved by a certain distance
- Reduces the number of candidates
- These particles are still tested so that they are within the 3D distance

Smart Solution



Smart Solution

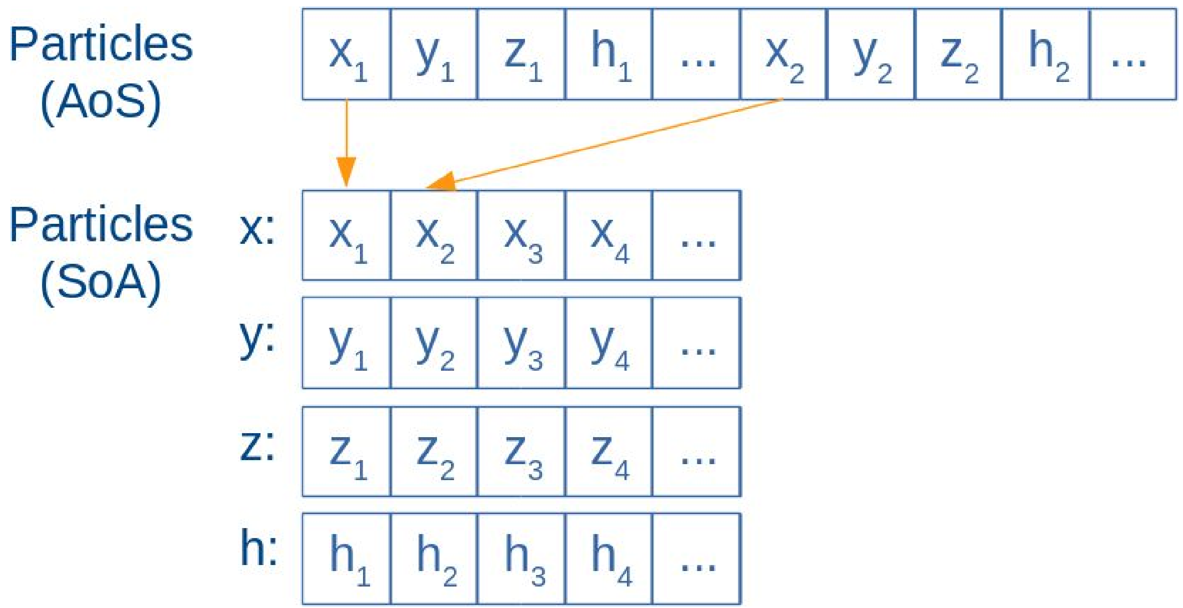
```
// Sort the particle on the axis
sort_parts(parts_i,parts_j);

// Pick particle pi from Cell A
for(int i=0; i<count_i; i++) {
  struct part pi = parts_i[i];
  float hi = pi.h;

  // Only loop over particles in Cell B that are within hi on the axis
  for(int j=0; j<count_j && dj<hi; j++) {
    struct part pj = parts_j[j];

    float dist = calc_dist(pi,pj);

    if(dist*dist < h*h) interact(pi,pj);
  }
}
```

SIMD Optimisations

- Use local particle cache (AoS -> SoA)
- Only read particles into cache that interact
- Calculate all interactions on a particle and store results in a set of intermediate vectors
- Perform horizontal add on intermediate vectors and update the particles with the result
- Pad caches to prevent remainders and mask out the result

Local Particle Cache

- The particles are stored in a global array of structs (AoS)
- Causes strided memory access when vectors are loaded
- We can improve performance by placing the required particle properties into a structure of arrays (SoA)

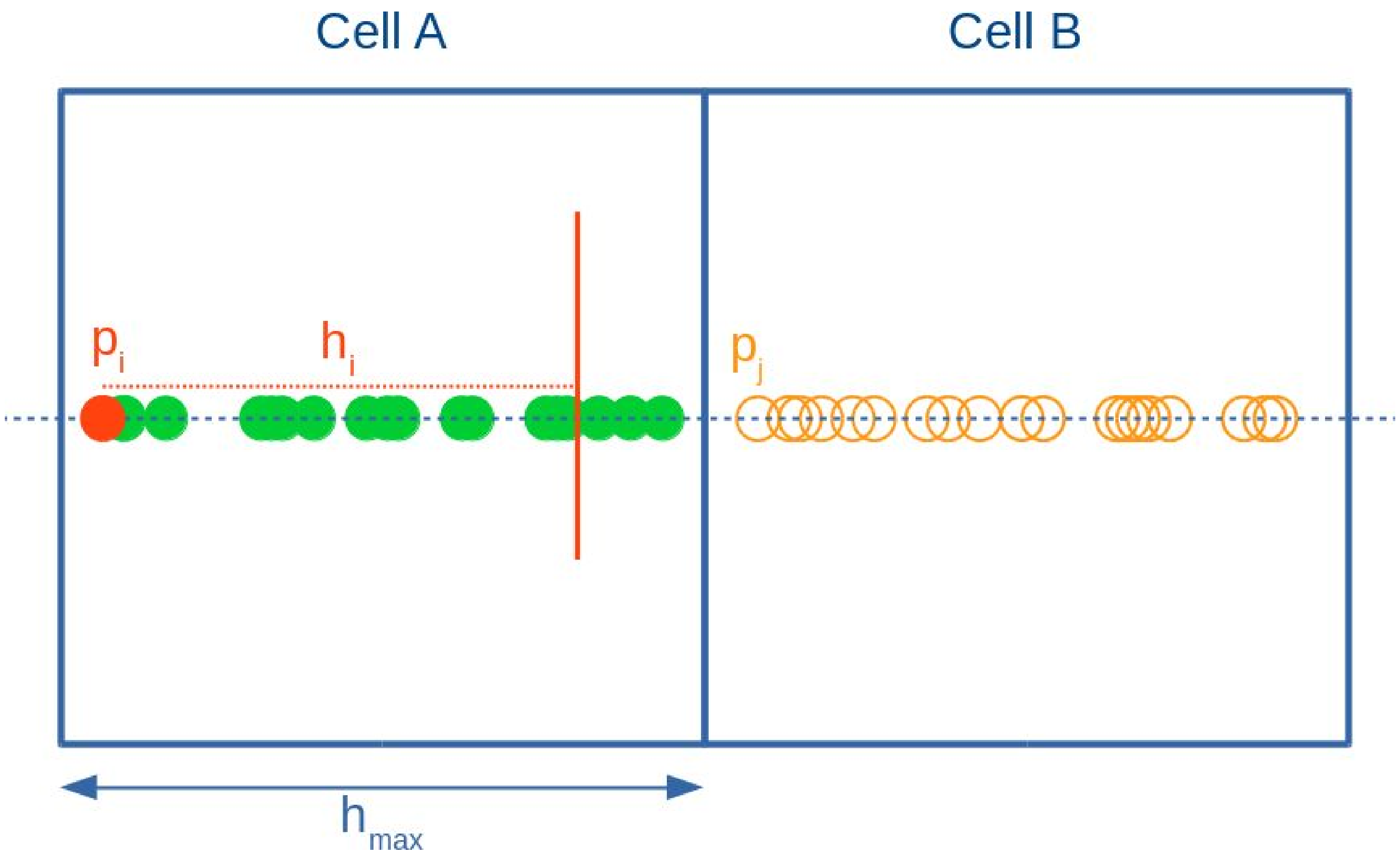


Populate Local Cache

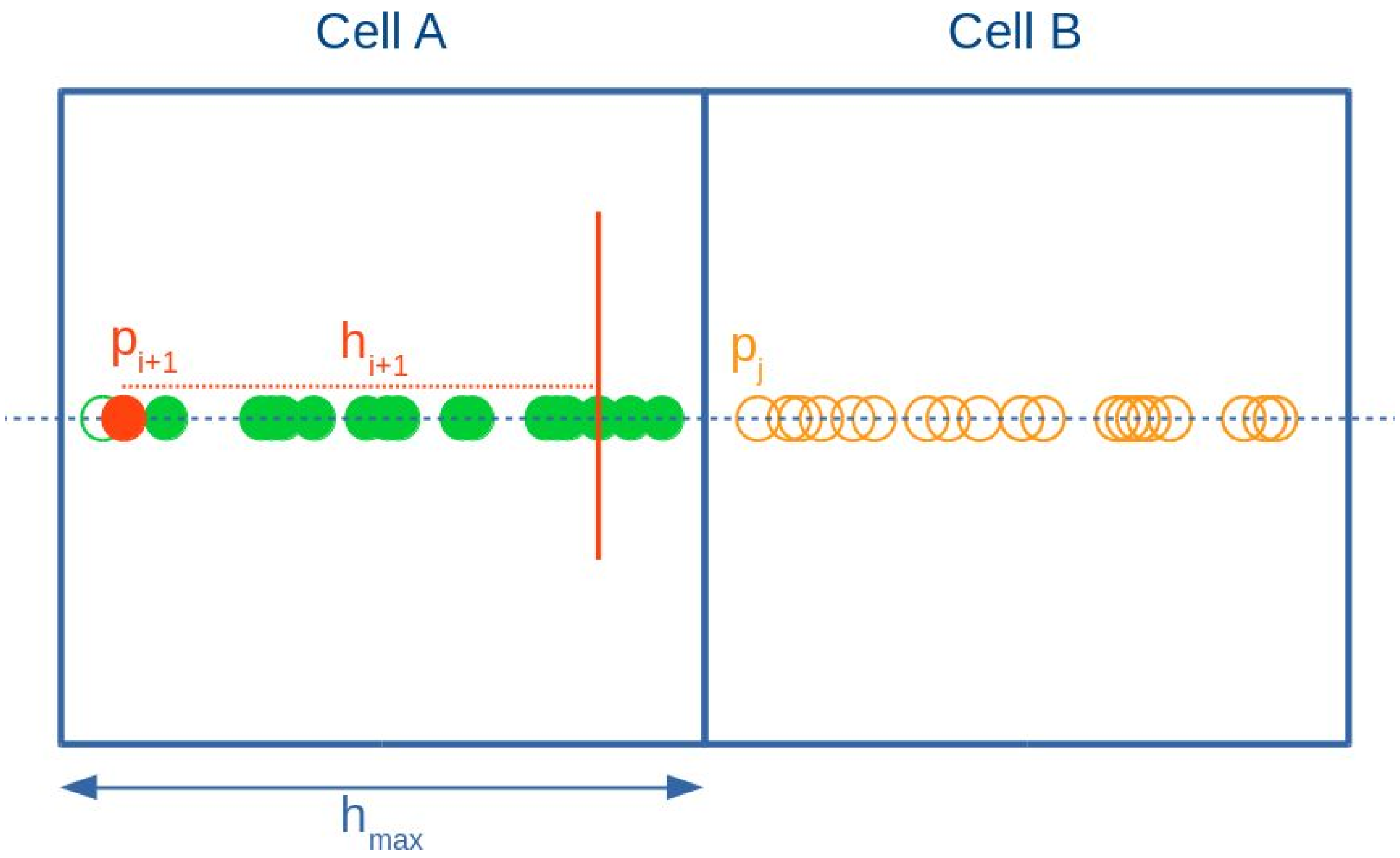
- In a uniform distribution of particles each cell pair orientation has a different number of interactions
- There are three cell pair orientations: *corner*, *edge* and *face*
- Number of interactions: *corner* < *edge* < *face*

- We want to reduce the cache overhead by only reading particles that are within range of each other
- Allows *edge* interactions to speedup instead of slowing down

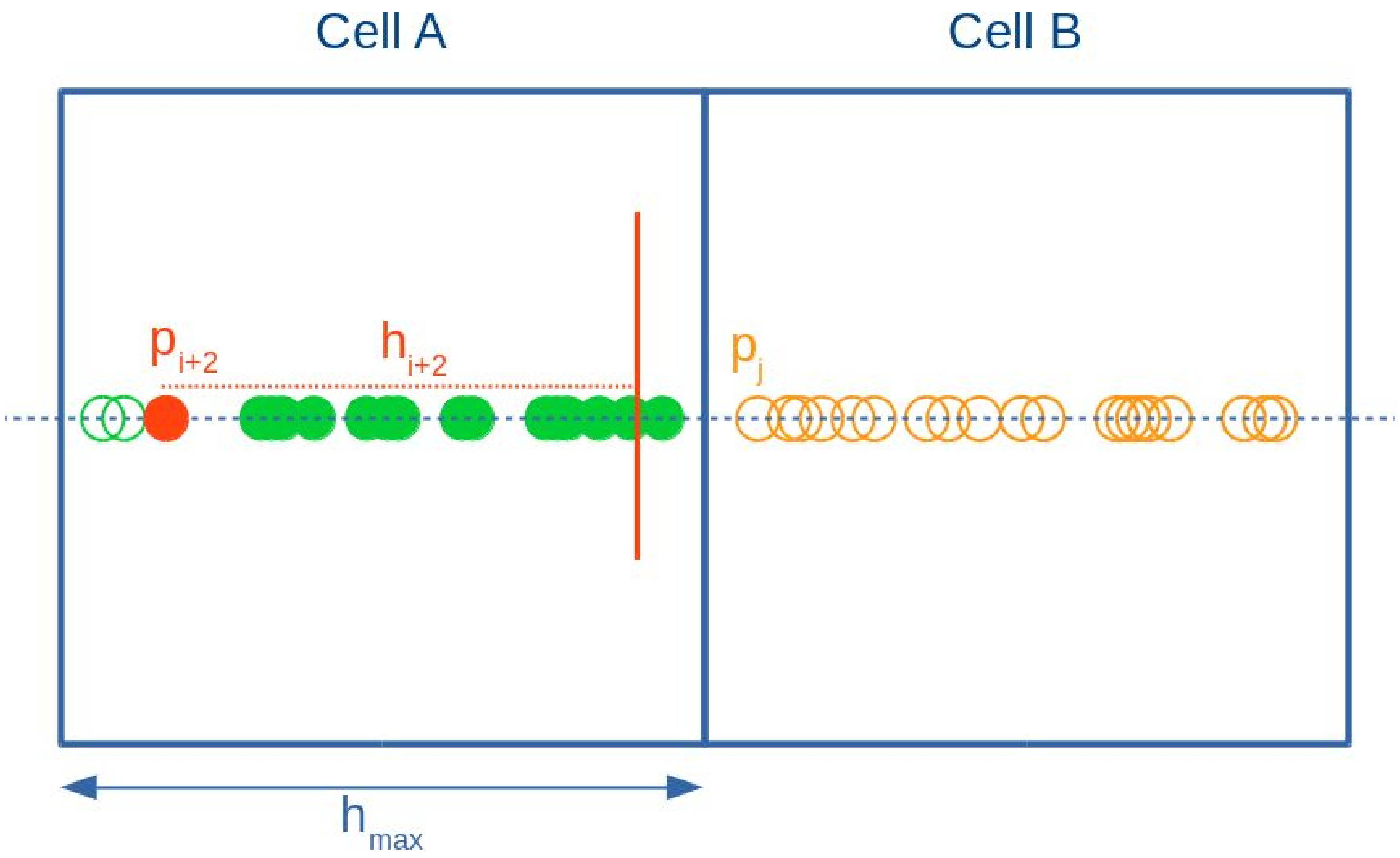
Populate Local Cache



Populate Local Cache



Populate Local Cache



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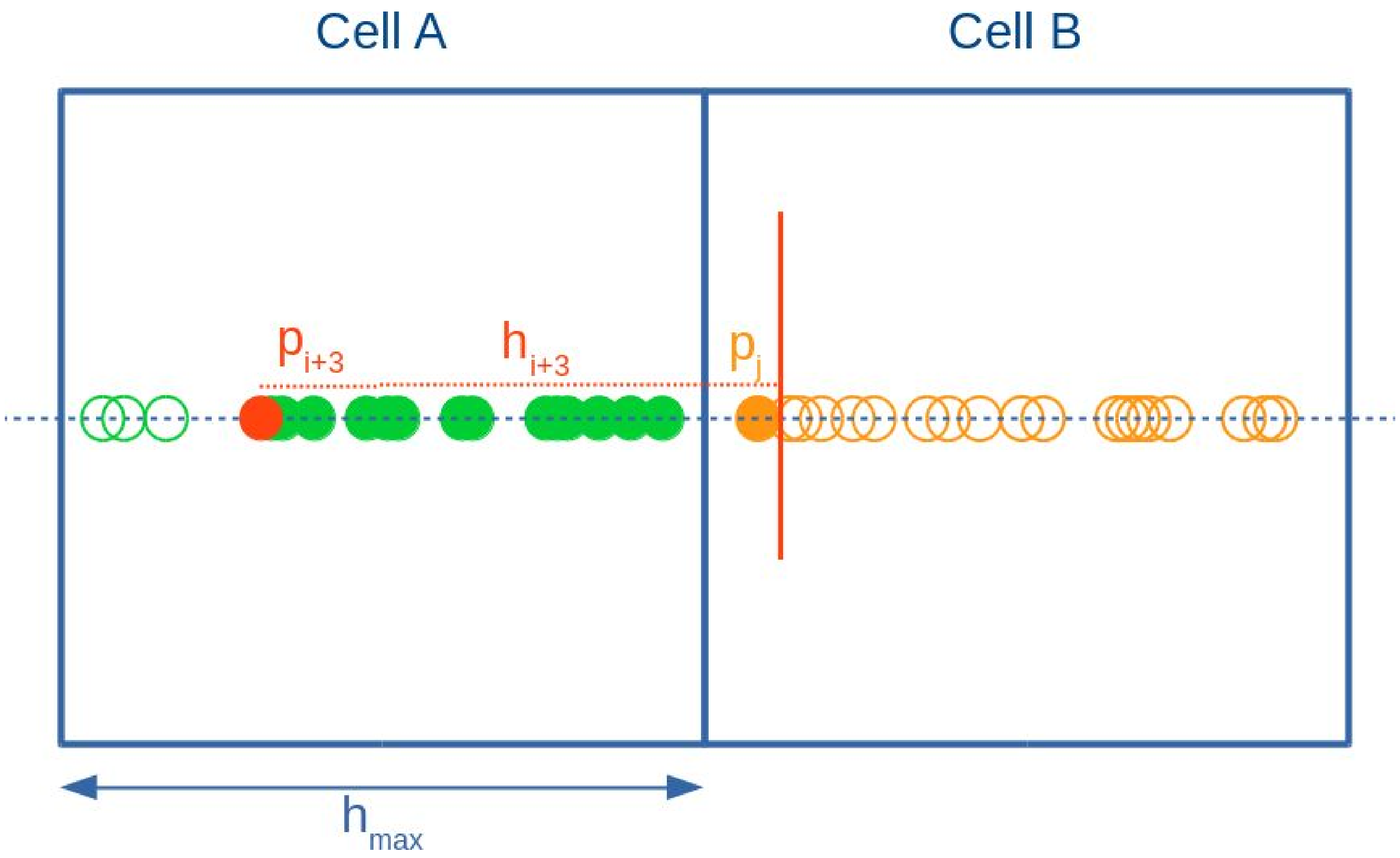

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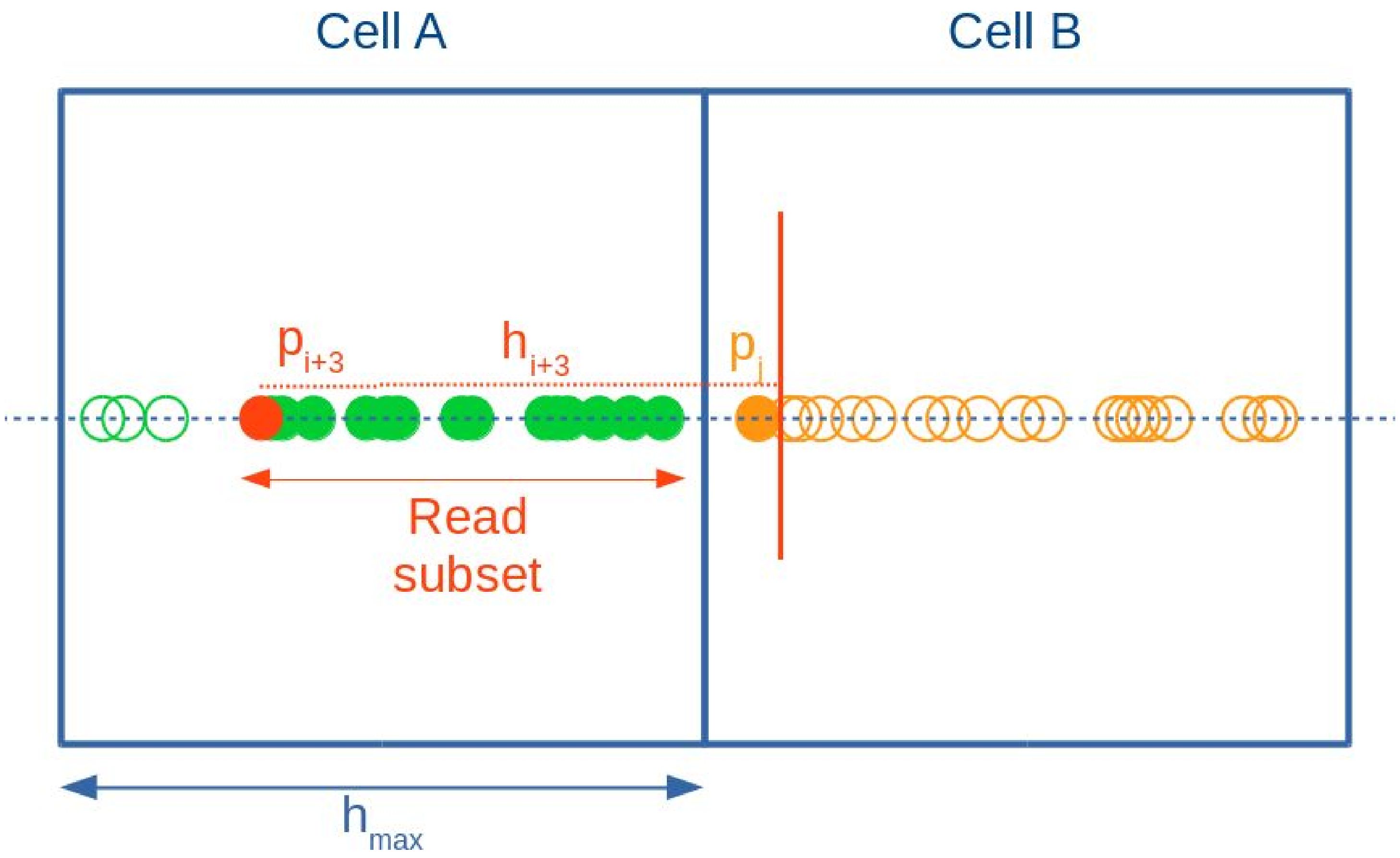
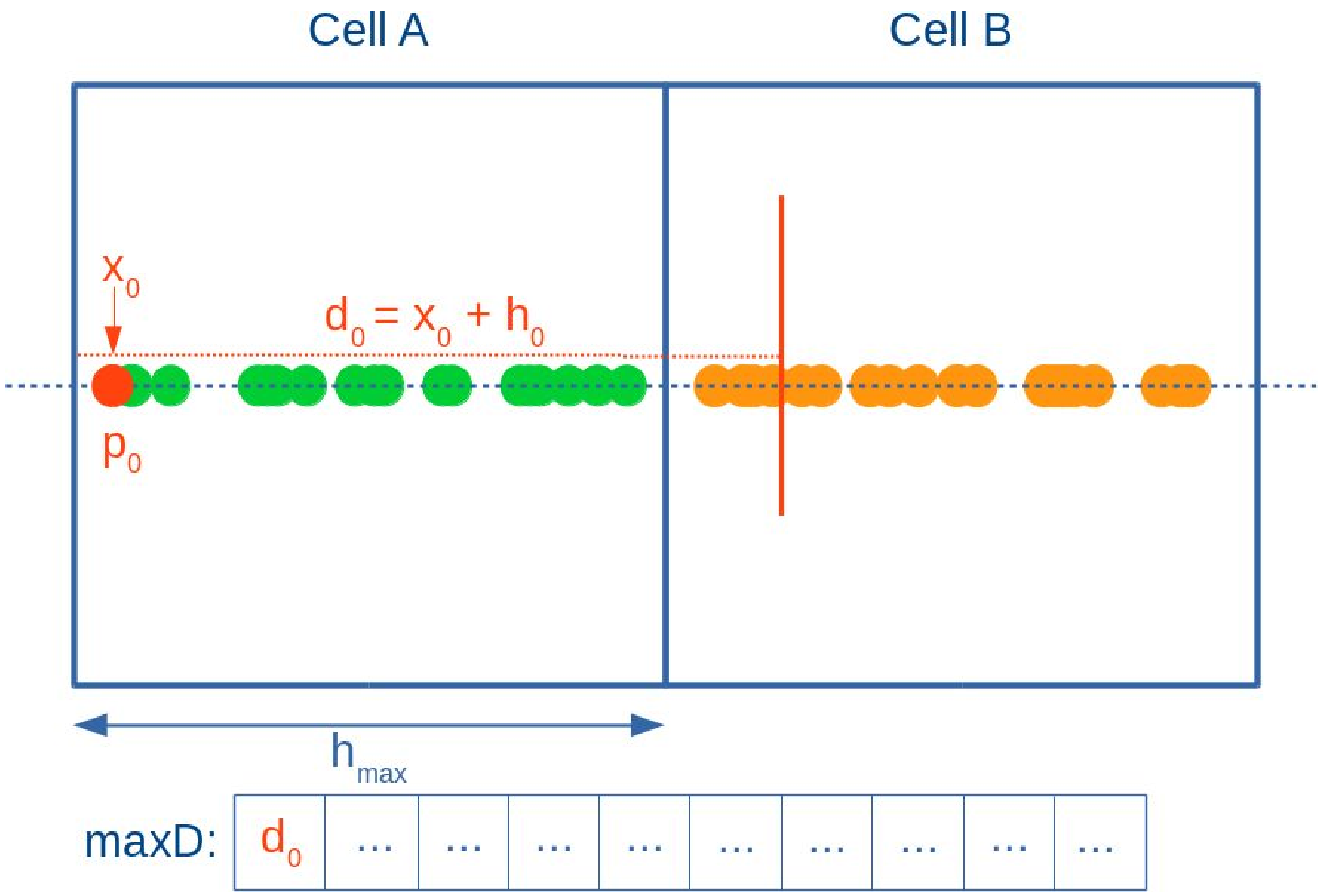


Limit Loop Bounds

- For each particle we loop over every candidate in the neighbouring cell
- Even though most will be out of range as we move further from the interface between the two cells
- We want to reduce the number of distance calculations even further

- Form array of maximum distances into neighbouring cell
- Use array to limit the number of particles looped over in the neighbouring cell

Limit Loop Bounds



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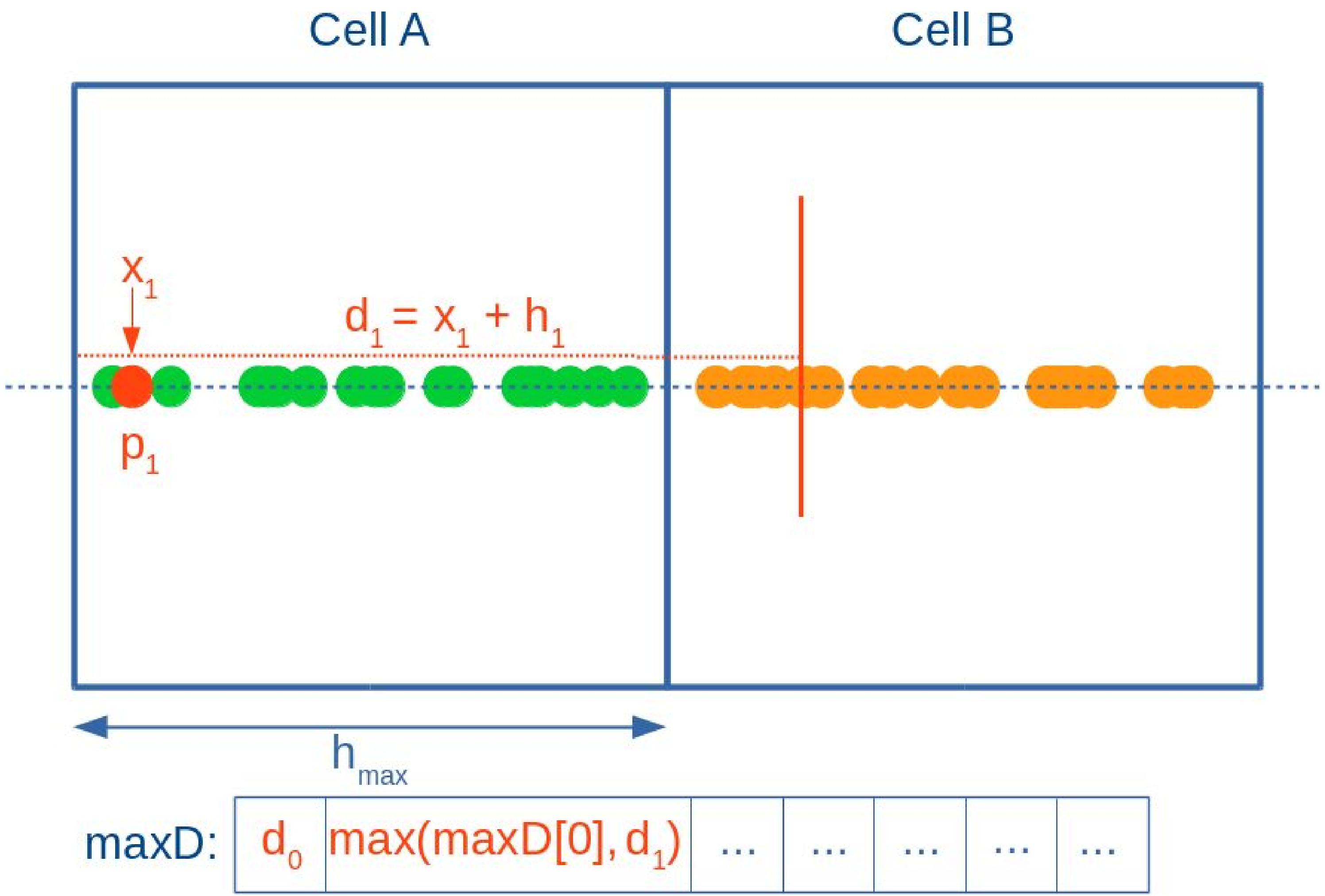

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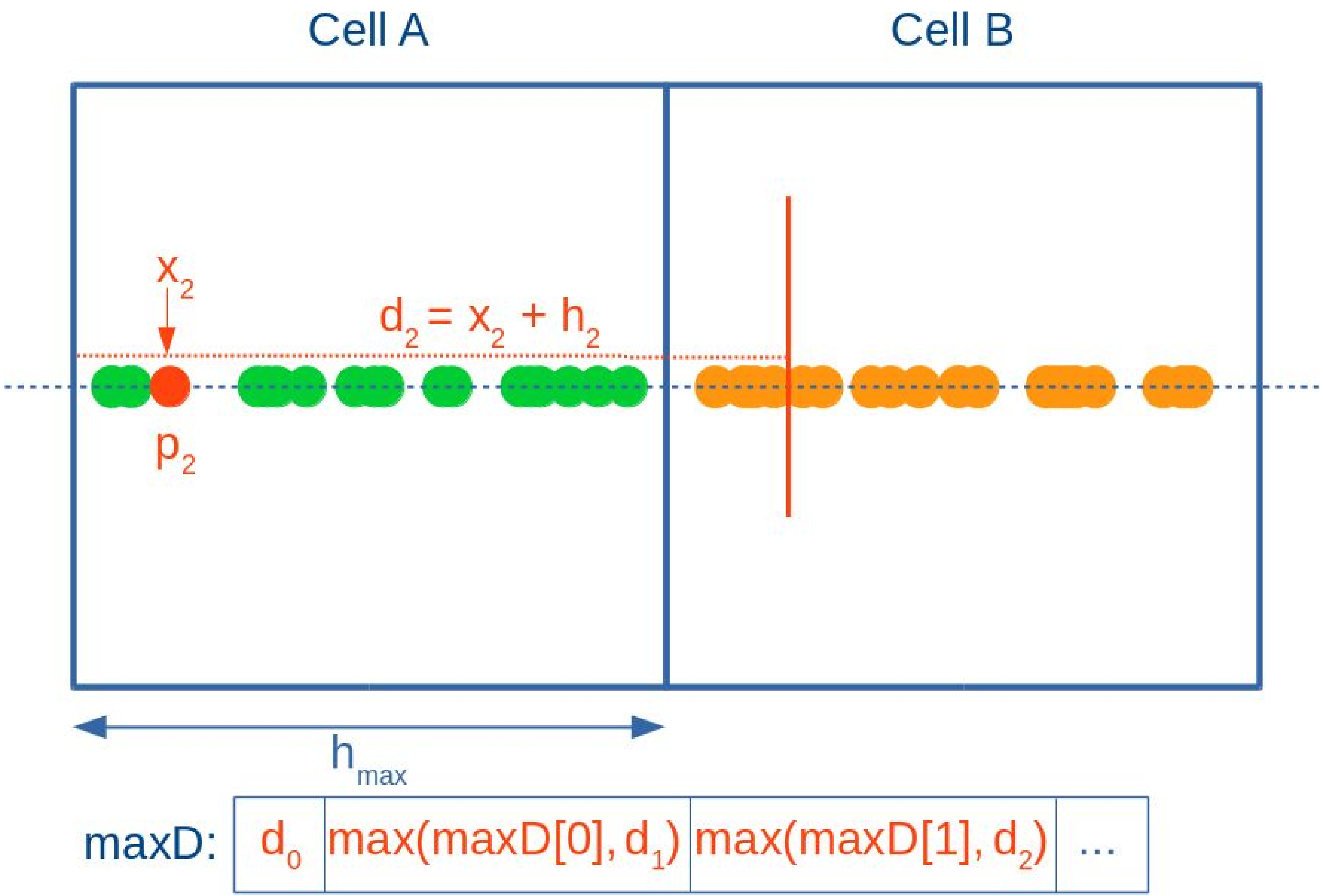

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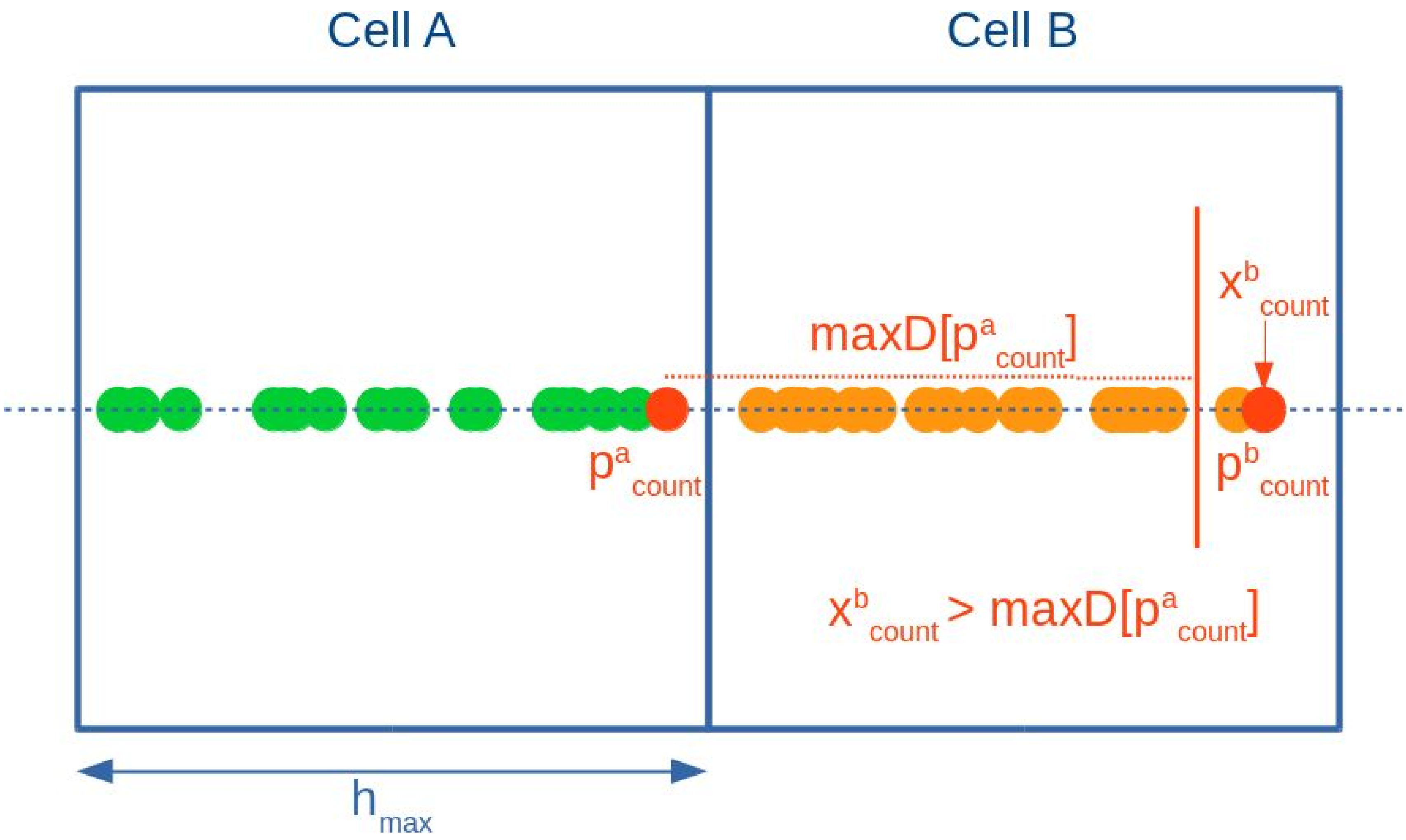

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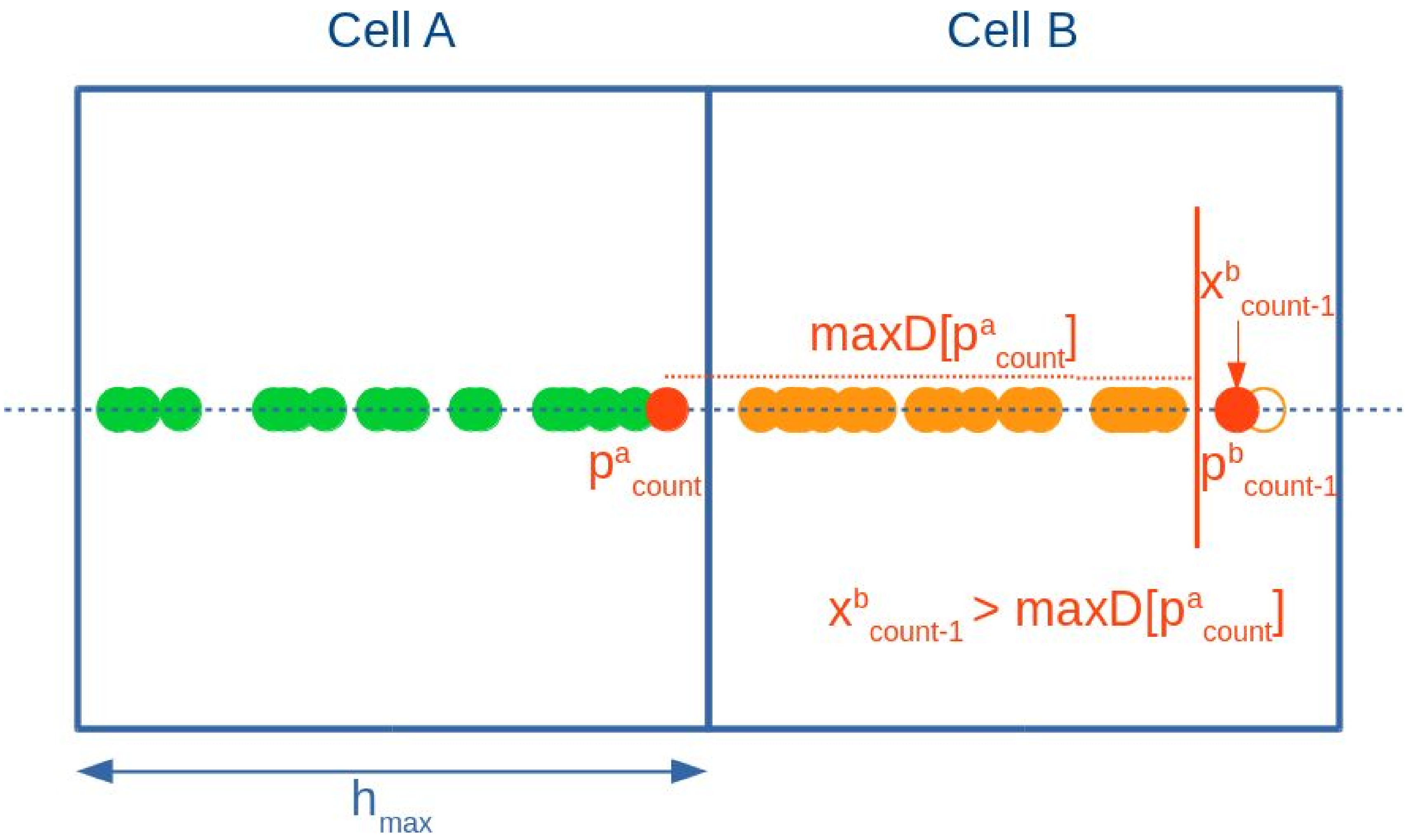

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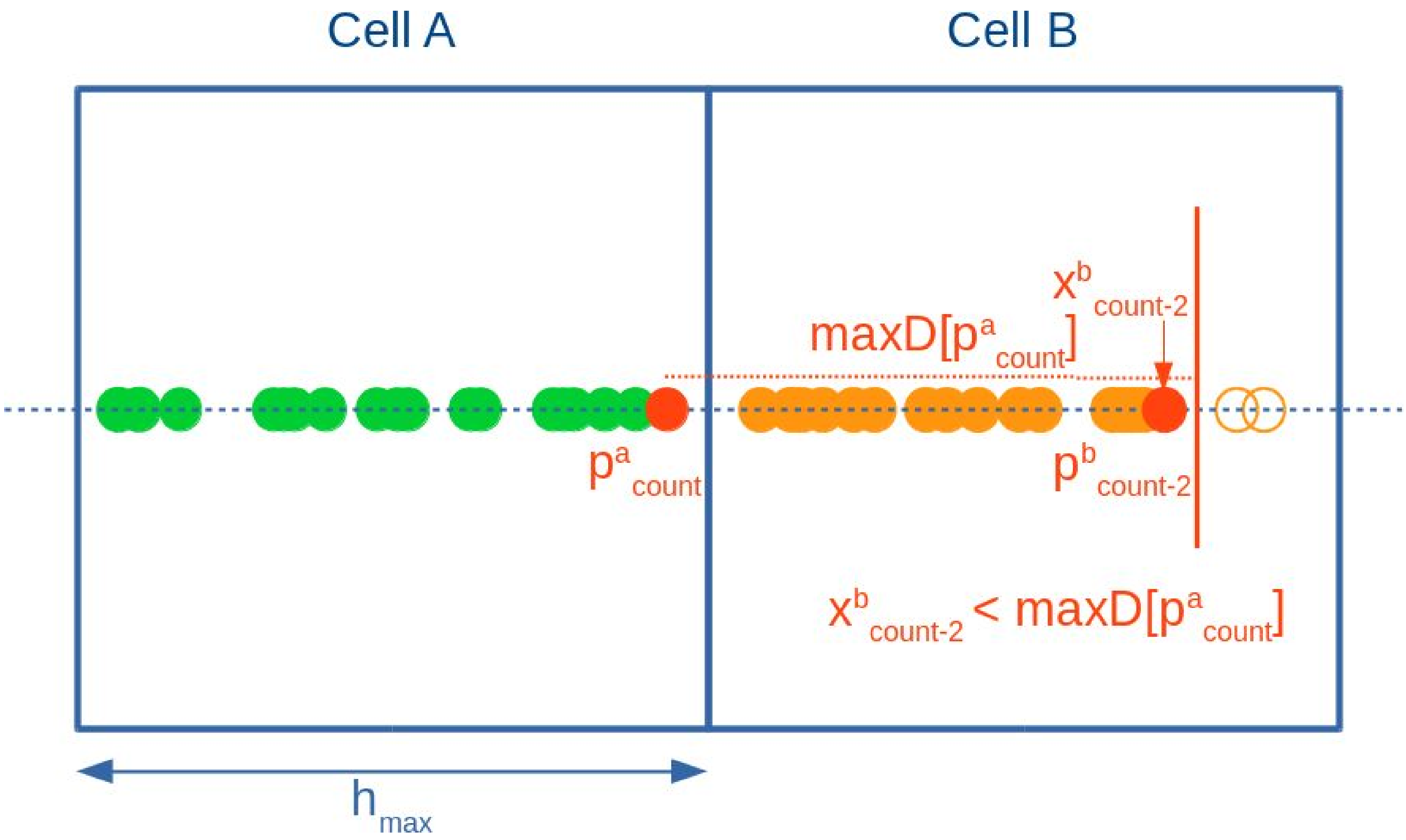


Calculating Interactions

- Particle density interactions are calculated using:

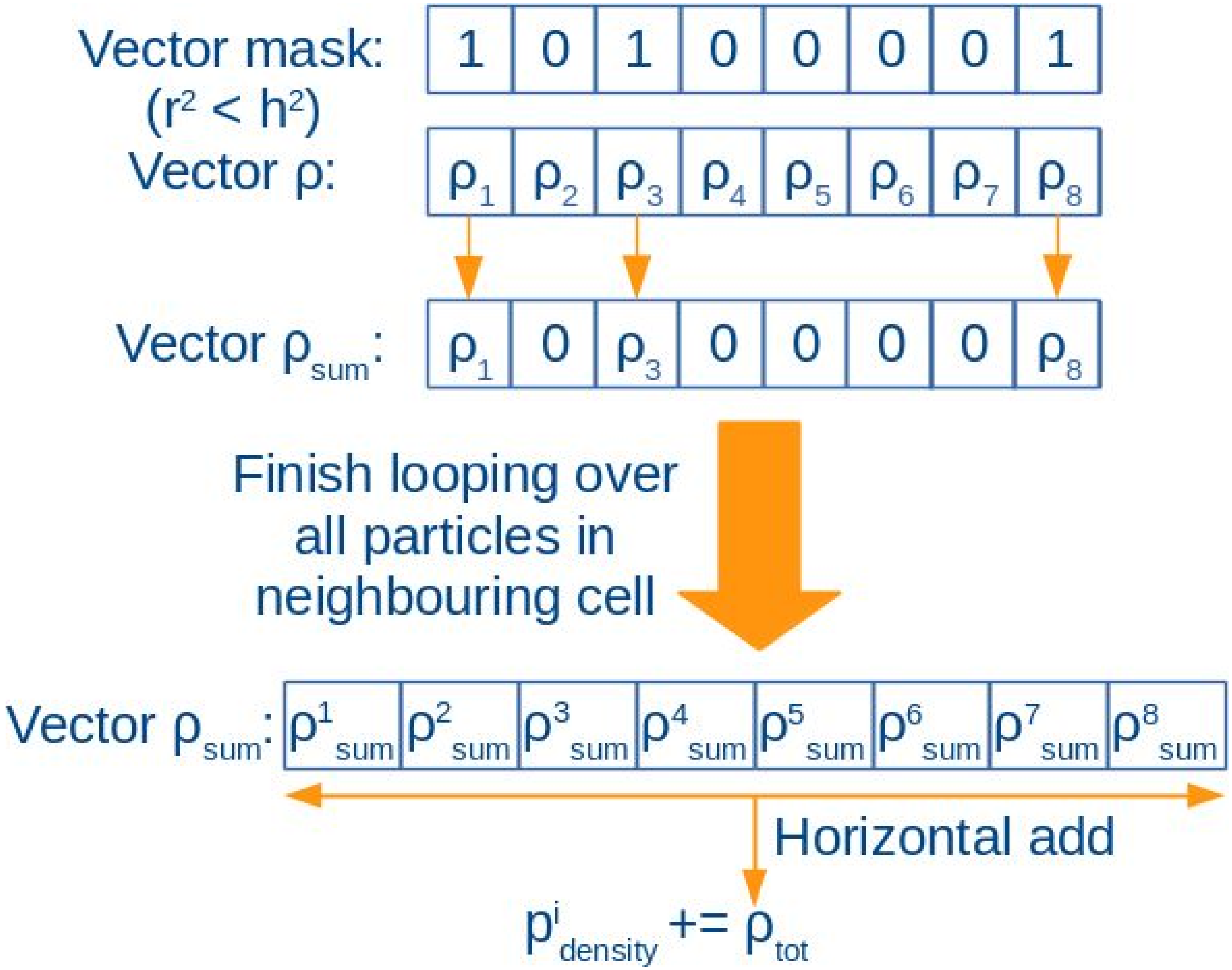
$$\rho(\mathbf{r}) = \sum_{b=1}^{N_{neigh}} m_b W(\mathbf{r} - \mathbf{r}_b, h)$$

- *W* is the weight function which is a low order polynomial

<u>SIMD Implementation</u>

- Use intermediate vectors to accumulate sum of particle updates in interaction function
- Perform horizontal add on these vectors and update the particles
- Decreases the amount of writes to memory

Calculating Interactions



Calculating Interactions

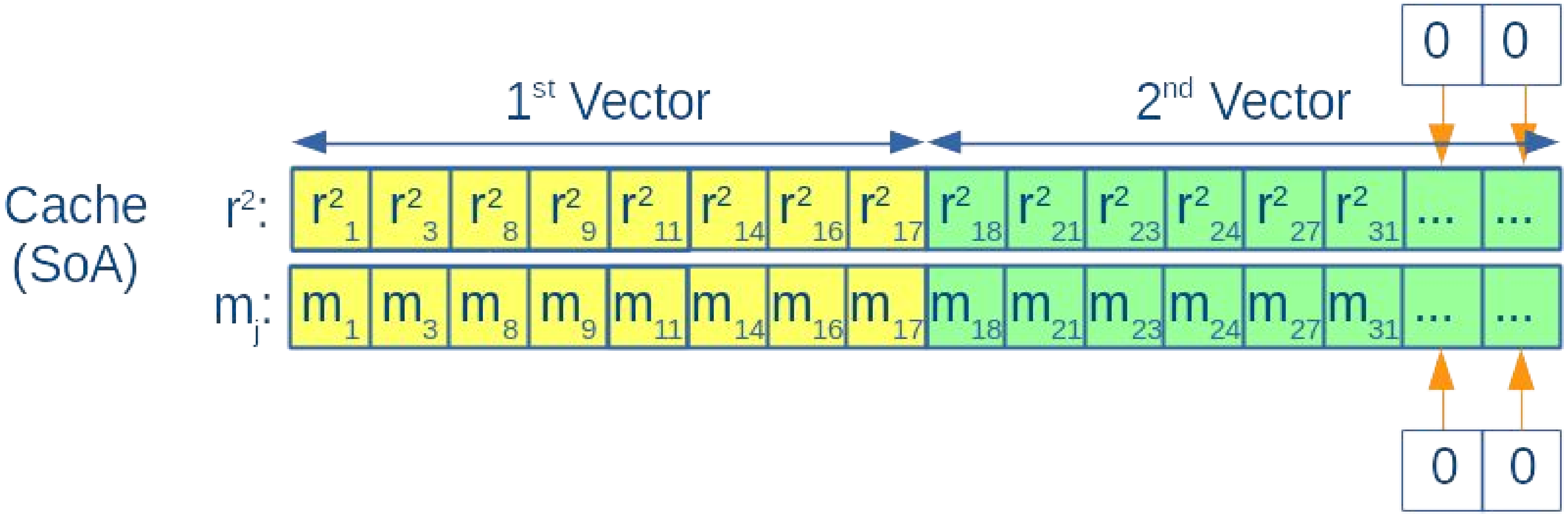
```
vector densitySum;
density = setzero();

for (int pjd = 0; pjd < icount; pjd+=VEC_SIZE) {
  INTERACT(&r2[pjd], &dx[pjd], &dy[pjd],
           &dz[pjd], &m[pjd], &v[pjd],
           &densitySum);
}

VEC_HADD(densitySum,pi); // _mm_hadd_ps
```

Calculating Interactions

```
// AVX intrinsics
vector interactionMask
vector v_densitySum;
vector v_mj, v_wi, v_r2, v_hi2;

// Form mask
interactionMask = _mm256_cmp_ps(v_r2, v_hi2, _CMP_LT_OQ);

// Mask and add to density sum
v_densitySum = _mm256_add_ps(v_densitySum,_mm256_and_ps(interactionMask, _mm256_mul_ps(v_mj, v_wi));

// AVX-512 intrinsics
__mmask16 interactionMask

// Form mask
interactionMask = _mm512_cmp_ps_mask(v_r2, v_hi2, _CMP_LT_OQ);

// Mask and add to density sum
v_densitySum = _mm512_mask_add_ps(v_densitySum, interactionMask, _mm512_mul_ps(v_mj, v_wi), v_densitySum);
```

Padding Local Cache

- Pad vectors to remove the serial remainders and mask the result



Performance Results

- Vectorisation performance was measured using AVX, AVX2 and AVX-512 instruction sets on the following hardware:

  - Intel Xeon CPU E5-4640 @ 2.4GHz (Sandy Bridge)

  - Intel Xeon CPU E5-2697 @ 2.6GHz (Haswell)

  - Intel Xeon Phi CPU 7210 @ 1.3GHz (Knights Landing)
    - 64 cores, configured in quadrant-cache mode
- Intel Compiler 17.0.1 20161005

Performance Results

CFLAGS	Speed-up of raw particle interactions over serial version	Speed-up over unsorted brute force solution	Speed-up over sorted solution
-O3 -xAVX -no-prec-sqrt -fp-model fast=2	6.50x	9.04x	2.20x
-O3 -xCORE-AVX2 -no-prec-sqrt -fp-model fast=2	6.65x	9.35x	2.32x
-O3 -xMIC-AVX512 -no-prec-sqrt -fp-model fast=2	17.35x	13.68x	3.90x

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Conclusions and Insights

- Increased performance of algorithm using a pseudo Verlet list and particle sorting
- Implemented a local particle cache (SoA)
- Implemented a vectorisation strategy
  - Only read particles into cache that interact
  - Calculate all interactions on a particle and store results in a set of intermediate vectors
  - Perform horizontal add on intermediate vectors and update the particles with the result
  - Pad caches to prevent remainders and mask out the result
- Obtained speed-up on AVX, AVX2 and AVX512 instruction sets

Future Work

- Reduce the impact of overheads even further
- Improve vectorisation efficiency to obtain speedup closer to 8x and 16x for AVX and AVX-512 instruction sets

Questions

- Thank you for your attention
- Any questions?
- Website: www.icc.dur.ac.uk/swift/