Massively Parallel OpenMP-MPI Implementation of the SPH Code DualSPHysics

Athanasios Mokos, Benedict D. Rogers

School of Mechanical, Aeronautical and Civil Engineering
University of Manchester, UK

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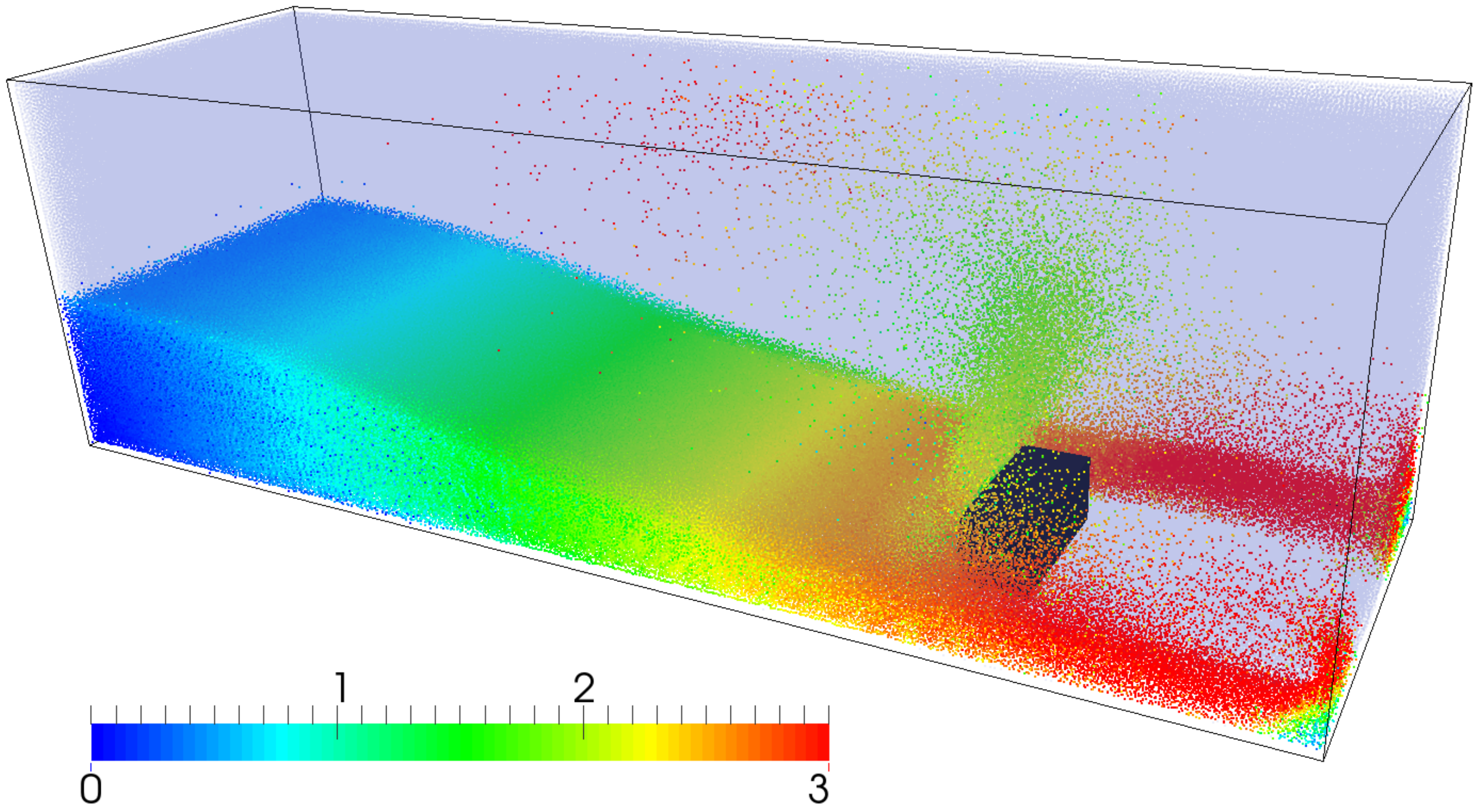
Outline of Presentation

- Motivation for Research
- Introduction to Meshless Methods
  - Introduction to SPH
- Message Passing Interface
  - Domain Division
  - Process Communication
  - Asynchronous communications
- Results
  - Runtime Results
- Optimization
  - Dynamic Load Balancing
  - Domain Decomposition
- 2D/3D Decomposition
  - Zoltan Library
  - Domain Decomposition Algorithms
- Conclusions and Future Work



Motivation for Research

- Primary focus on violent water flows with breaking free surface, e.g. wave impact/slamming or potentially explosive pipe flows

- Applications:
  - Coastal Defence
  - Offshore structures
  - Dam and river flooding

- Experiments are expensive and require significant investment

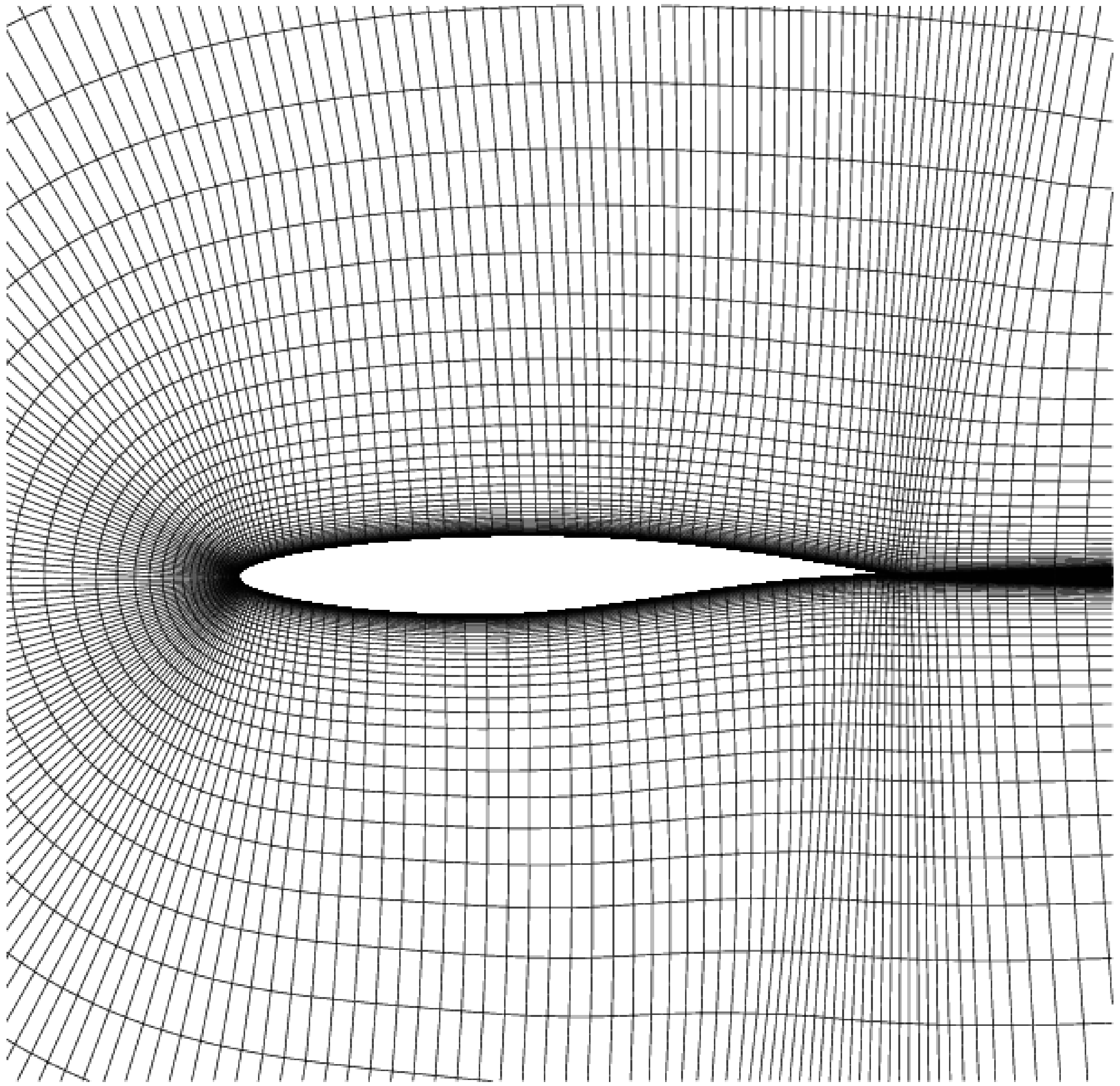
- Focus on computational methods

Whitehaven 2013 (North News)

Mesh-based Methods

- Most common methods used in both industry and academia:
  - Finite Difference Method (FDM)
  - Finite Element Method (FEM)
  - Finite Volume Method (FVM)
- Robust, well-developed and mature
  - Multiple algorithms and models
  - Adapted for every application

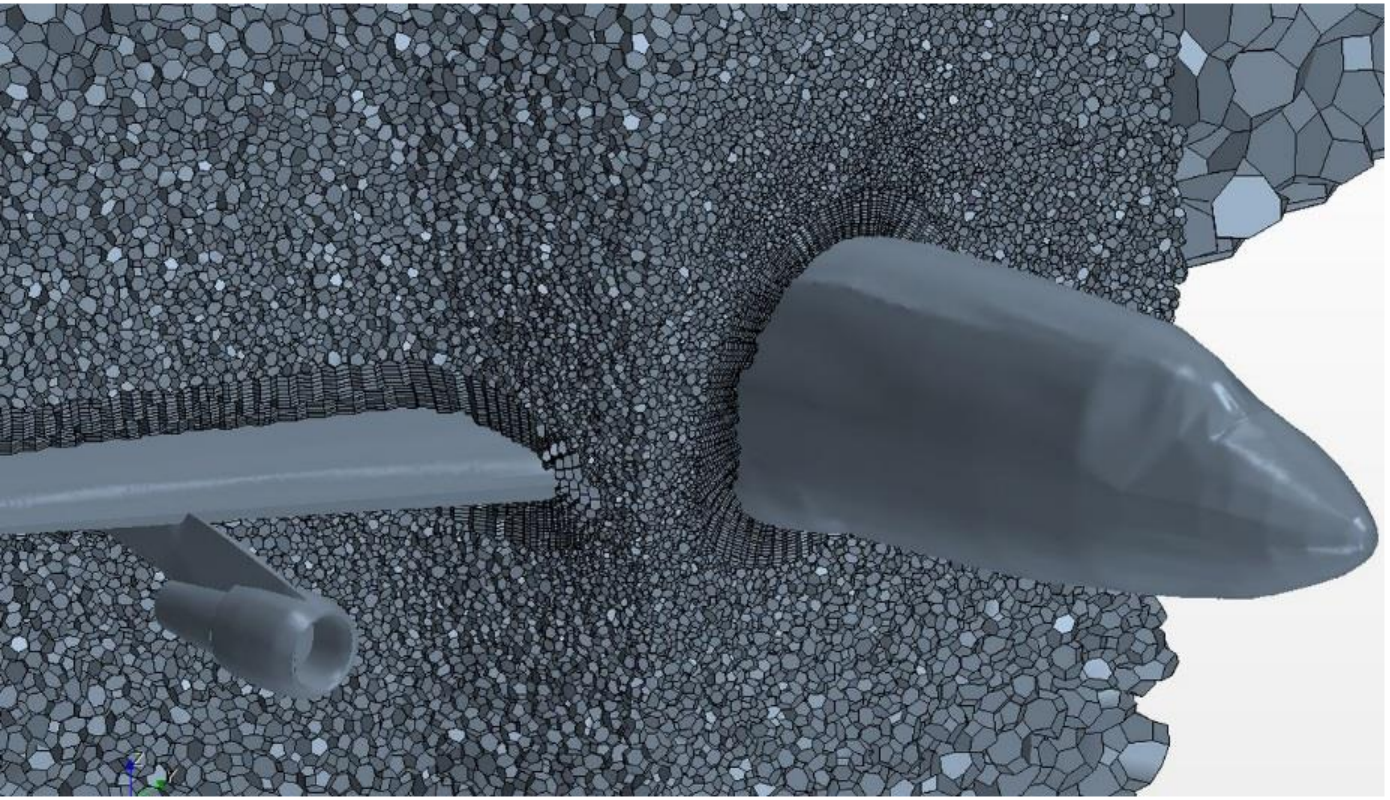
However…


Mesh around a RAE 2822 transonic aerofoil (NASA)

Mesh-based Methods

Meshing can be complex

Deformation?



Mesh around an airplane hull

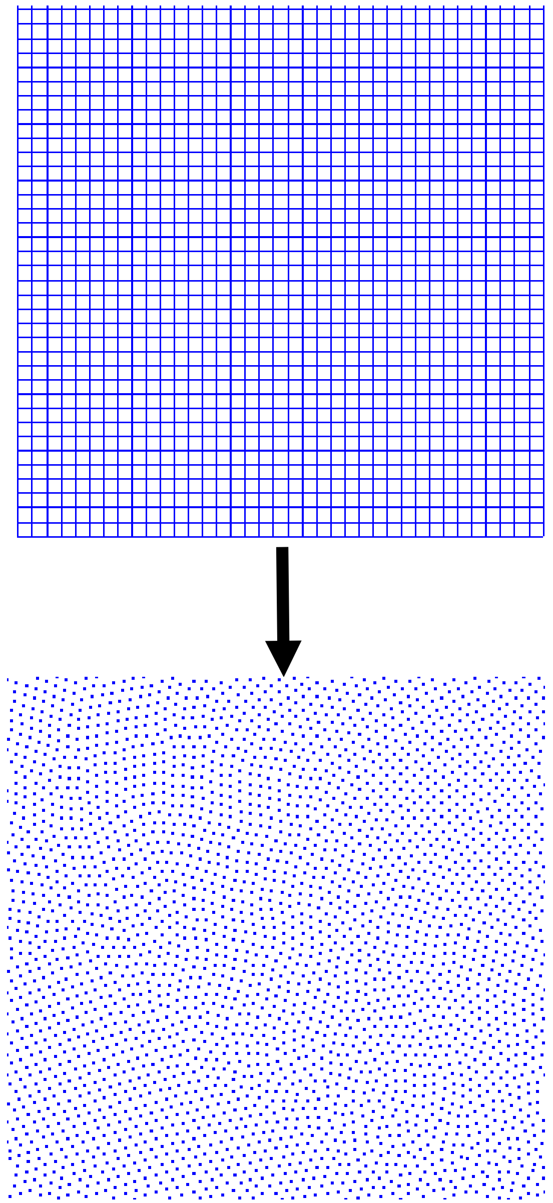
(Photo courtesy of Siemens)

Waves breaking on the shore

(Photo courtesy of the University of Plymouth)

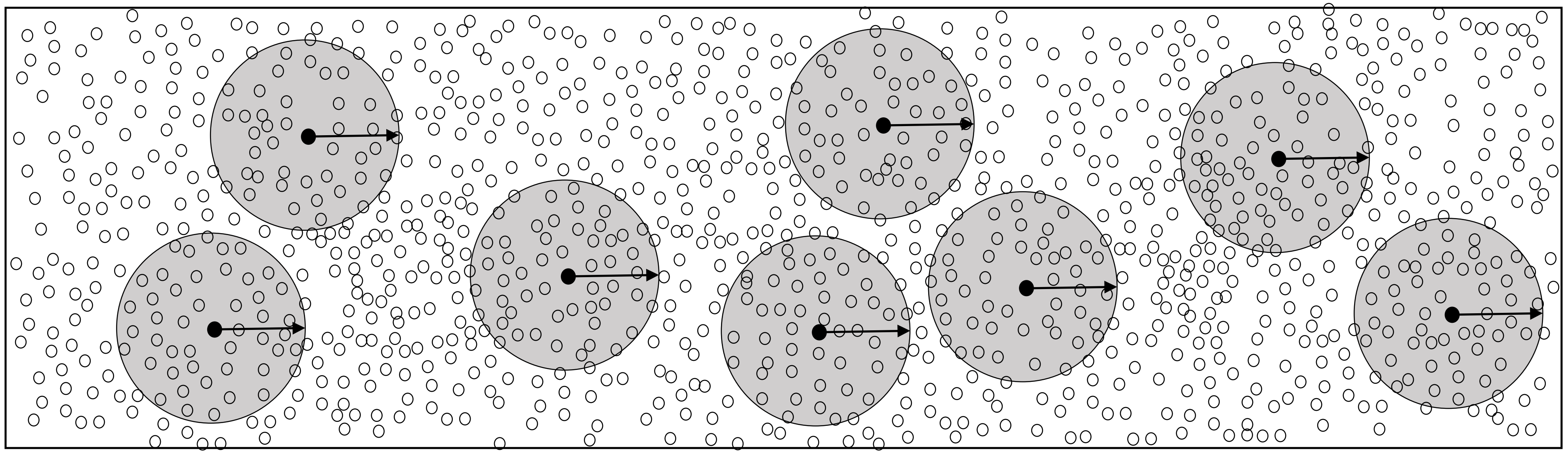
Meshless Methods

- Computation Points: Nodes -> **Particles**
- Particles are not connected with a grid
- Particles are not fixed but **move** with their own velocity and acceleration
- Each particle follows a unique trajectory
- Particles are described through **Lagrangian** derivatives: Rate of change along a trajectory



Local Interpolation

- Particles possess **properties** (density, pressure etc.) travelling with them
- Particles are linked to their current **neighbouring particles in space**
- Neighbours' values affect the properties of the particle through a summation
- Particle movement also affected by neighbours



Introduction to Smoothed Particle Hydrodynamics

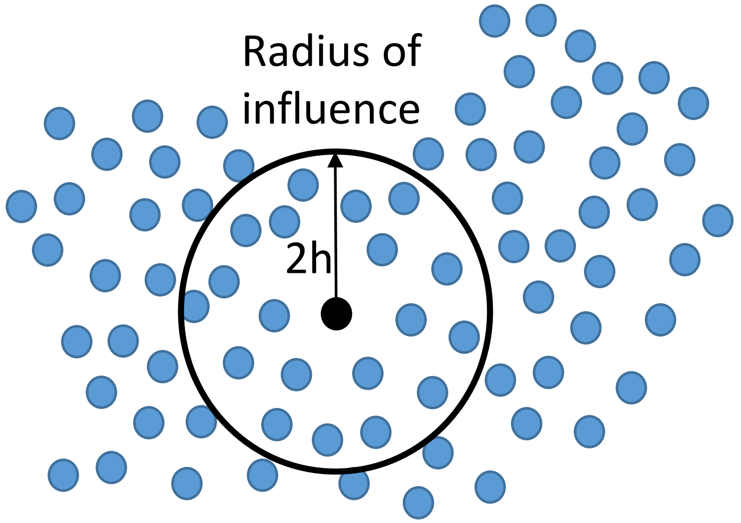
- SPH is a **Lagrangian meshless** method: Computation points (**particles**) move according to governing equations (Navier-Stokes Equations)

- **Basic idea**: The value of a function A(**r**) at point **r** in space is approximated as:

$$A(\boldsymbol{r}) = \int_{\Omega} A(\boldsymbol{r}')\delta(\boldsymbol{r}-\boldsymbol{r}')\,\mathrm{d}\Omega$$

- Properties computed through **local interpolation** with a weighting function (**kernel**) around each particle

$$\langle A(\boldsymbol{r})\rangle \approx \sum_{j=1}^{N} \frac{m_j}{\rho_j} A(\boldsymbol{r}_j) W(\boldsymbol{r}-\boldsymbol{r}_j, h)$$



Introduction to SPH

- Navier-Stokes Equations
  - Continuity $$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\nabla \boldsymbol{v} \quad \rightarrow \quad \left\langle \frac{\mathrm{d}\rho_i}{\mathrm{d}t} \right\rangle = \sum_j m_j \left(\boldsymbol{u}_i - \boldsymbol{u}_j\right) \cdot \nabla_i W_{ij}$$
  - Momentum $$\frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = -\frac{1}{\rho}\nabla p + \nu\nabla^2 \boldsymbol{u} + \boldsymbol{F} \rightarrow \left\langle \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} \right\rangle = -\sum_j m_j \left[\frac{p_j}{\rho_j^2} + \frac{p_i}{\rho_i^2}\right] \nabla_i W_{ij} + \Pi_{ij} + \boldsymbol{F}_i$$

- Fluid Compressibility
  - Incompressible SPH ⟶ Poisson Equation
  - Weakly Compressible SPH ⟶ Equation of State

SPH for real problems

- Real-life applications are complex 3D flows
- Multi-scale problems with long runtimes
- SPH requires over 10^8 particles to model them
- Must do so as quickly as possible

OPTION: Use the inherent parallelism of the **GPU**

Photo by University of Plymouth

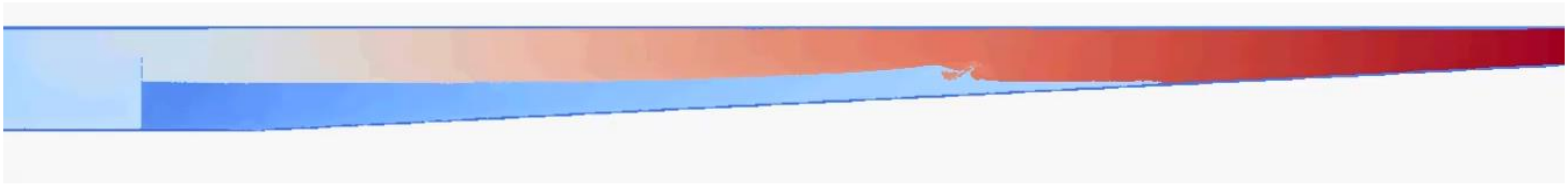
SPH Solver DualSPHysics

http://dual.sphysics.org/

- Open-source project, co-developed with the Universities of Vigo, Manchester, Parma and Lisbon

- Validated for violent water flows[1]

- Includes pre- and post processing software

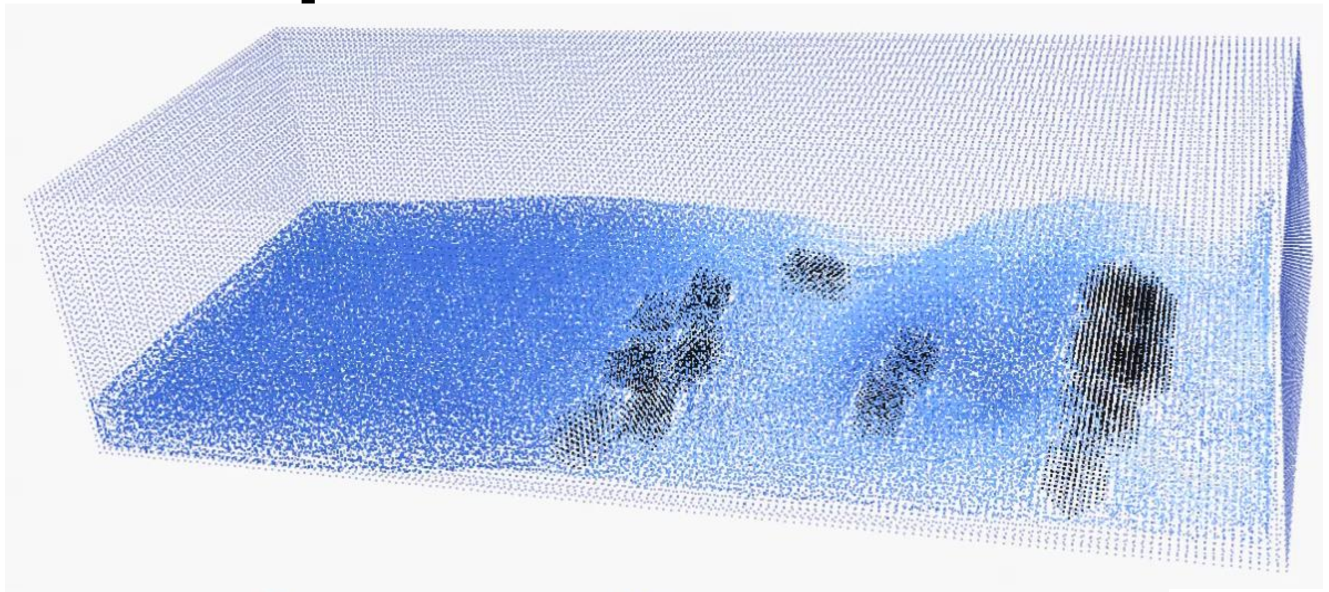


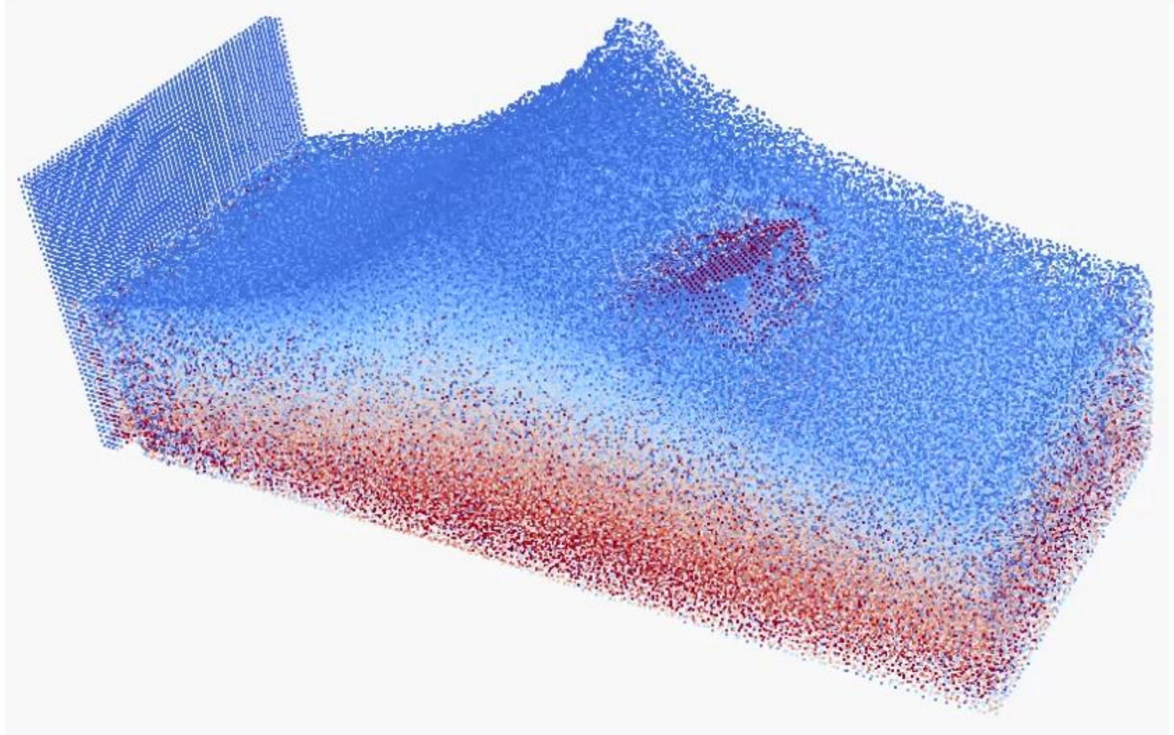
http://www.youtube.com/user/DualSPHysics/videos

Additional Capabilities

Integration with all existing capabilities of DualSPHysics

- Wave Generator
- DEM model
- Floating Bodies
- Air-Water multiphase model
- Solid-Water multiphase model
- Object motion





Current State of DualSPHysics

GPU

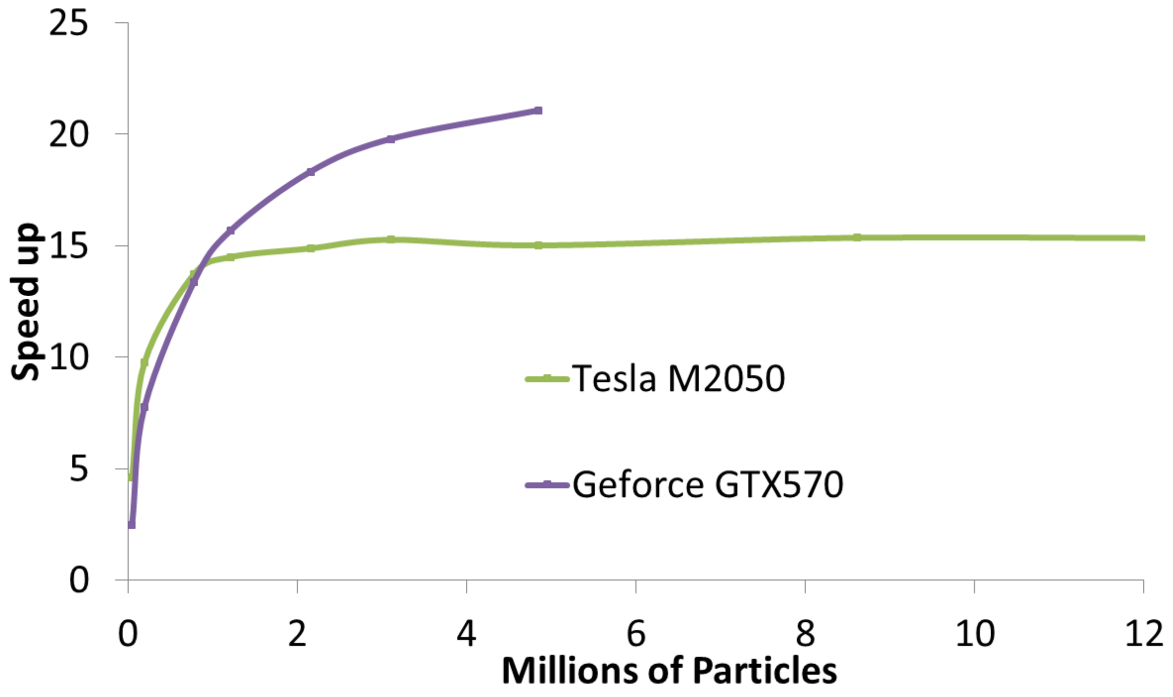
- Highly optimised code
- Multiple options
- Pre- and post-processing tools
- Able to take advantage of the inherent parallelism
- Simulates millions of particles in a few **hours**

CPU

- Highly optimised code
- Multiple options
- Pre- and post-processing tools
- OpenMP implementation
- Simulates millions of particles in a few **months**

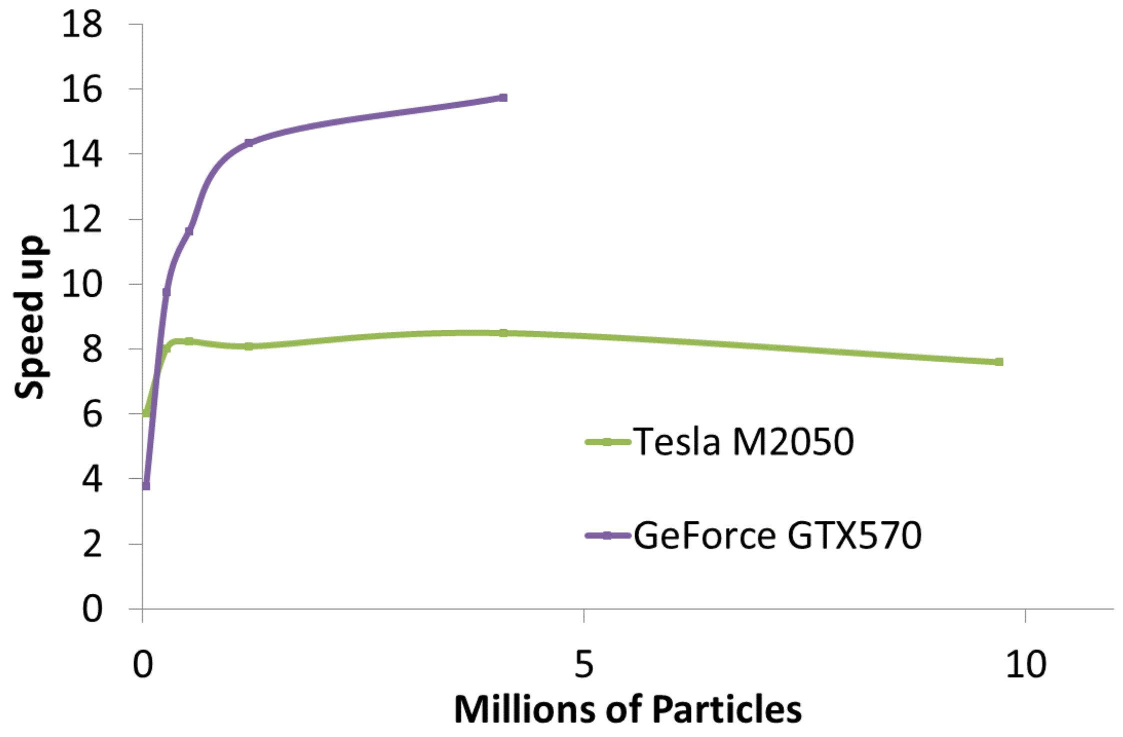
Current State of DualSPHysics

2D



Speedup up to **21** for a 6-year old card compared to an 8-thread OpenMP simulation

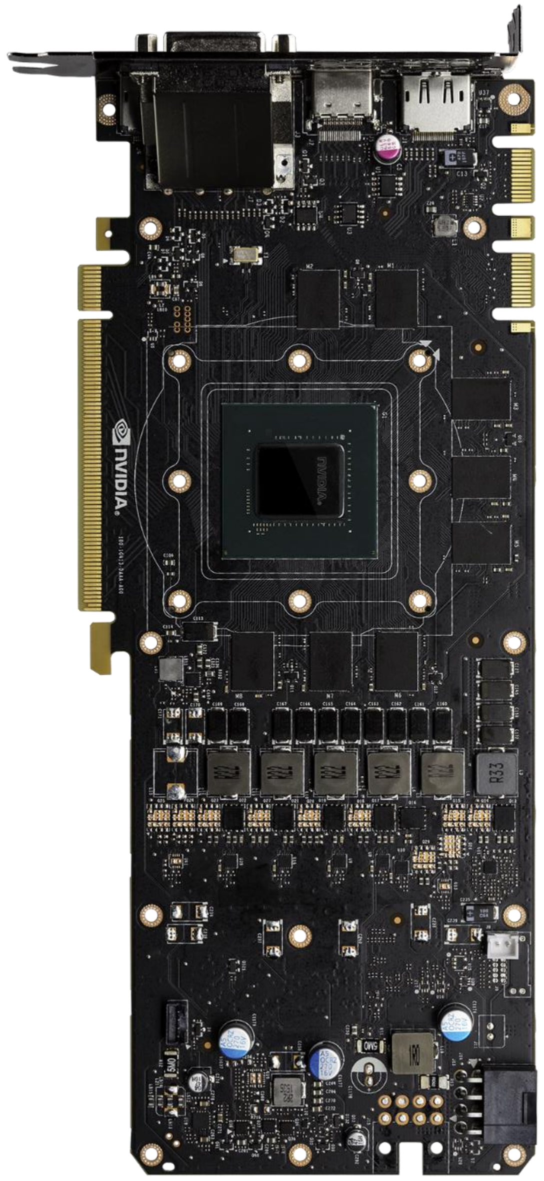
3D



Speedup up to **16** for a 6-year old card compared to an 8-thread OpenMP simulation

Current State of DualSPHysics

- GPUs are fantastic:
  - Massively Parallel, ideal for n-body simulations
  - Low cost and energy consumption (**Green Computing**)
- But…
  - Still in their infancy (less developed tools and compilers)
  - Single precision to maintain speed
  - The multi-GPU code is not easily portable
  - Require specialised hardware and additional investment (cannot take advantage of existing HPC infrastructure)
  - Industrial engineering companies still need convincing to invest resources and personnel


NVidia GTX1080

Motivation for Research

- Develop a **CPU code** with similar capabilities to the existing GPU code that can be used in HPC installations
- Massive Parallelism required: Ability to scale for **1000s** of cores
- Currently only local parallelism (OpenMP) -> Communication between different processors required
- Implementation of the **Message Passing Interface (MPI)** standard

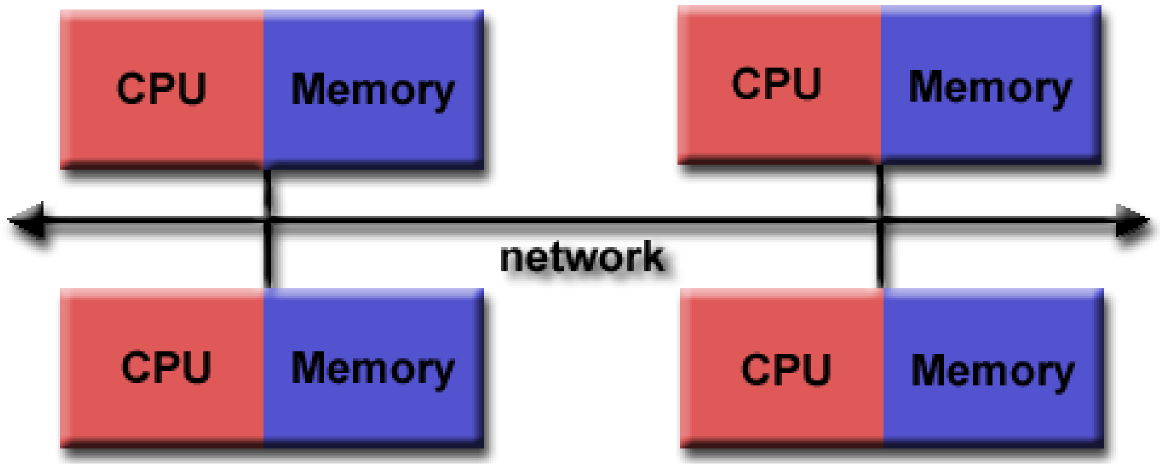
- **AIM: Develop a hybrid OpenMP-MPI program that can scale to 1000s of cores**

Message Passing Interface

- Standardised, independent and portable message parsing library specification

- **Message Passing**: Data is moved from one process to another through cooperative operations on each process. The recipient then selects the appropriate code to be executed.

Distributed memory model



Message Passing Interface

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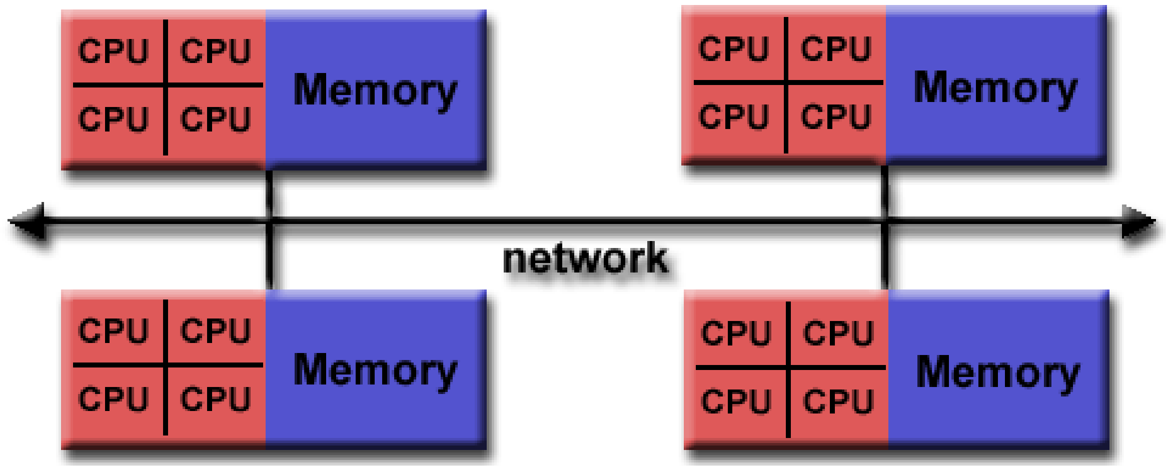
OpenMP already developed so…

Hybrid memory model



Challenges of Integrating MPI

- Maintain DualSPHysics optimisation and structure
  - Cell-linked neighbor list[3]
  - Ease of use
  - Reduce changes in SPH computation
  - Limits options when creating particles and cells

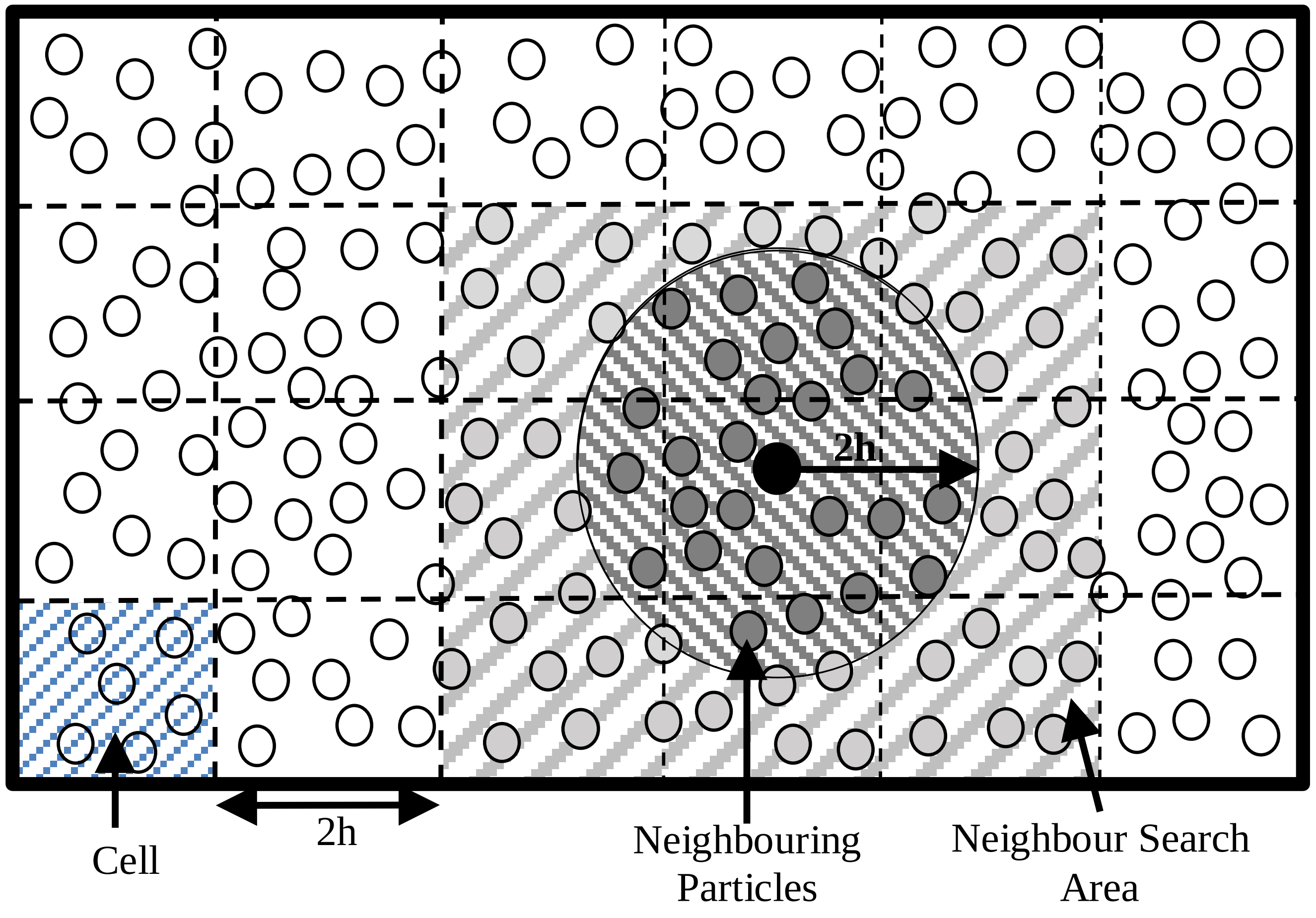
- Need to introduce new features
  - Focus on updating existing functions to work with multiple nodes
  - Create new files to handle communication and data transfer

SPH Solver DualSPHysics

http://dual.sphysics.org/

Cell-linked neighbour list[3]

- Algorithm that optimises neighbour searching
- Divide the domain into cells
- Cells remain constant throughout the computation
- Create a list linking particles and cells
- Search for neighbour particles only in adjacent cells



Integrating MPI in DualSPHysics

Single node files

- JCellDivCpuSingle
- JPartsLoad4
- JSphCpuSingle

MPI files

- CellDivCpuMPI
- ParticleLoadMPI
- SphCpuMPI

- Changes focused on:
  - Loading data from pre-processing software
  - Creating and updating the assignment of particles in cells
  - Handling and integrating the new features

Integrating MPI in DualSPHysics

Single node files

- JCellDivCpuSingle
- JPartsLoad4
- JSphCpuSingle

MPI files

- CellDivCpuMPI
- ParticleLoadMPI
- SphCpuMPI

New files created to handle:

- Node communication
- Domain Decomposition
- Halo Exchange

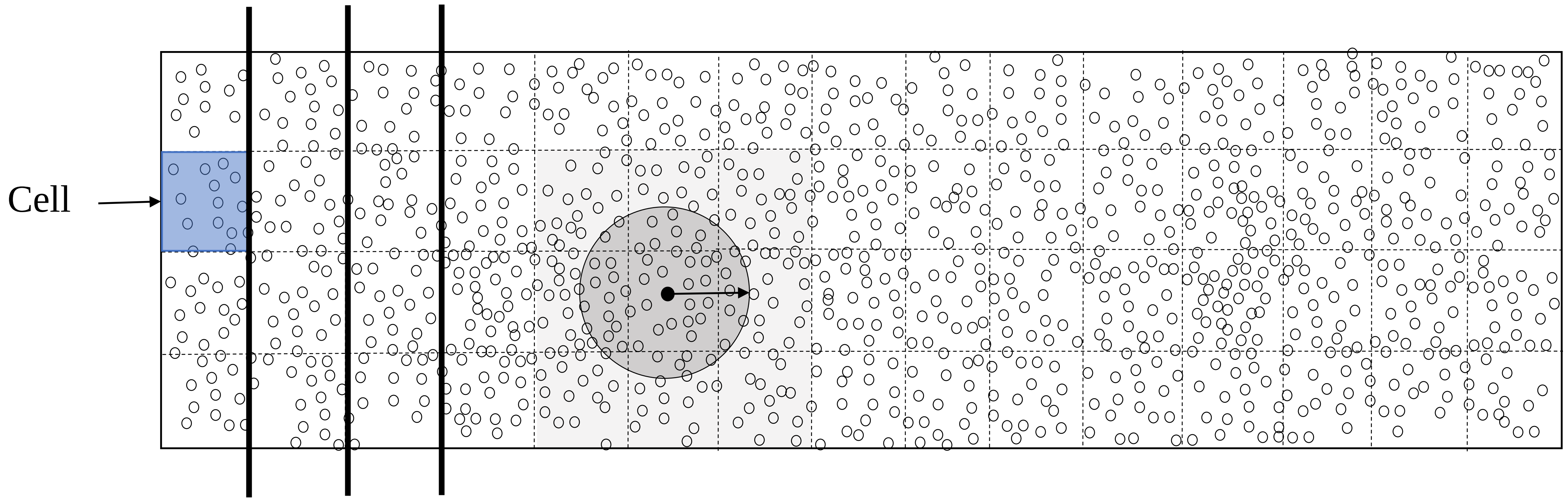
- BufferMPI
- DataCommMPI
- HostMPI
- InfoMPI
- SliceMPI
- SphMPI
- SphHaloMPI

Domain Decomposition

- Divide the domain between nodes
- Unique particle and cell list
- 1D decomposition through slices[2]

⇒

- Allows the simulation to use more particles
- Reduces local and global memory footprint
- Reduces the load on each CPU core



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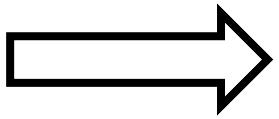

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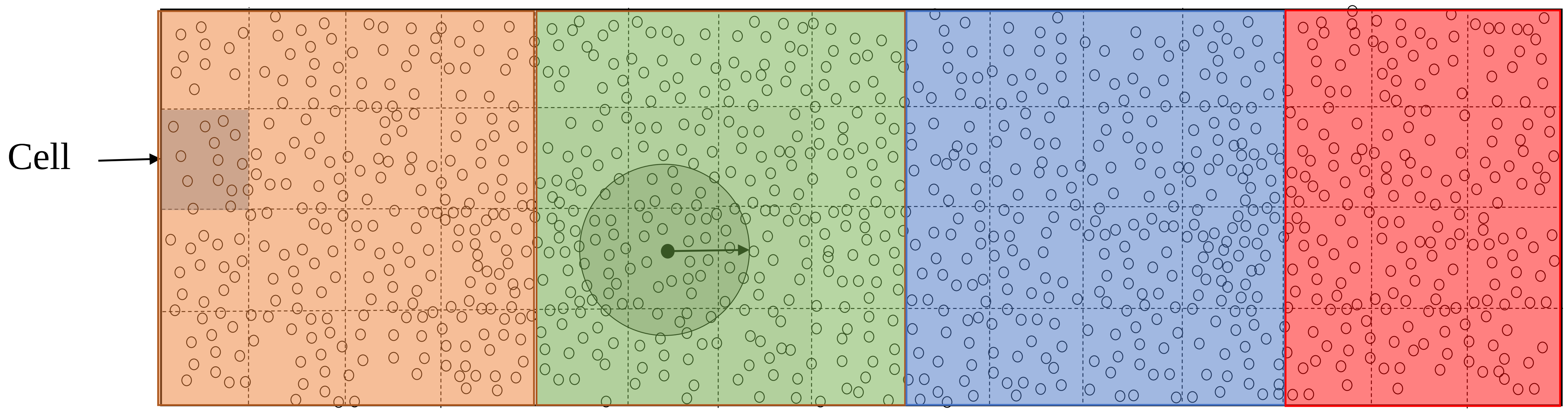
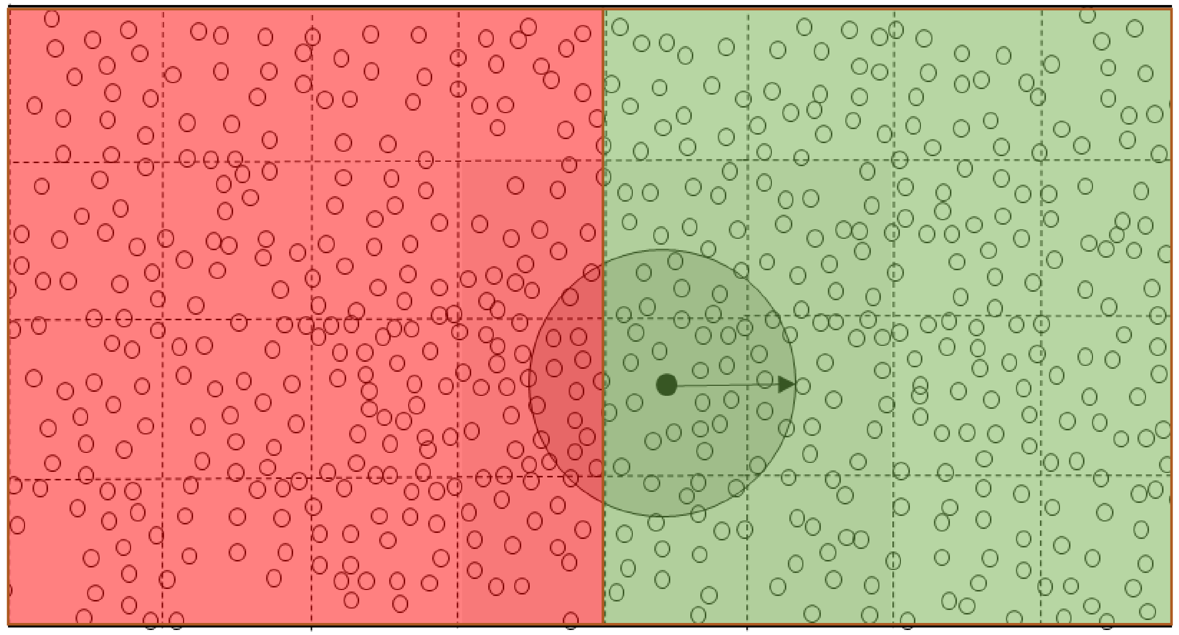
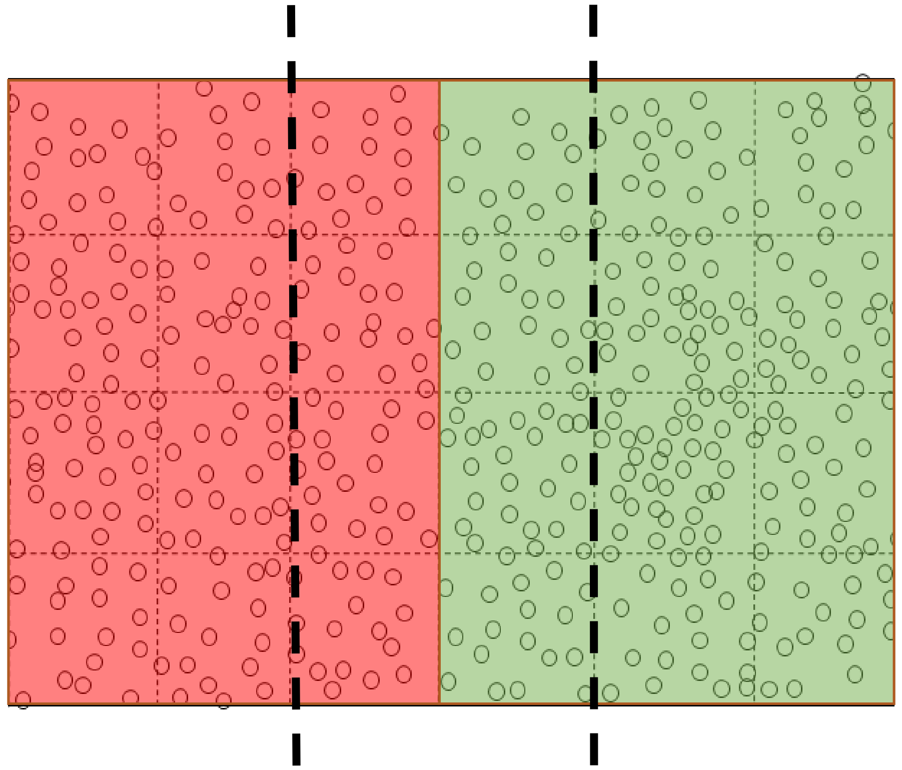


Halo Exchange





- Identify neighbouring particles in another process or particles moved from another process

- Transfer only the data of all potential neighbours

- Use a **halo** system for more efficiency[3]

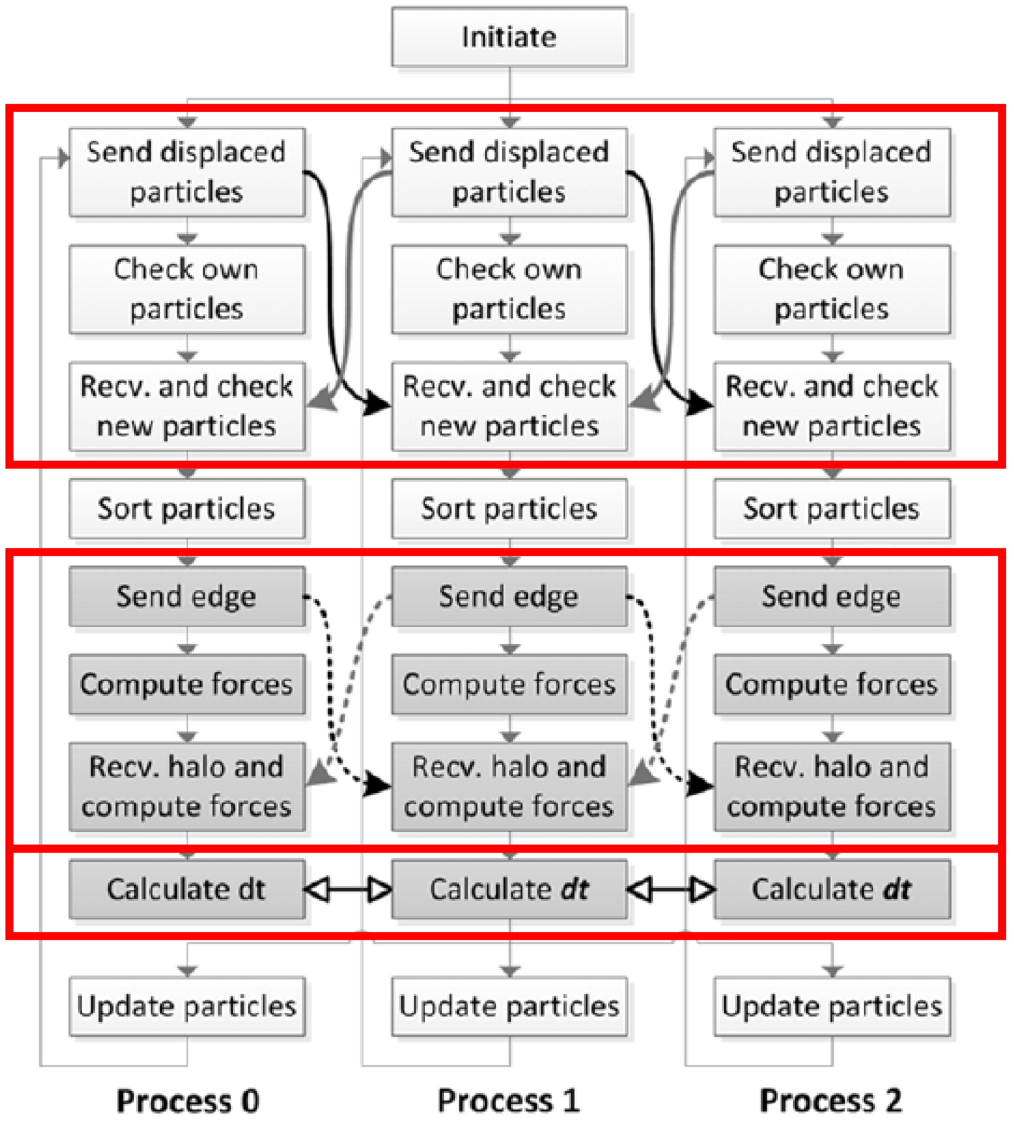
- Only data from the neighbouring slice (distance 2h) are transferred

- Edge particles form the **halo** of the subdomain

- Similar procedure on every subdomain border

Asynchronous Communications

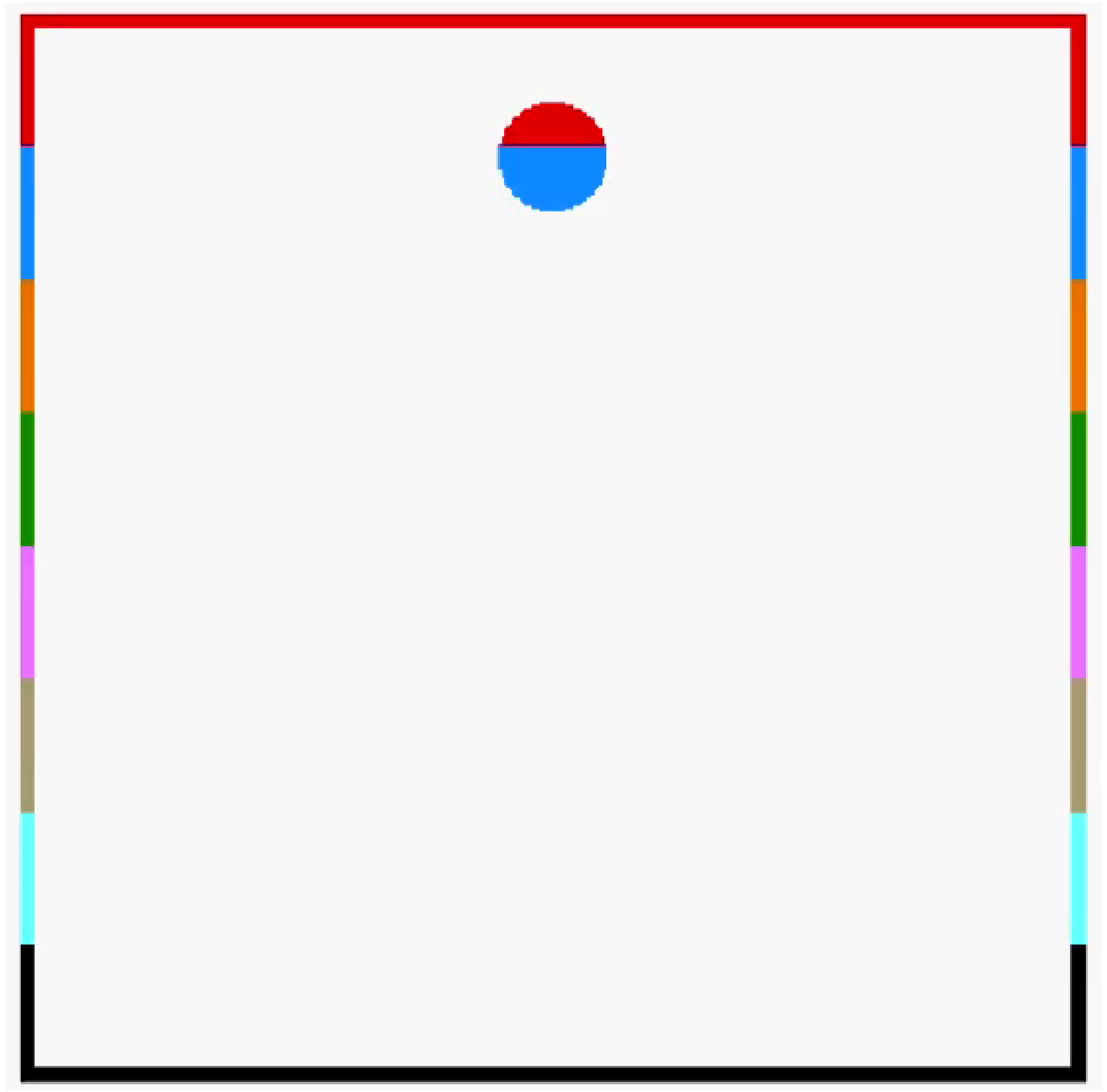
- Objective: Minimise waiting time for data transfer
- Neighbour list of interior particles processed while sending data of displaced particles
- Compute forces on interior particles while receiving halo data
- Processes synchronise when calculating the time step



(Dominguez et al. 2013)[2]

Results

- Execution for 8 processes
- Results identical to single-node DualSPHysics
- Results independent of the number of processes
- Portability: Code operates for both Windows and Linux in different processor architectures



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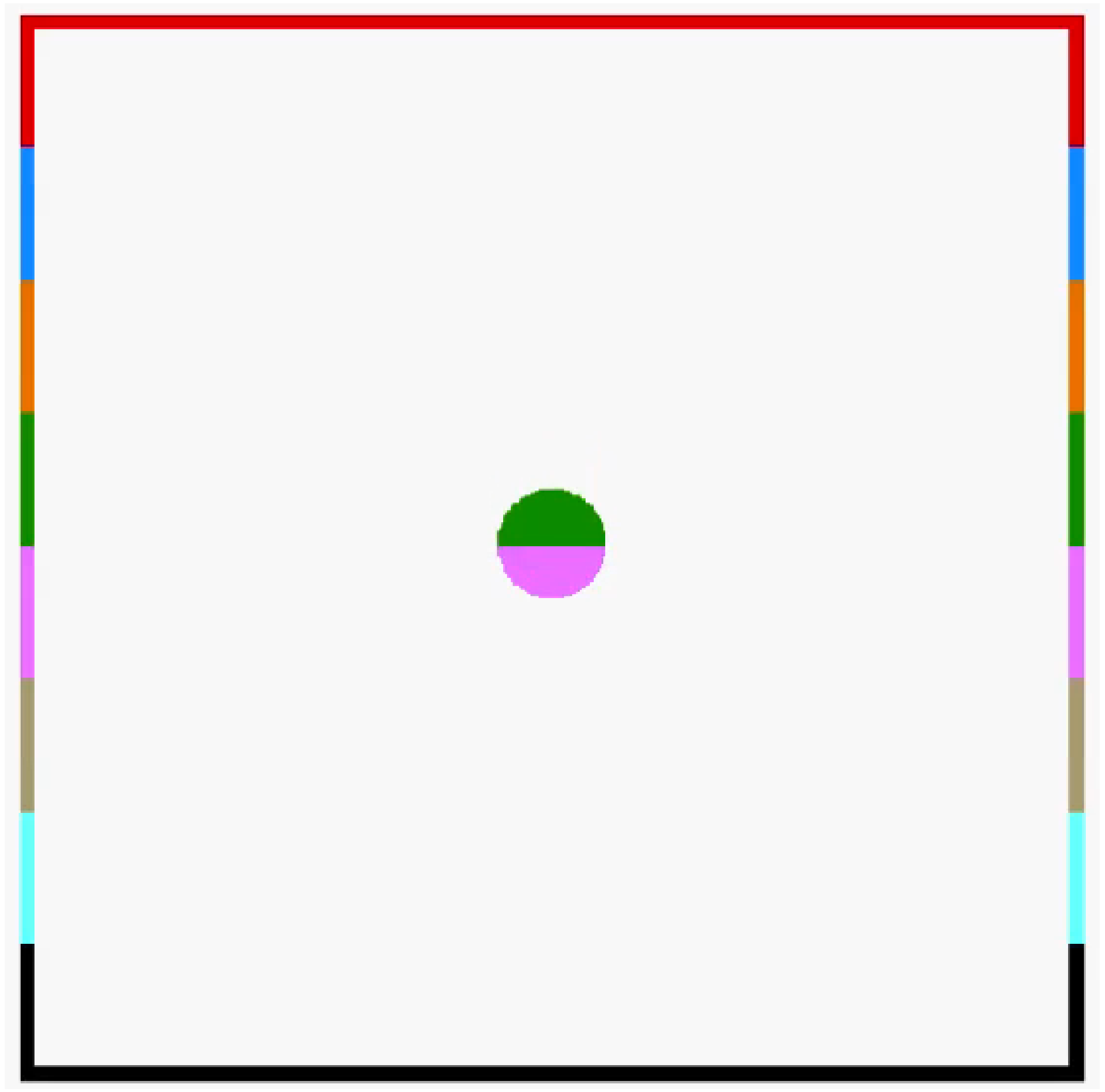

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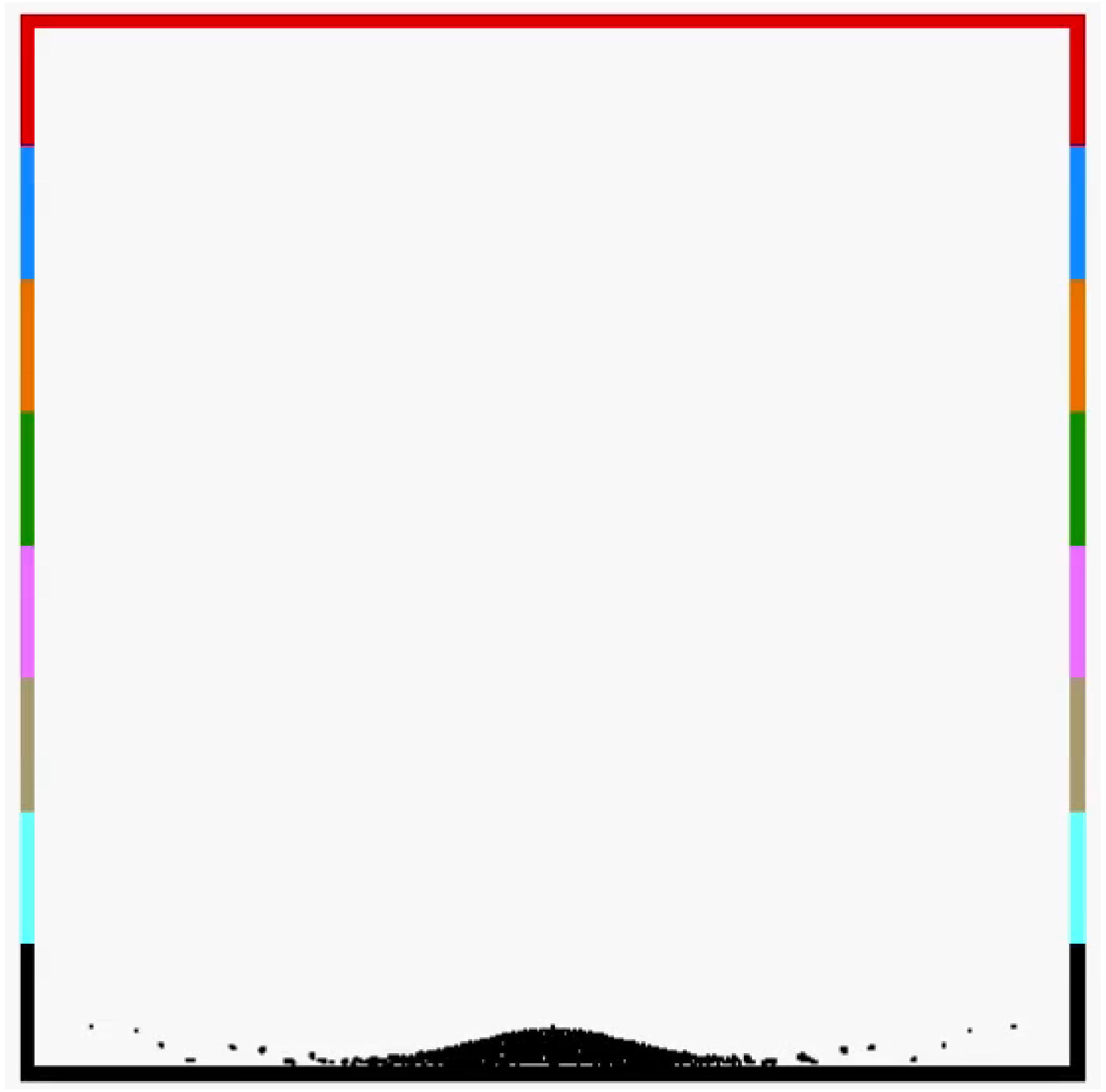
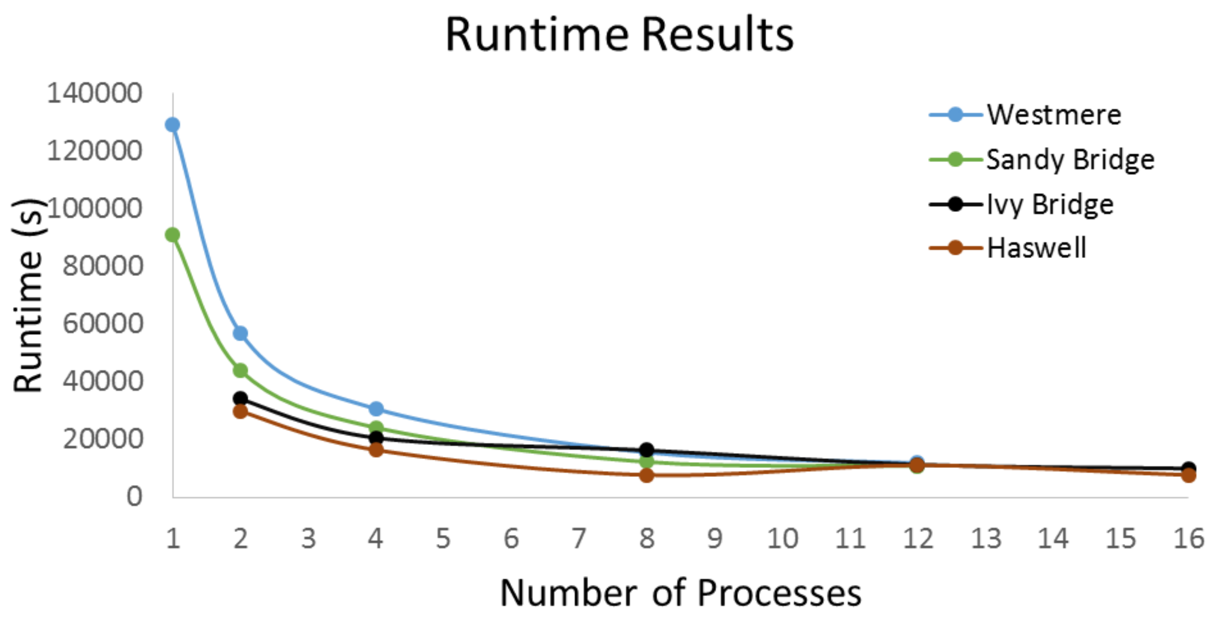


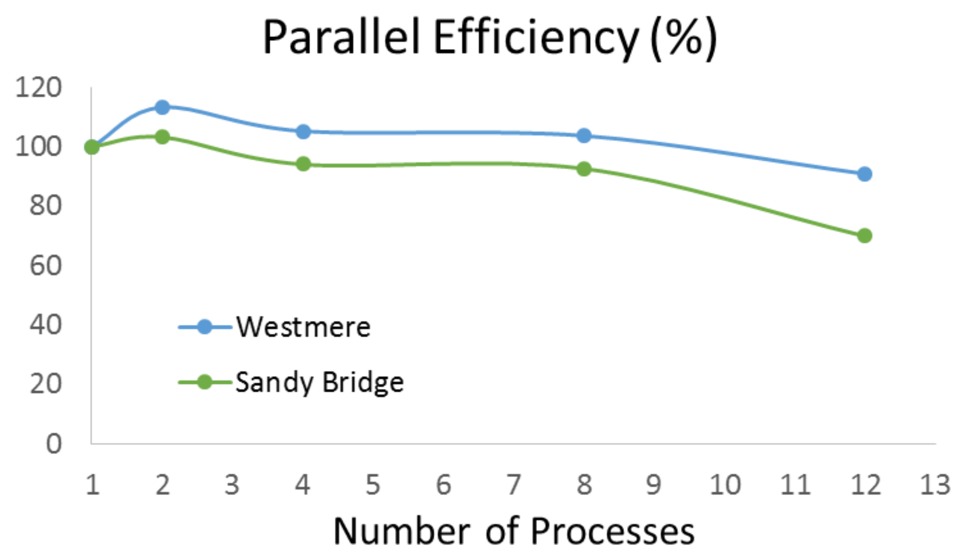
Runtime Results (small scale)

- Local execution for 1-16 processes
  - Westmere: Xeon X5650 - 2.66GHz (2x6-core)
  - Sandy Bridge: Xeon E5-2640 - 2.5GHz (2x6-core)
  - Ivy Bridge: Xeon E5-2650 v2 – 2.6GHz (2x8-core)
  - Haswell: Xeon E5-2690 v3 – 2.6GHz (2x12-core)

- Still Water case for 700,000 particles

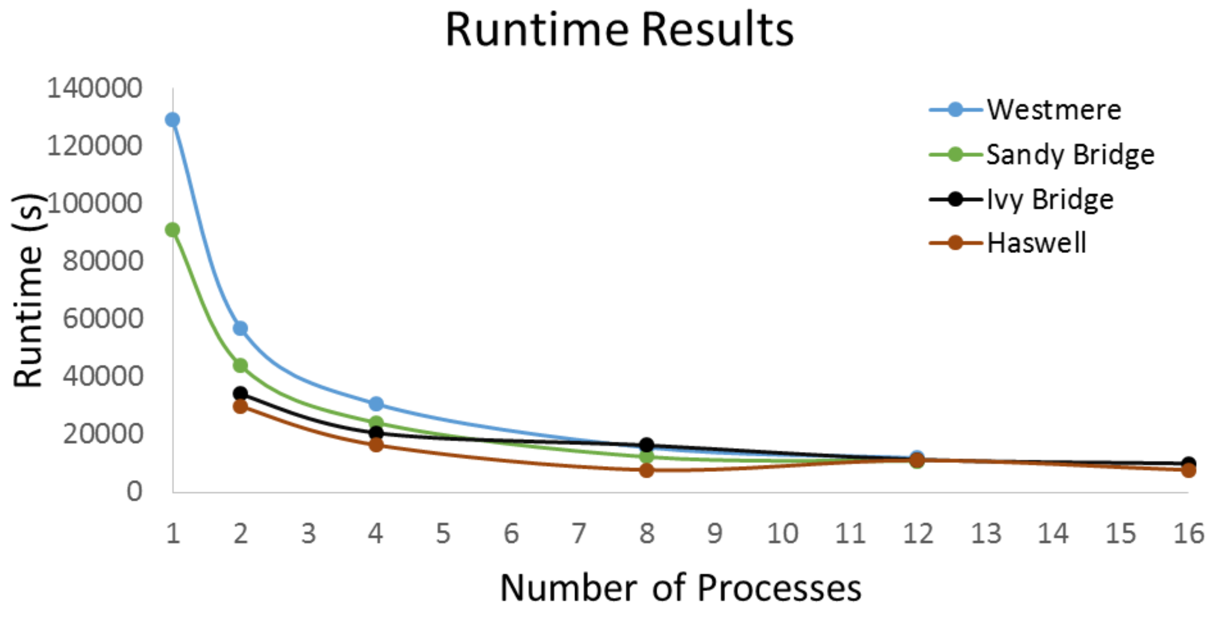
- Parallel Efficiency $$E_p = \frac{T_p}{pT_1} 100\%$$

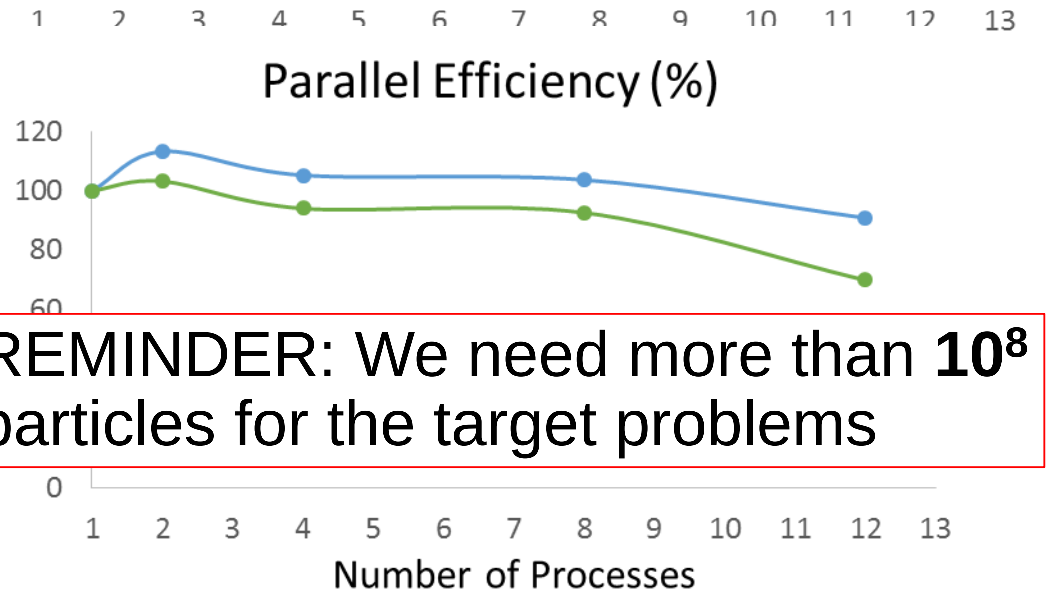




Scalability (small scale)

- Code can be further optimised
- Parallel Efficiency $$E_p = \frac{T_p}{pT_1} 100\%$$
- Scalability issues do not allow efficient computation with ~100 processes
- 1D decomposition not scalable
- No load balancing

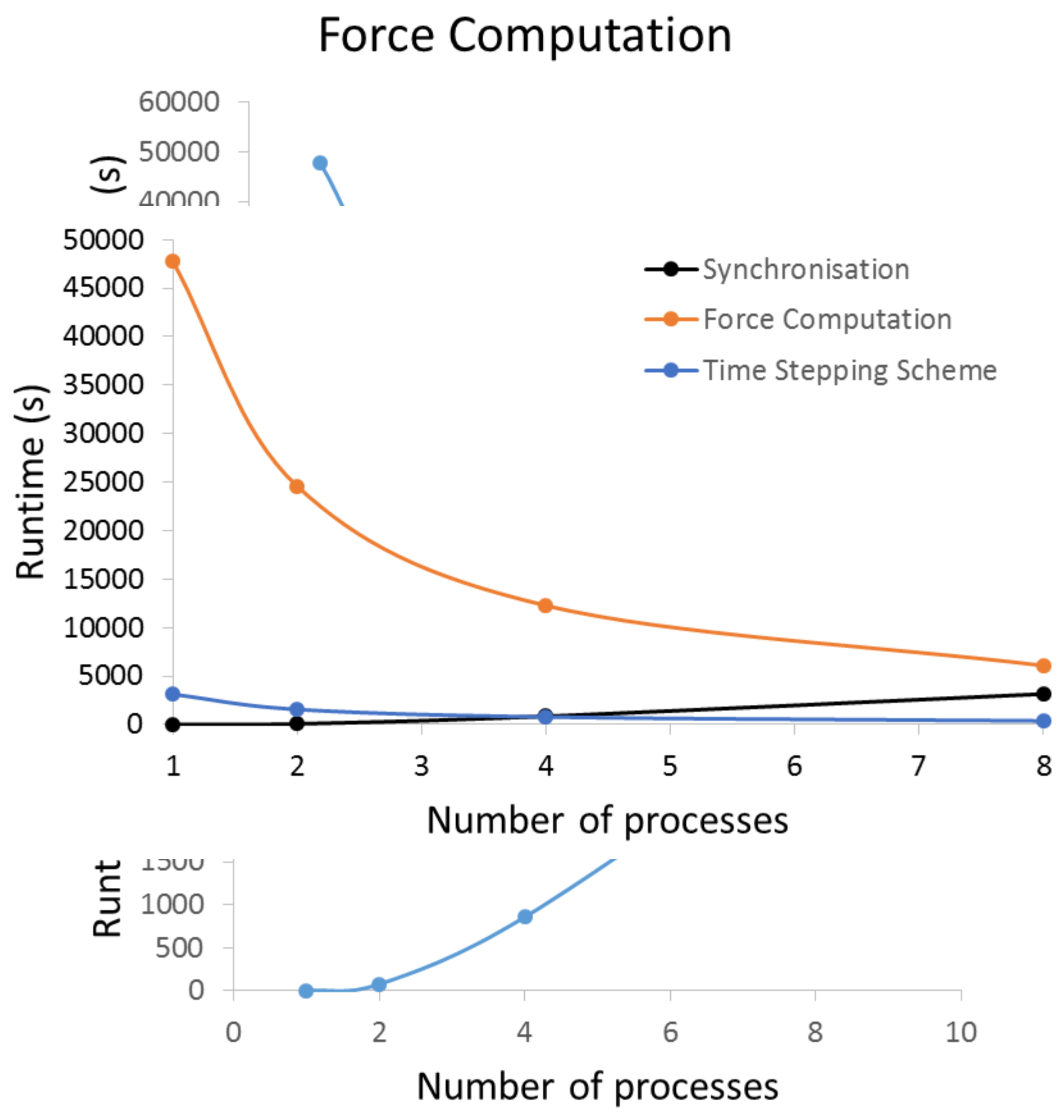




REMINDER: We need more than **10^8** particles for the target problems

Runtime Results (small scale)

- Local execution for 8 processes
  - Intel Xeon E5507 at 2.27GHz
- Still Water case for 160,000 particles
- Synchronisation at the end of the time step slows the computation
- Current implementation : *MPI_Allreduce*



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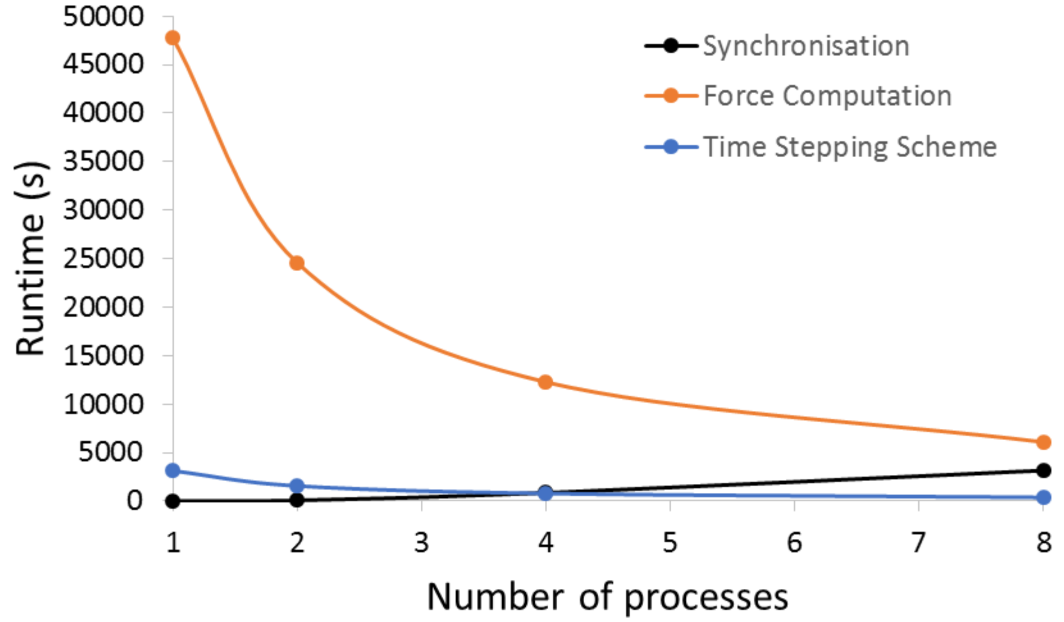
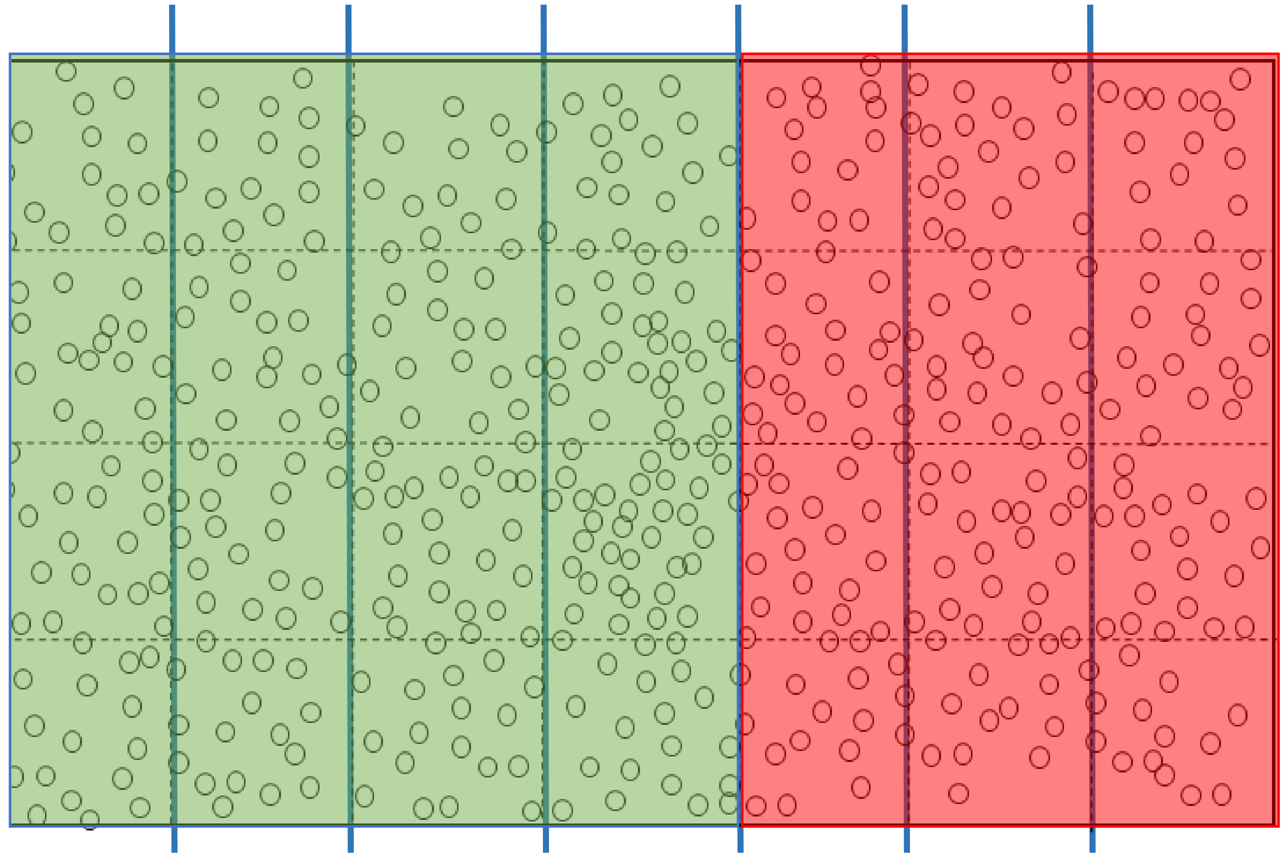


Dynamic Load Balancing

- Processes do not have the same workload (number of particles, inter-particle forces)
- Dynamic simulations – workload of each process changes constantly
- Options:
  1. Same number of particles
  2. Same execution time
- Option 1 is simpler to enforce
- Option 2 has higher potential but difficult to enforce



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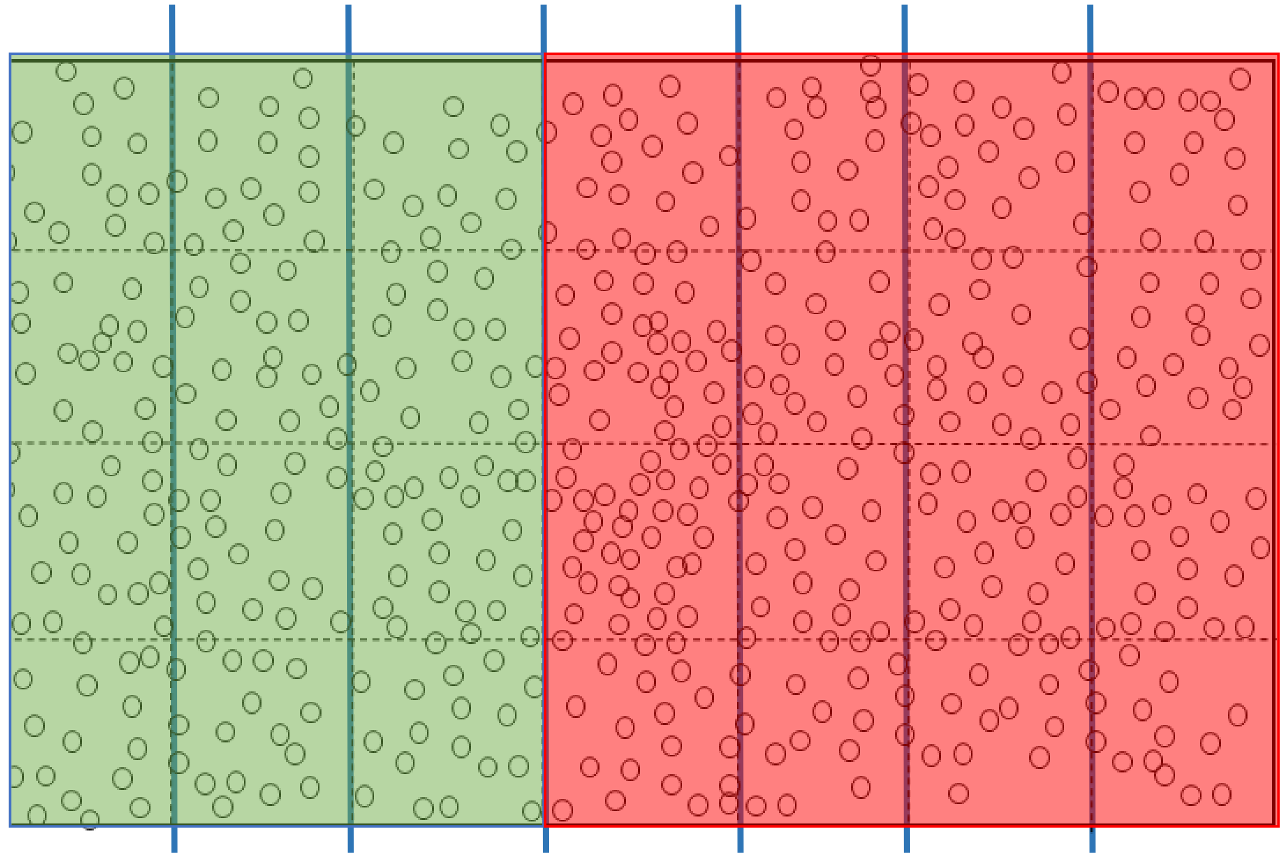
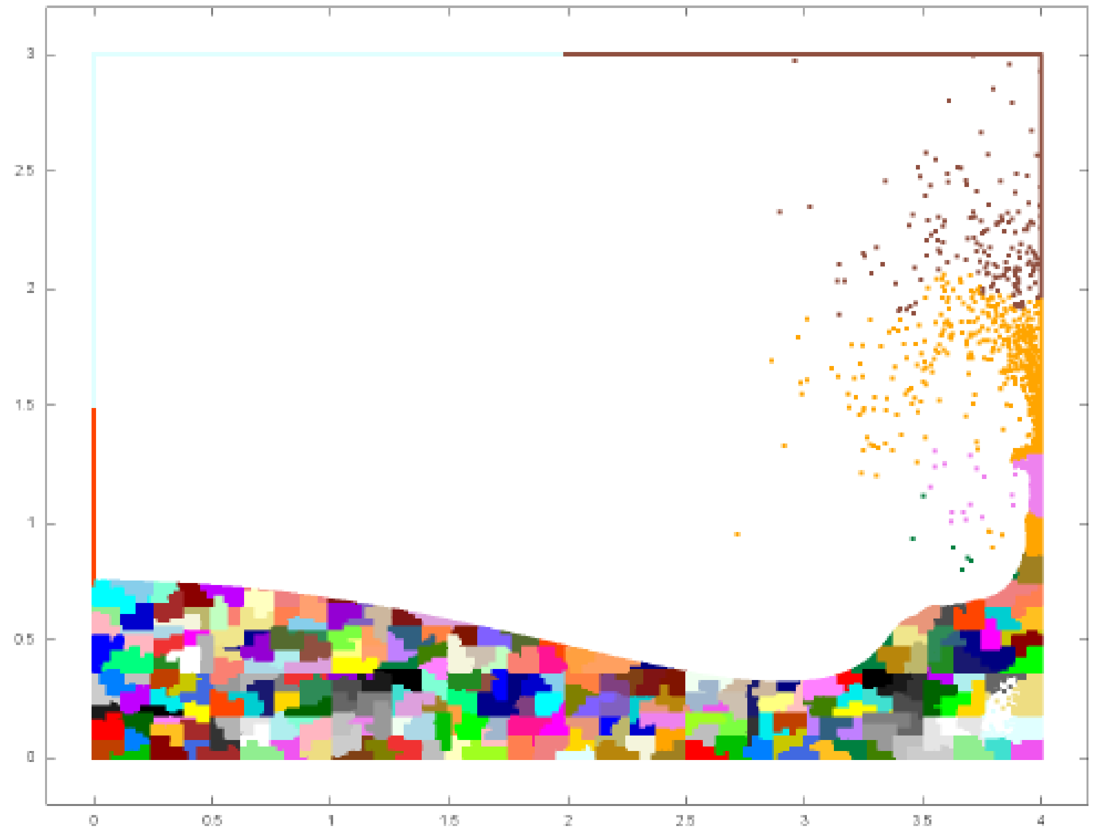


The Zoltan Library

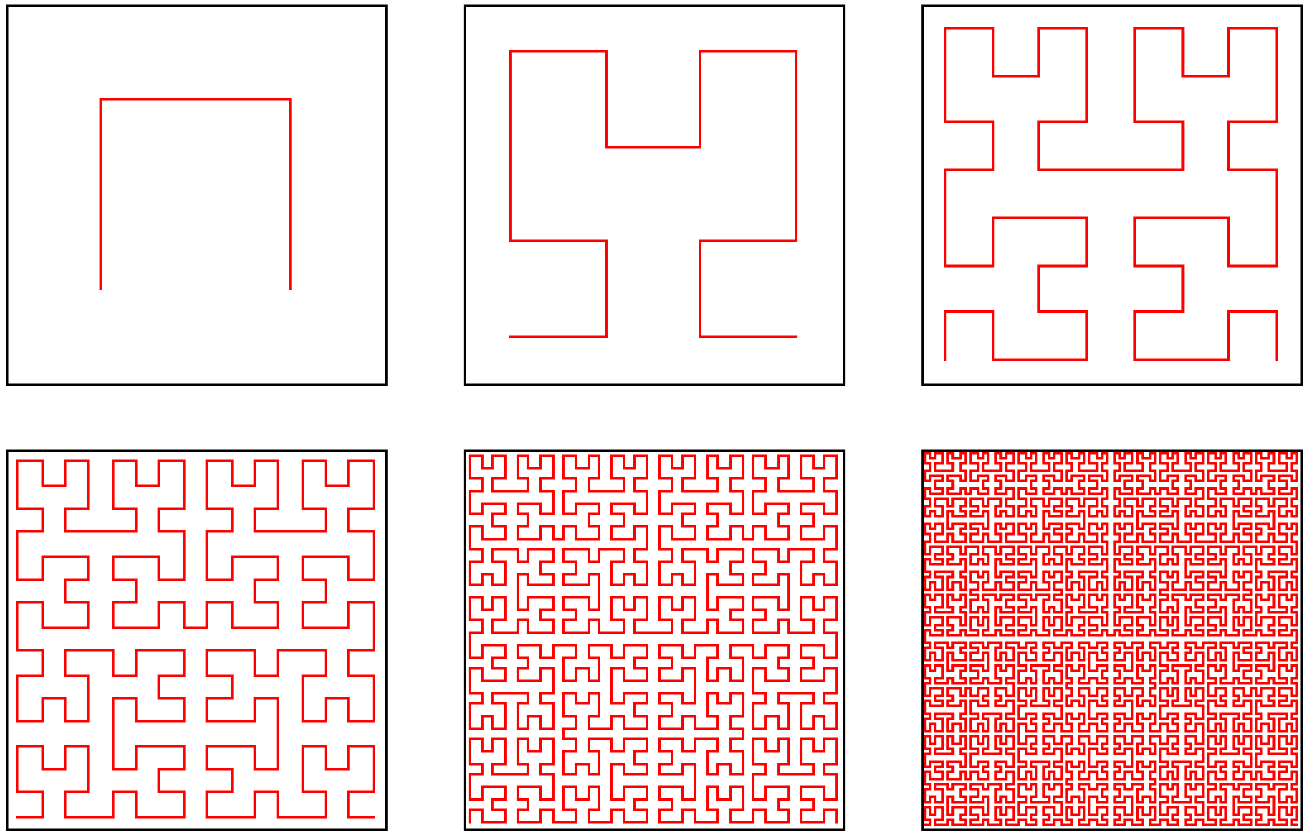
- Use of the Zoltan data management library[4]
- Library for the development and optimization of parallel, unstructured and adaptive codes
- Scalable up to 10^6 cores[4]
- Includes a suite of spatial decomposition and dynamic load balancing algorithms and an unstructured communication package
- Geometric Decomposition Algorithm:
  Hilbert Space Filling Curve (HSFC)



Dambreak at 1.1s for 256 partitions[5]

Hilbert Space Filling Curve

- A continuous fractal space-filling curve (containing the entire 2D unit square)
- Maps 2D and 3D points to a 1D curve
- Maintains spatial locality
- Already used for SPH[5]
- Irregular subdomain shapes (increased complexity of data transfer)



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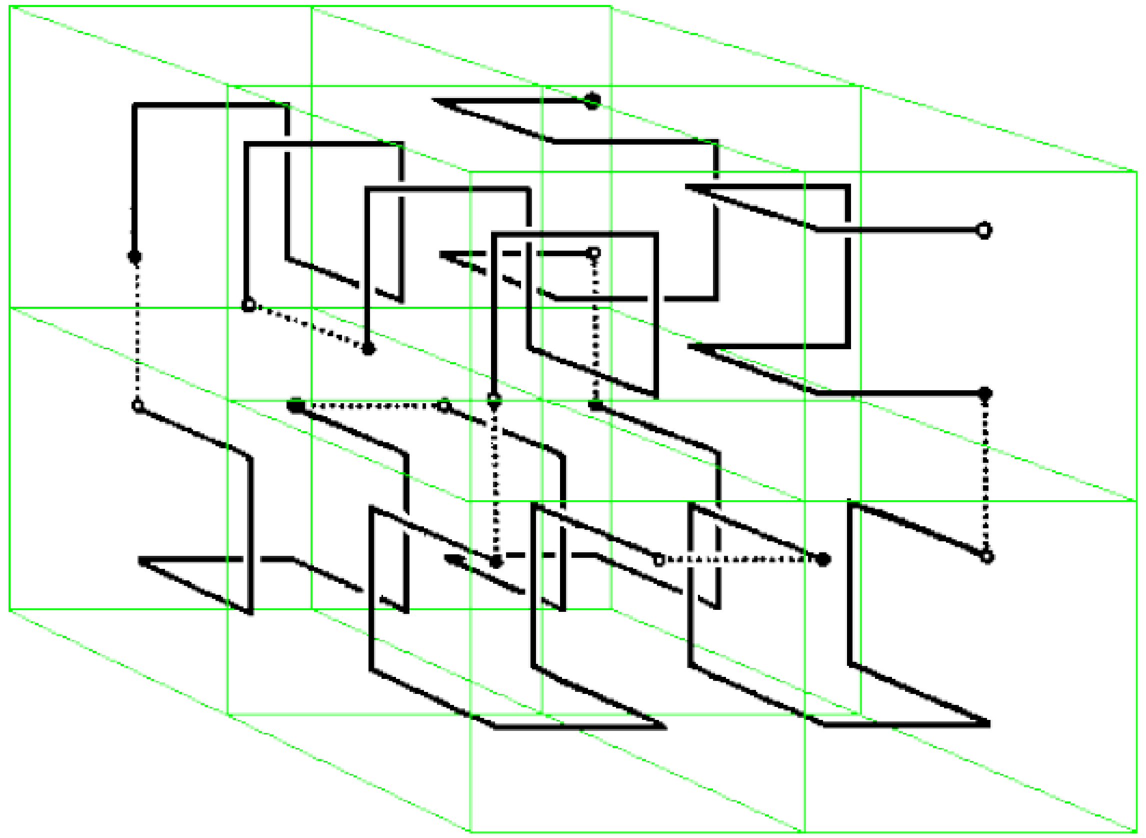
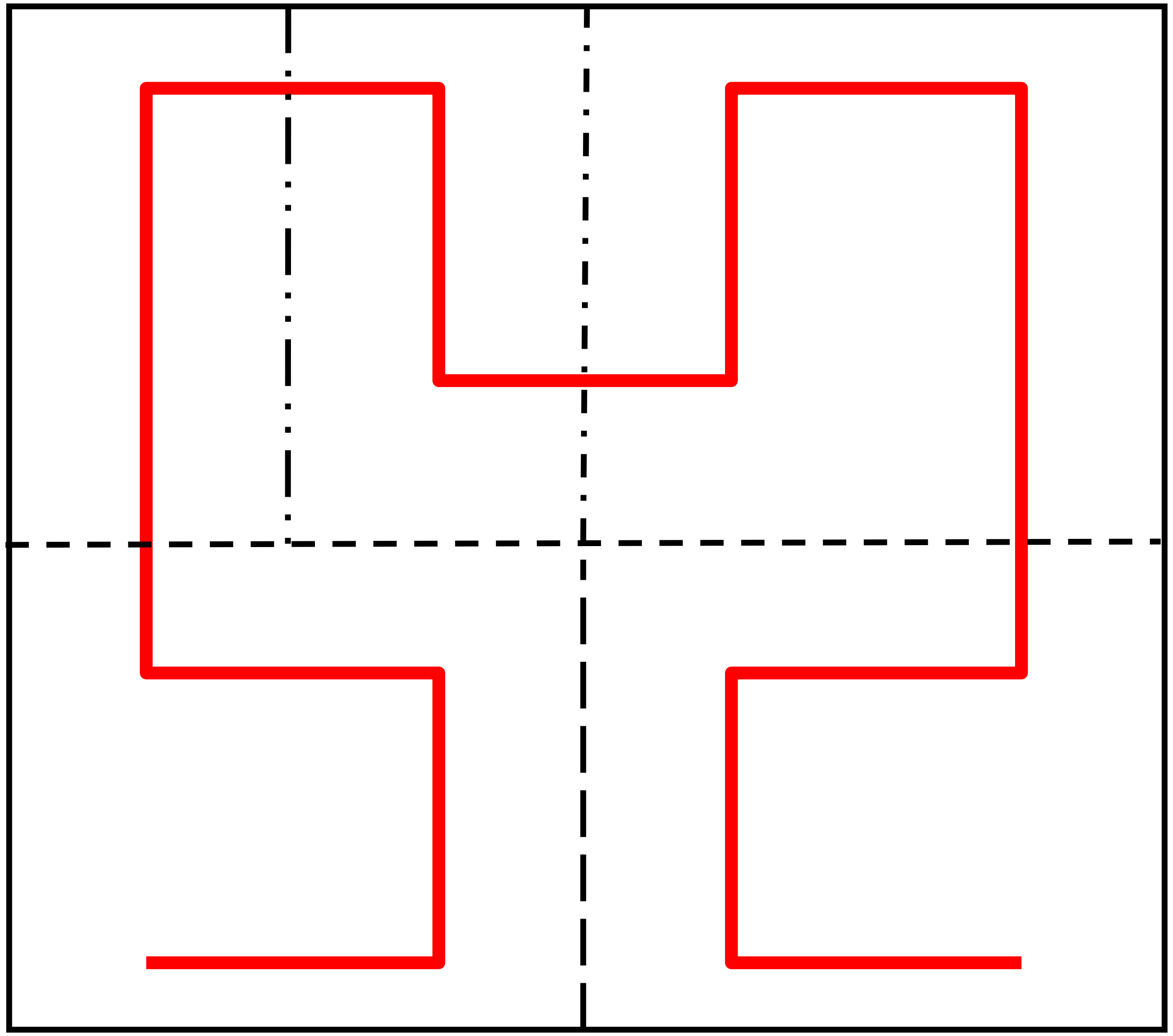


Guo et al. (2015)[7]

HSFC Algorithm

- HSFC maps cells on a 1D curve into the interval [0,1]
- Divides the curve into N ‘bins’ where N is larger than the amount of processes
- Sums bin weights from starting point, cutting off whenever the desired weight is reached
- Bins containing a cutting off point are further refined until the desired balance is achieved



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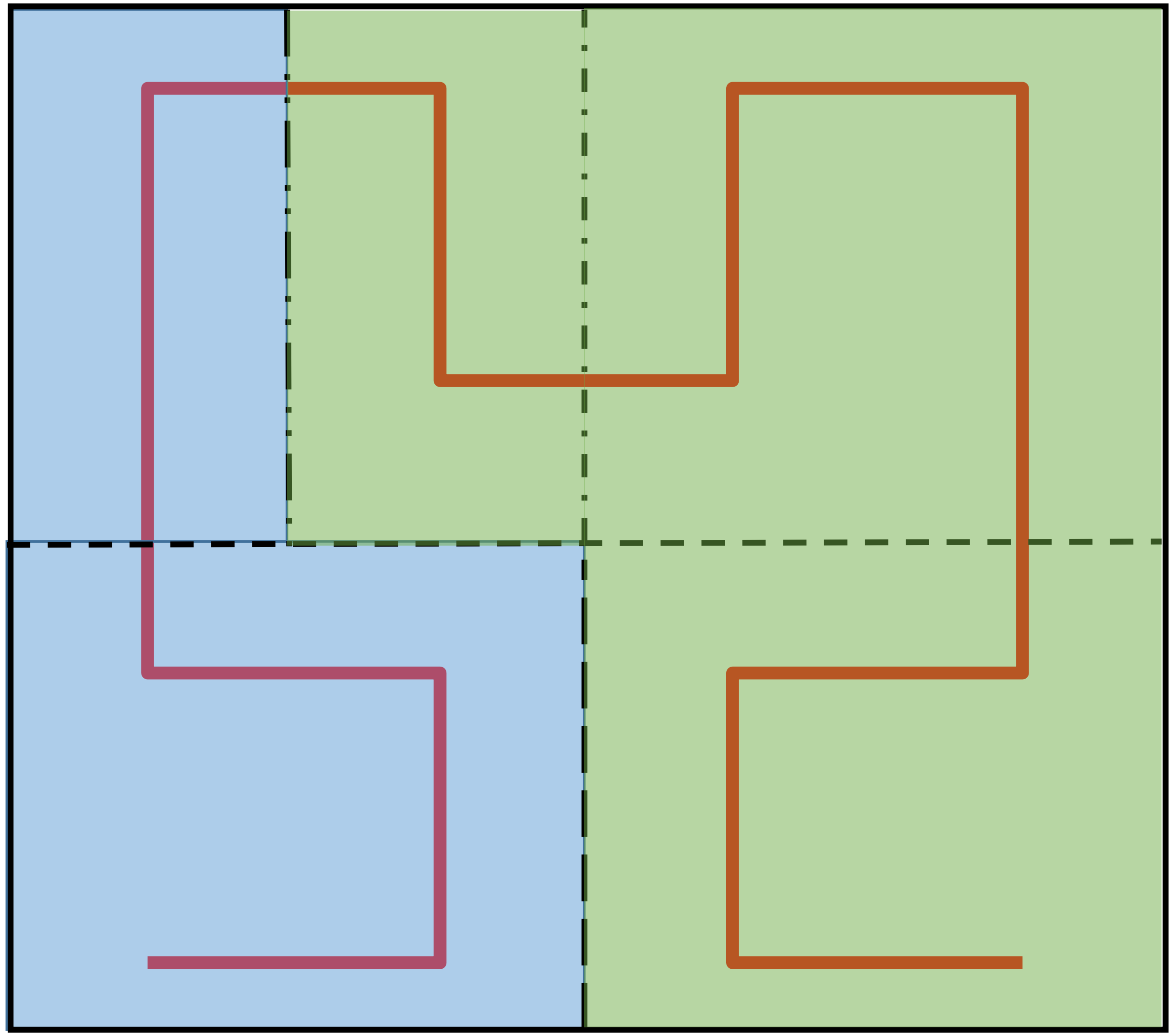


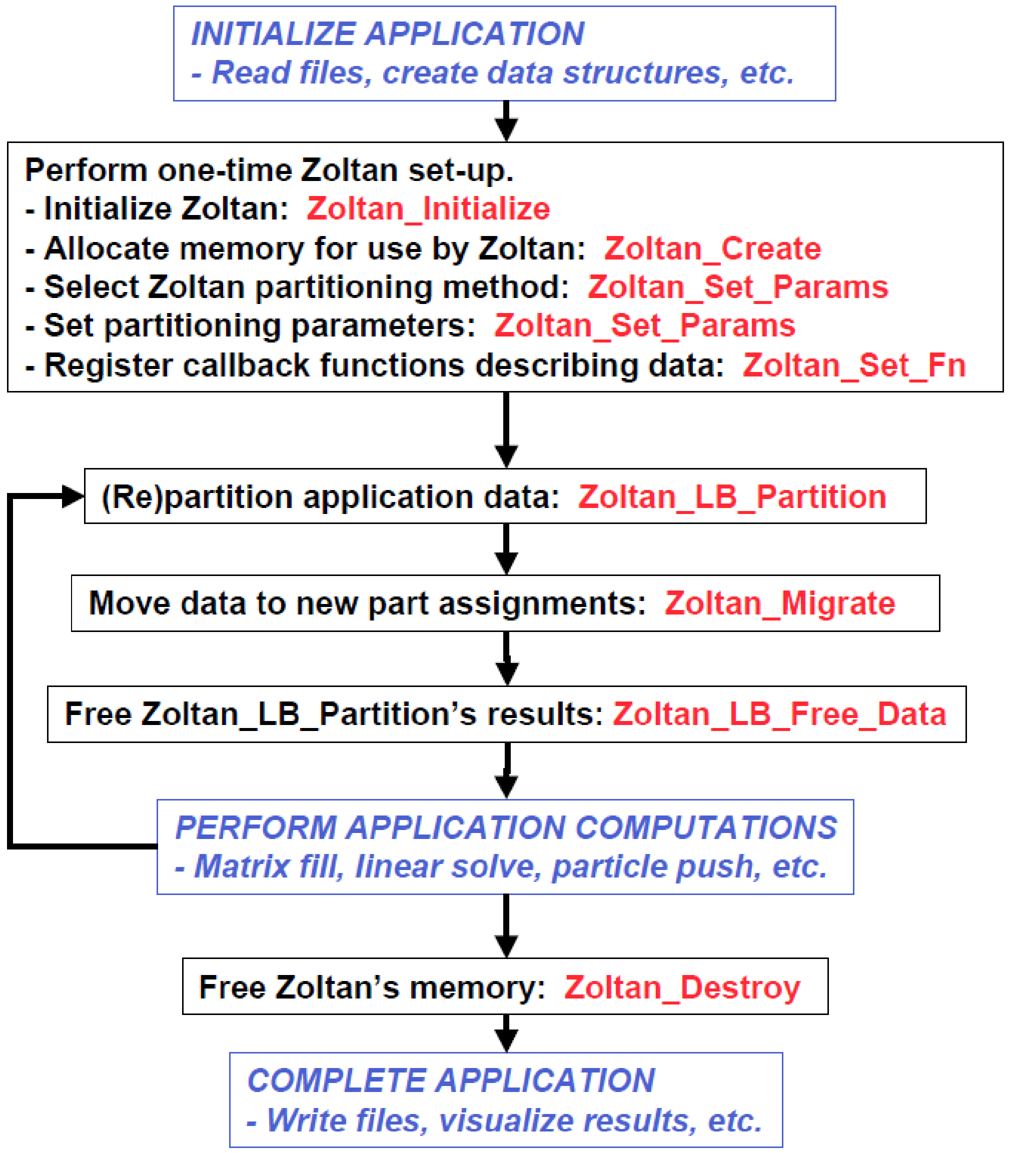
Using Zoltan in DualSPHysics

- Domain Decomposition and Load Balancing through Zoltan

- Main Partitioning Parameter: Cells
  - Significantly smaller number than particles
  - Allow for load balancing
  - Position does not change

- Load Balancing through Cell Weights
  - Based on particle number[5] (Current)
  - Based on execution time

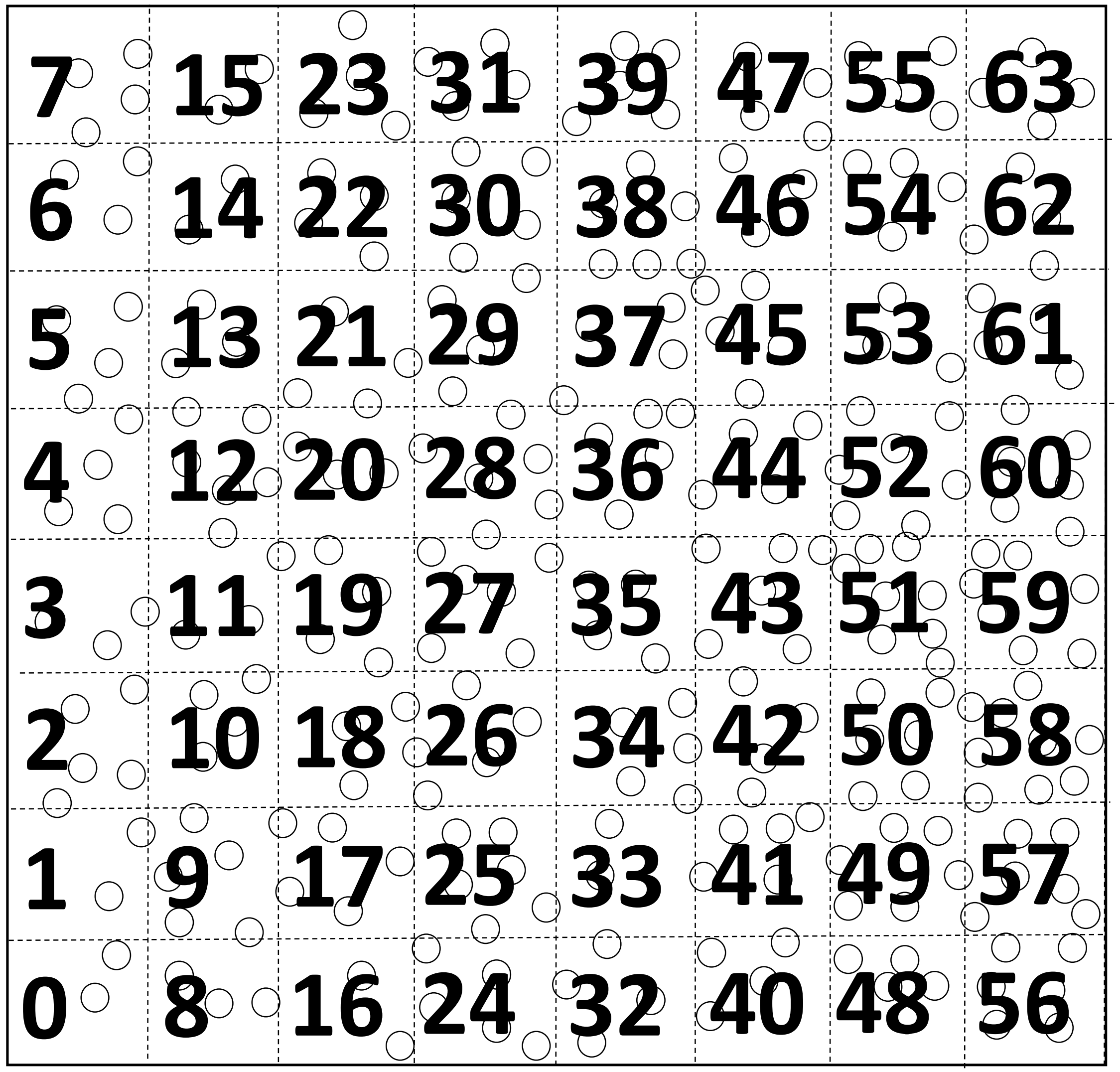
- Automatic migration through Zoltan_Migrate
  - Low complexity of data transferred


INITIALIZE APPLICATION
- Read files, create data structures, etc.
Perform one-time Zoltan set-up.
- Initialize Zoltan: Zoltan_Initialize
- Allocate memory for use by Zoltan: Zoltan_Create
- Select Zoltan partitioning method: Zoltan_Set_Params
- Set partitioning parameters: Zoltan_Set_Params
- Register callback functions describing data: Zoltan_Set_Fn
(Re)partition application data: Zoltan_LB_Partition
Move data to new part assignments: Zoltan_Migrate
Free Zoltan_LB_Partition's results: Zoltan_LB_Free_Data
PERFORM APPLICATION COMPUTATIONS
- Matrix fill, linear solve, particle push, etc.
Free Zoltan's memory: Zoltan_Destroy
COMPLETE APPLICATION
- Write files, visualize results, etc.

Devine et al. (2009)[4]

Using Zoltan in DualSPHysics

- New arrays created:
  - Global Cell ID
  - Local Cell ID
  - Cell Coordinates
  - Cell Weights
- Each process only holds local data
- Example: Domain divided in 64 cells containing 285 particles
- Initial domain split by 1D decomposition (Slices)



Global Cell ID

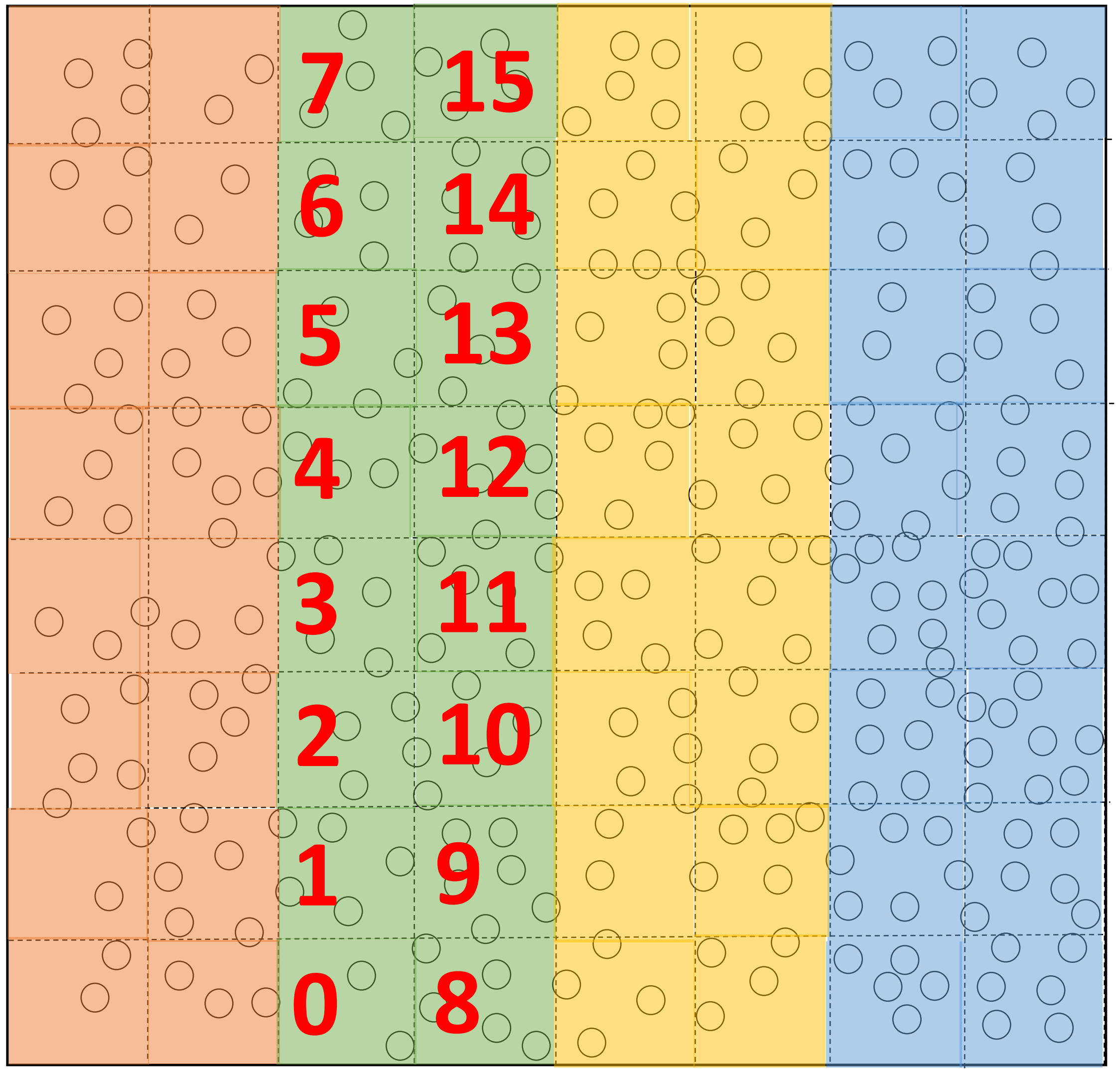
Using Zoltan in DualSPHysics

- New arrays created:
  - Global Cell ID
  - Local Cell ID
  - Cell Coordinates
  - Cell Weights

- Each process only holds local data

- Example: Domain divided in 64 cells containing 285 particles

- Initial domain split by 1D decomposition (Slices)



Local Cell ID

Using Zoltan in DualSPHysics

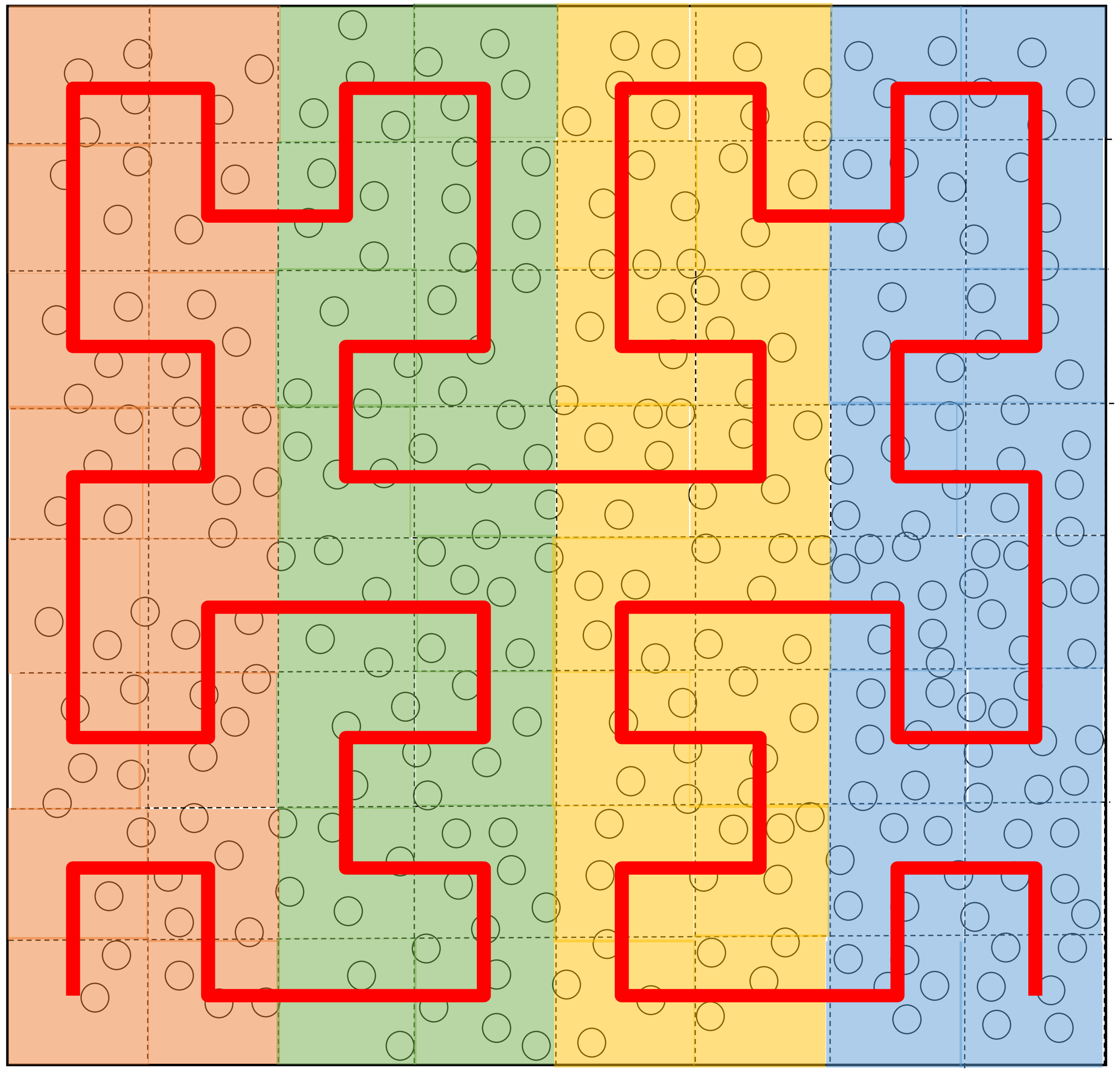
- Cell weights[5]: $w_C = \dfrac{N_{pc}}{N_{pt}}$

- Data is sent to Zoltan

- HSFC algorithm is applied

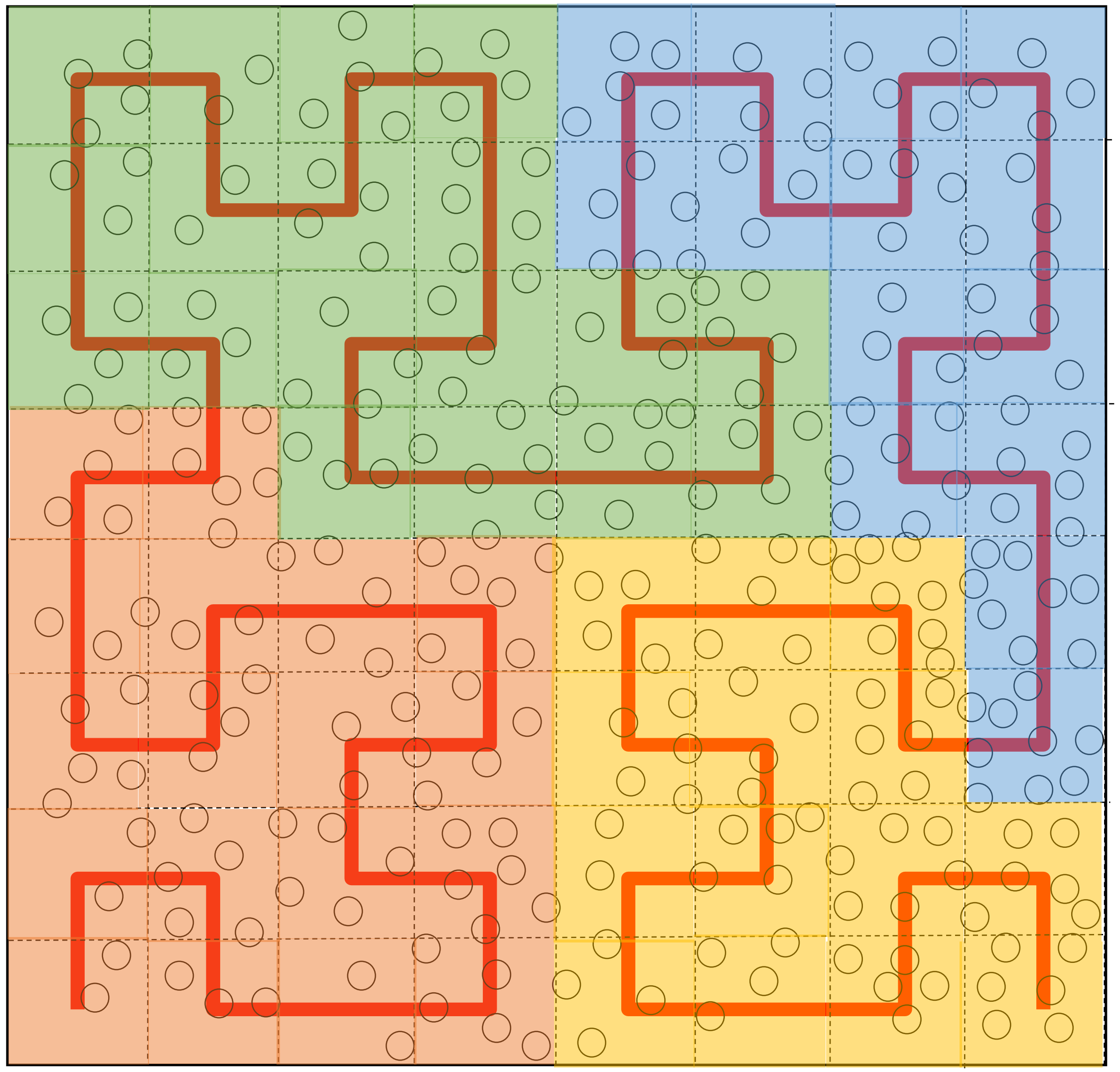
- Zoltan Output:
  - Global Cell IDs of imported cells
  - Global Cell IDs of exported cells
  - Destination process

- Cell data automatically migrated using AUTO_MIGRATE option



Using Zoltan in DualSPHysics

- GlobalCellID is updated:
  - Exported cells removed
  - Imported cells added
- Particles are also imported and exported
- Data reordered creating new cell-linked neighbour list
- LocalCellID is updated
- Algorithm applied only when imbalance exceeds 20%



Particle Mapping

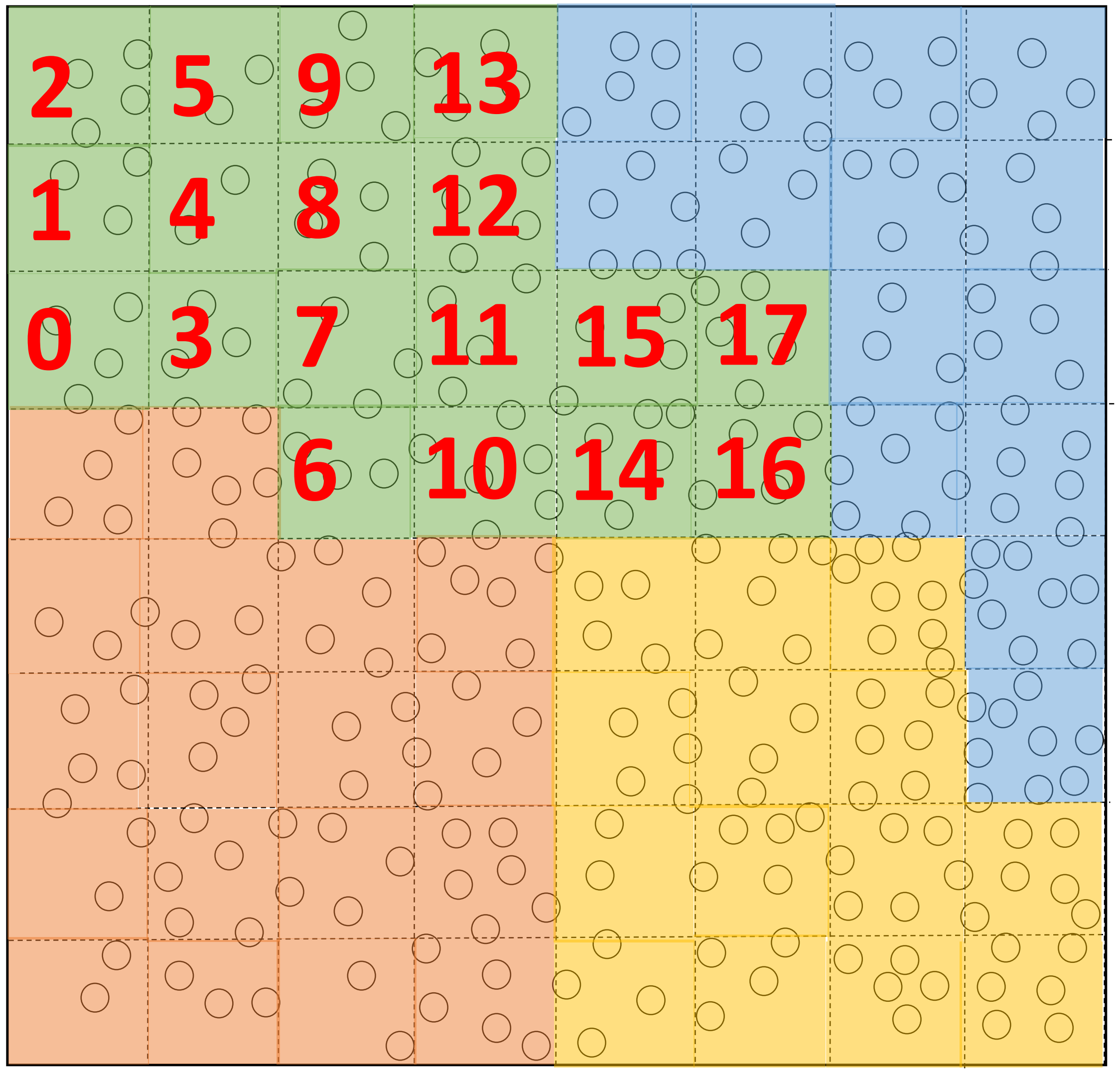
- Connection between cells and particles needed
- Existing DualSPhysics array: **CellPart**
- CellPart can be easily mapped on LocalCellID
- LocalCellID acts as intermediary between CellPart and GlobalCellID

If N_c number of local cells

$$\begin{tikzcd}
\begin{array}{c}\text{CellPart}\\(2N_c+5)\end{array} \arrow[r, Leftrightarrow] & \begin{array}{c}\text{LocalCellID}\\(N_c)\end{array} \arrow[r, Leftrightarrow] & \begin{array}{c}\text{GlobalCellID}\\(N_c)\end{array}
\end{tikzcd}$$

Particle Reordering

- Particles need reordering to maintain local spatial locality
- Currently, particle data reordered using single node algorithm
- Same for LocalCellID – allows mapping to Cellpart
- GlobalCellID is constant
- Better option: reorder along HSFC path[5]



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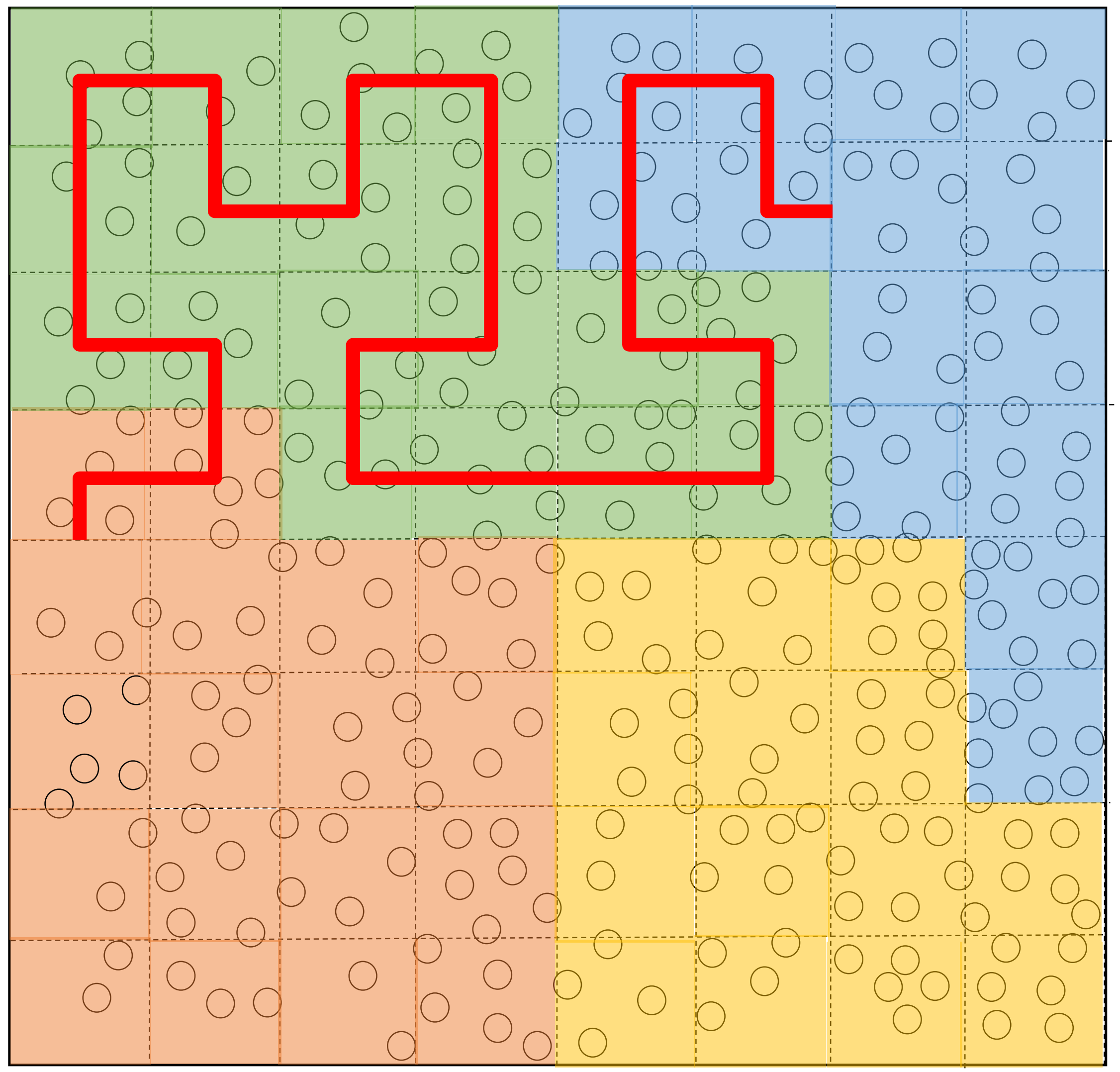

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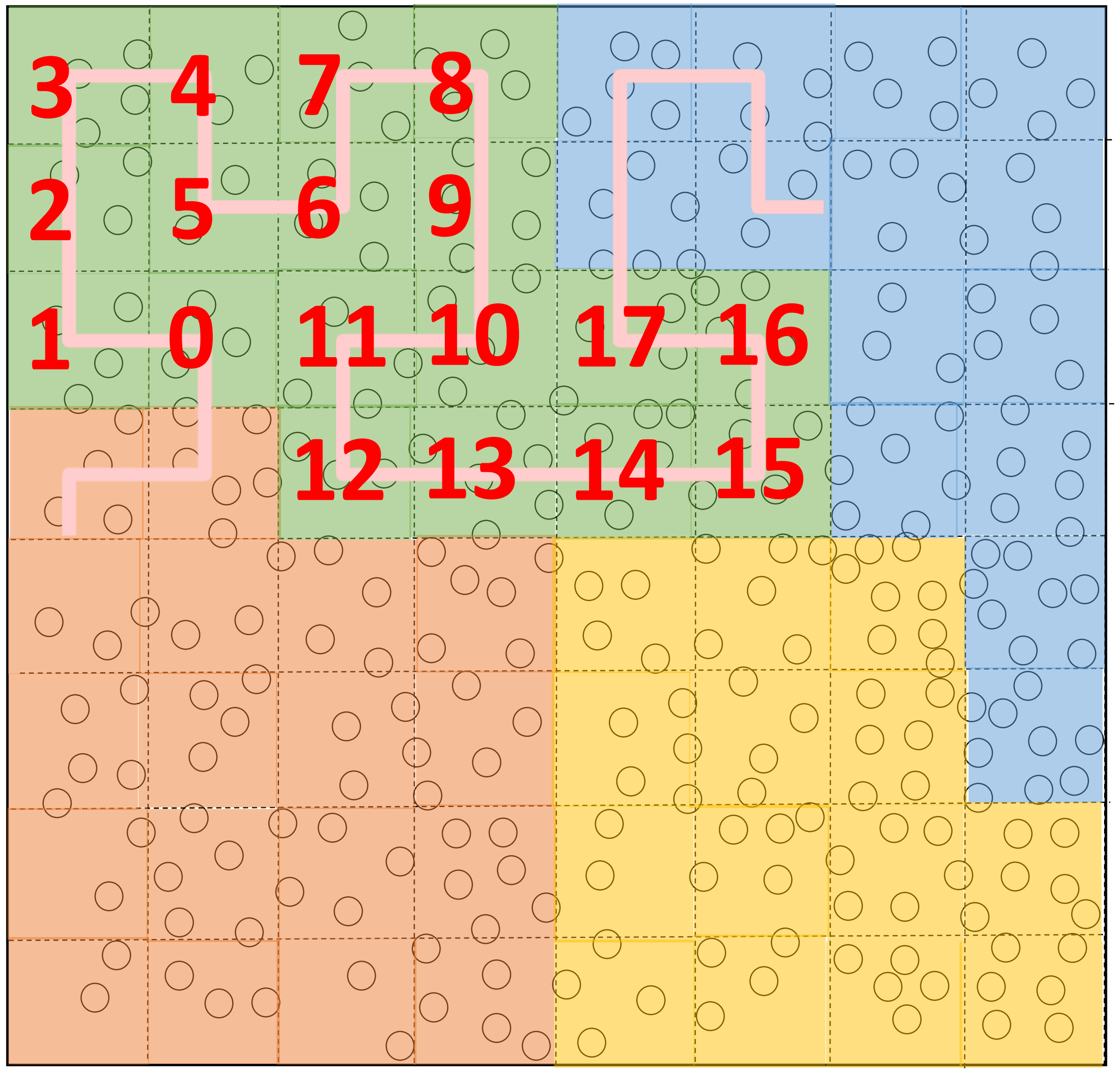
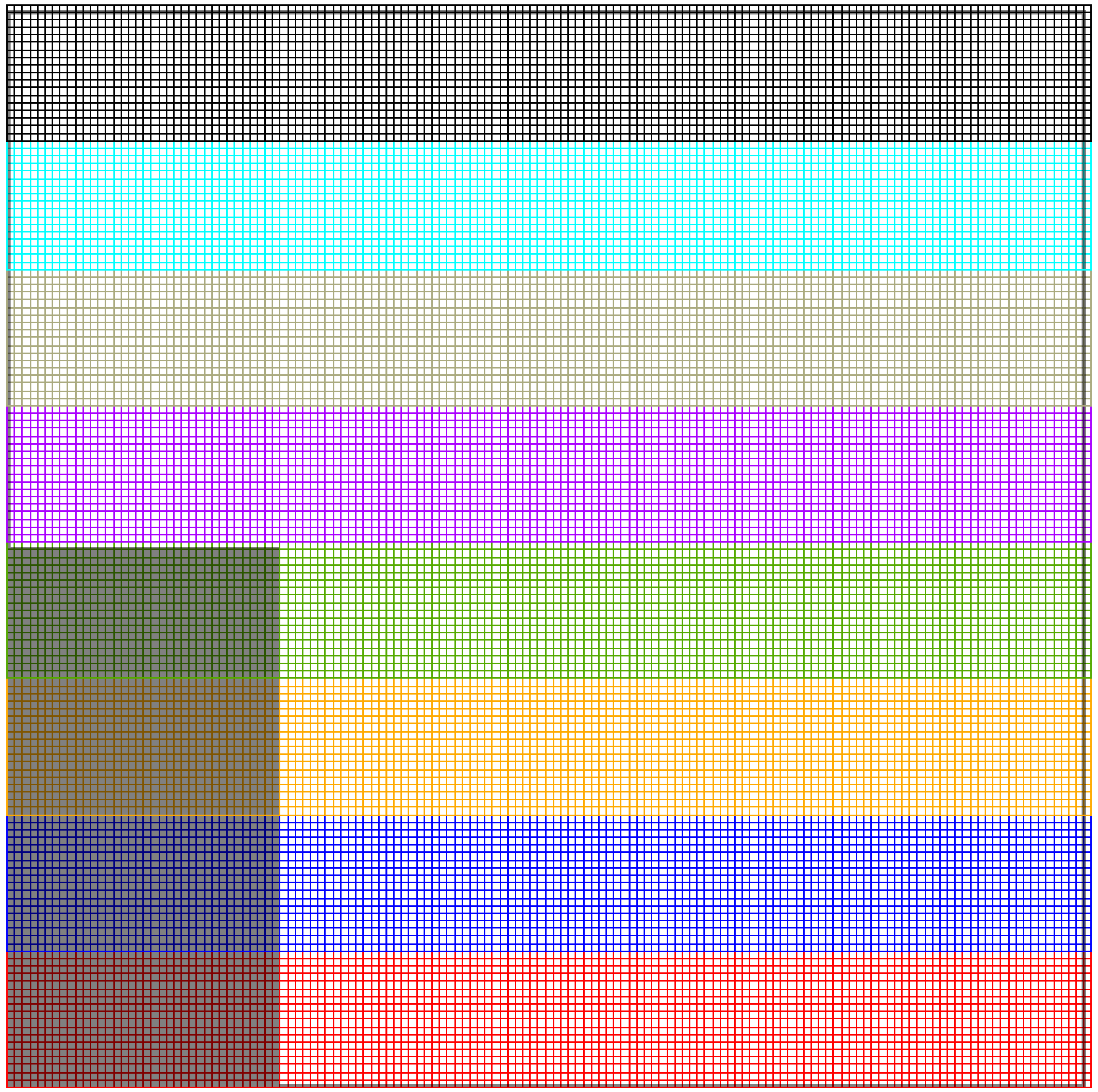
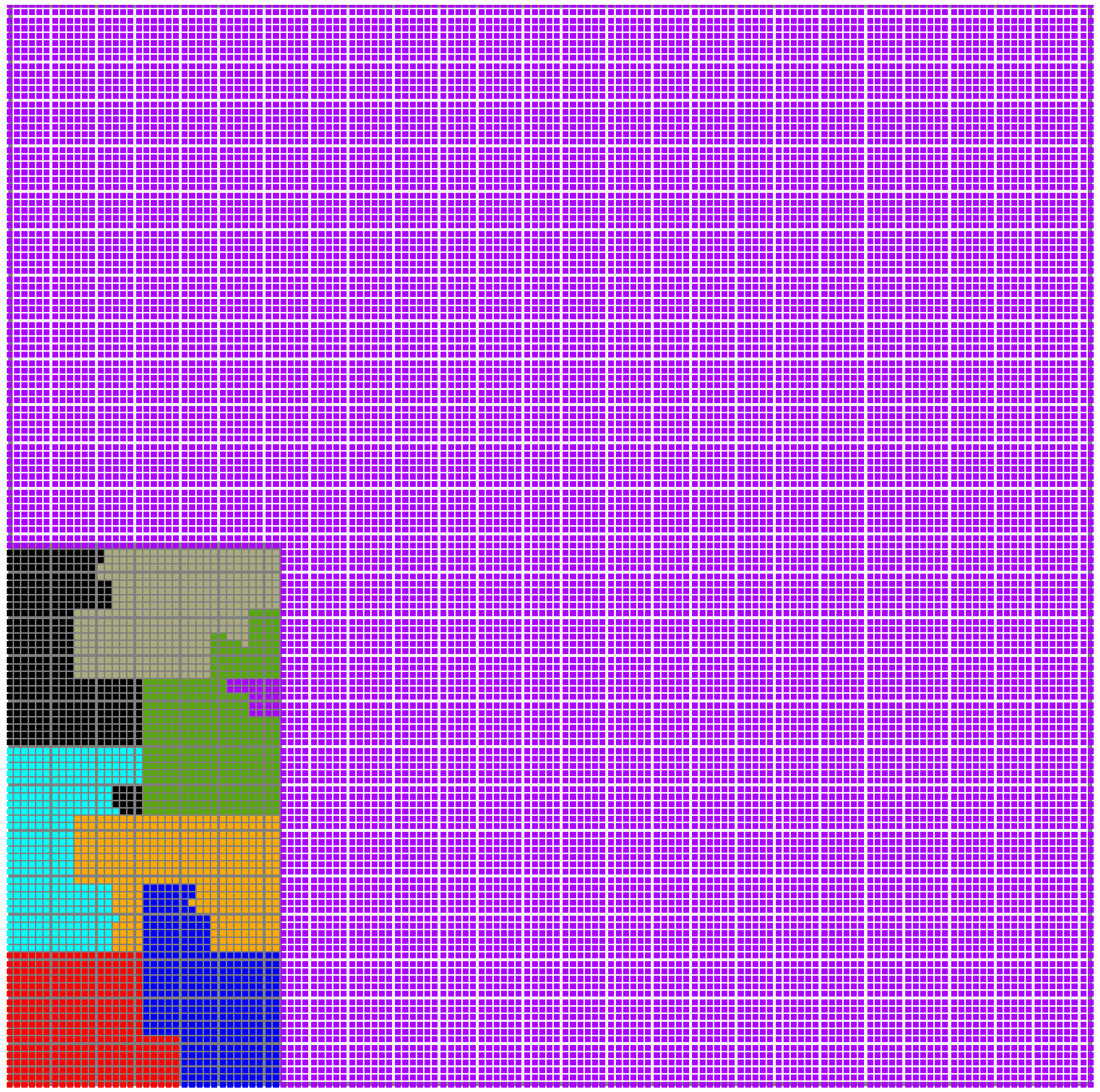
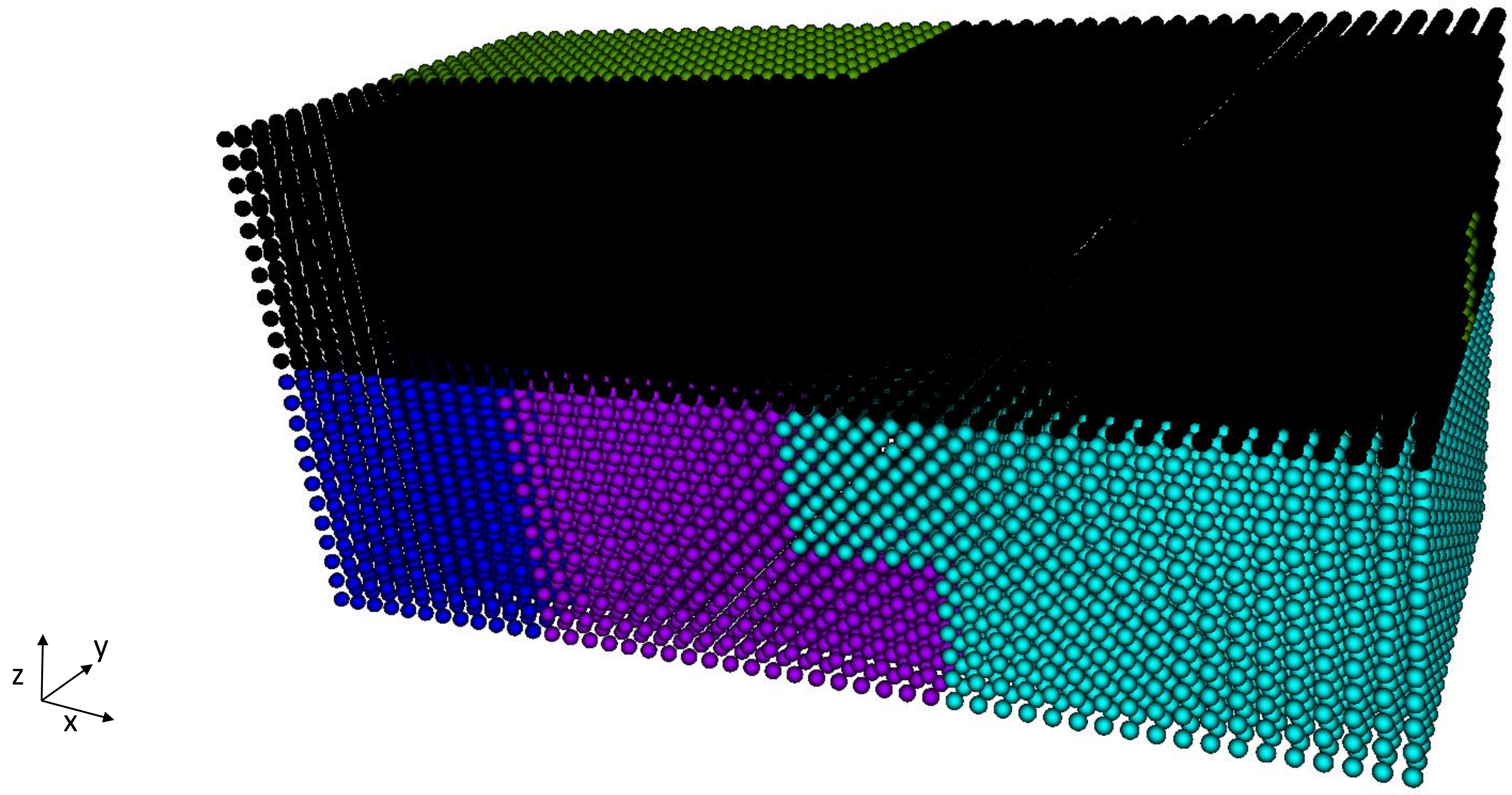


Partition Results





Partition Results



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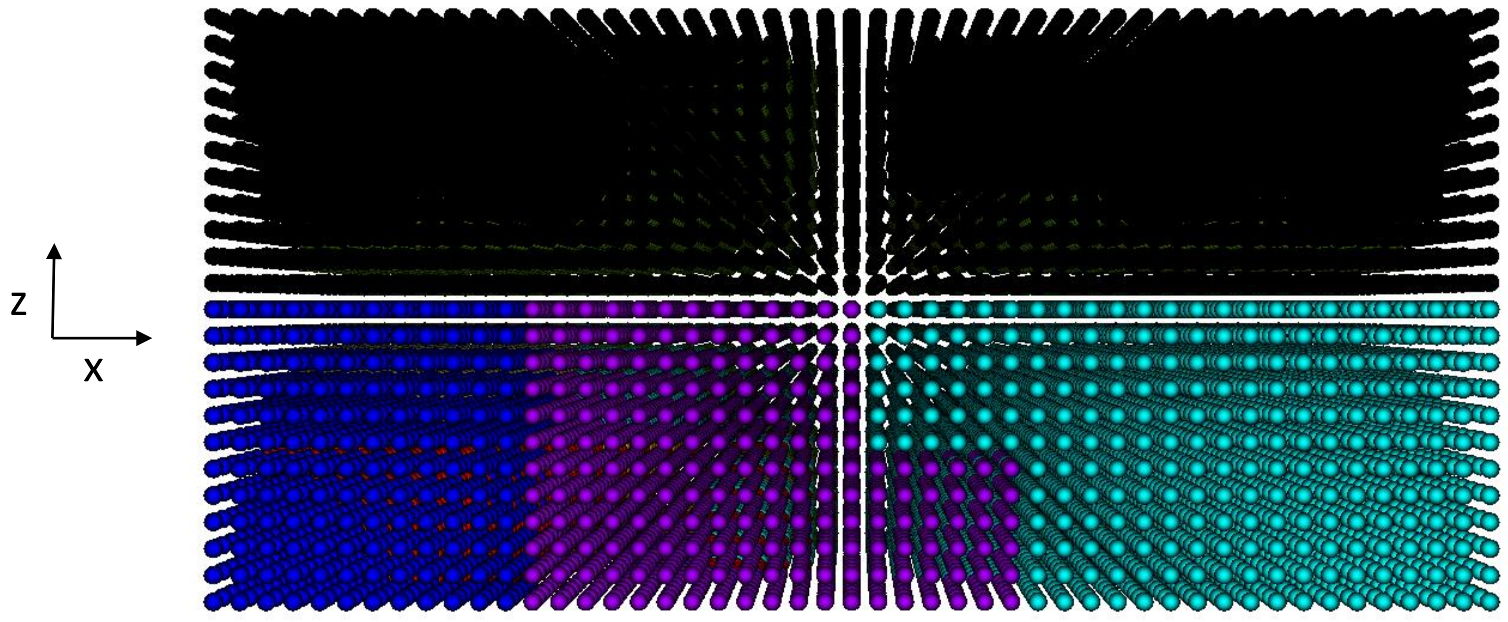
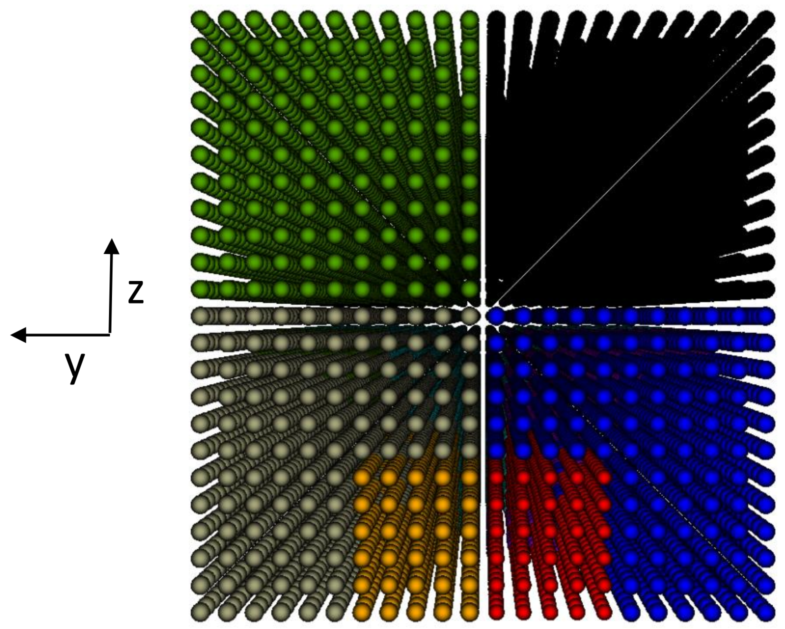
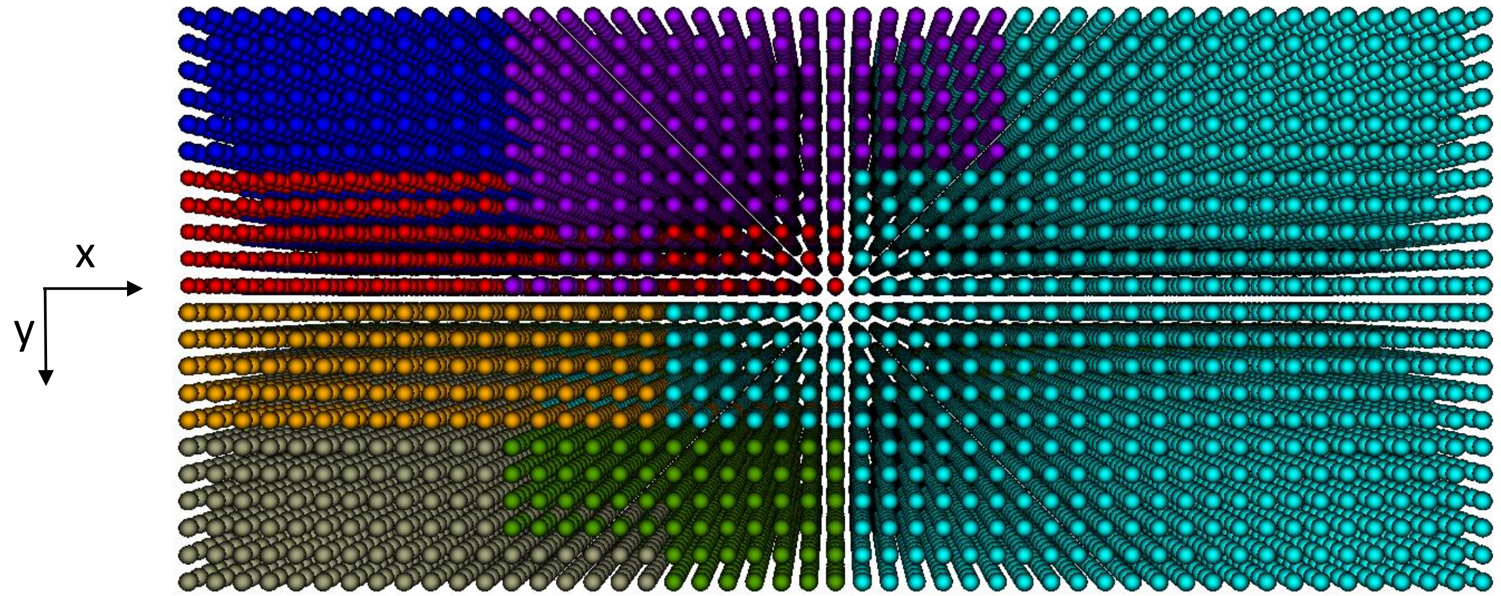




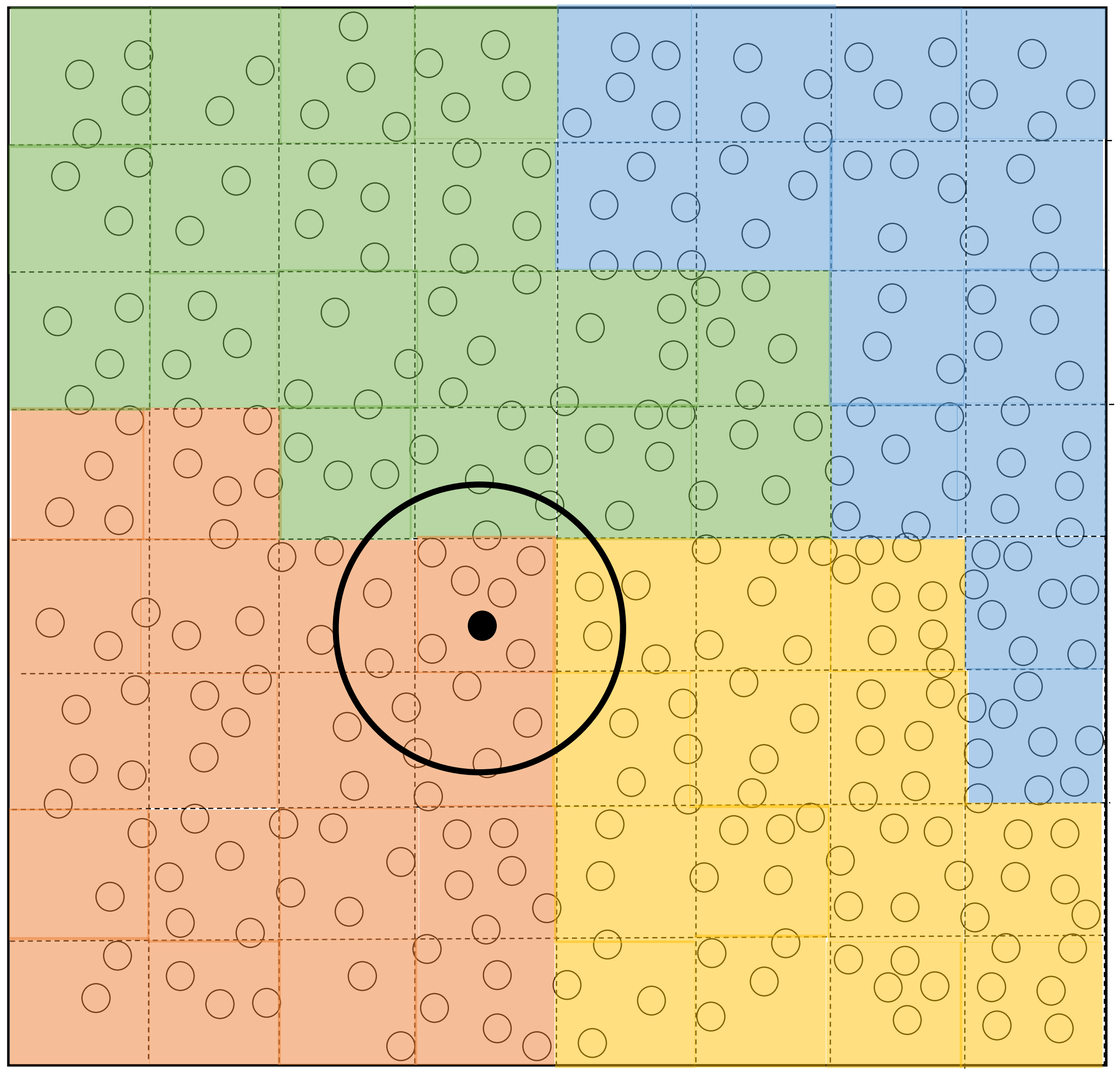


Future Work

- Complete a fully working version of the DualSPHysics MPI code
  - Halo Exchange
  - Particle Exchange
- Assess the code capabilities and validate
- Optimisation
- New I/O functions required – Transition to the Hierarchical Data Format (HDF5)
- Execution to large HPC clusters for 1000s of cores

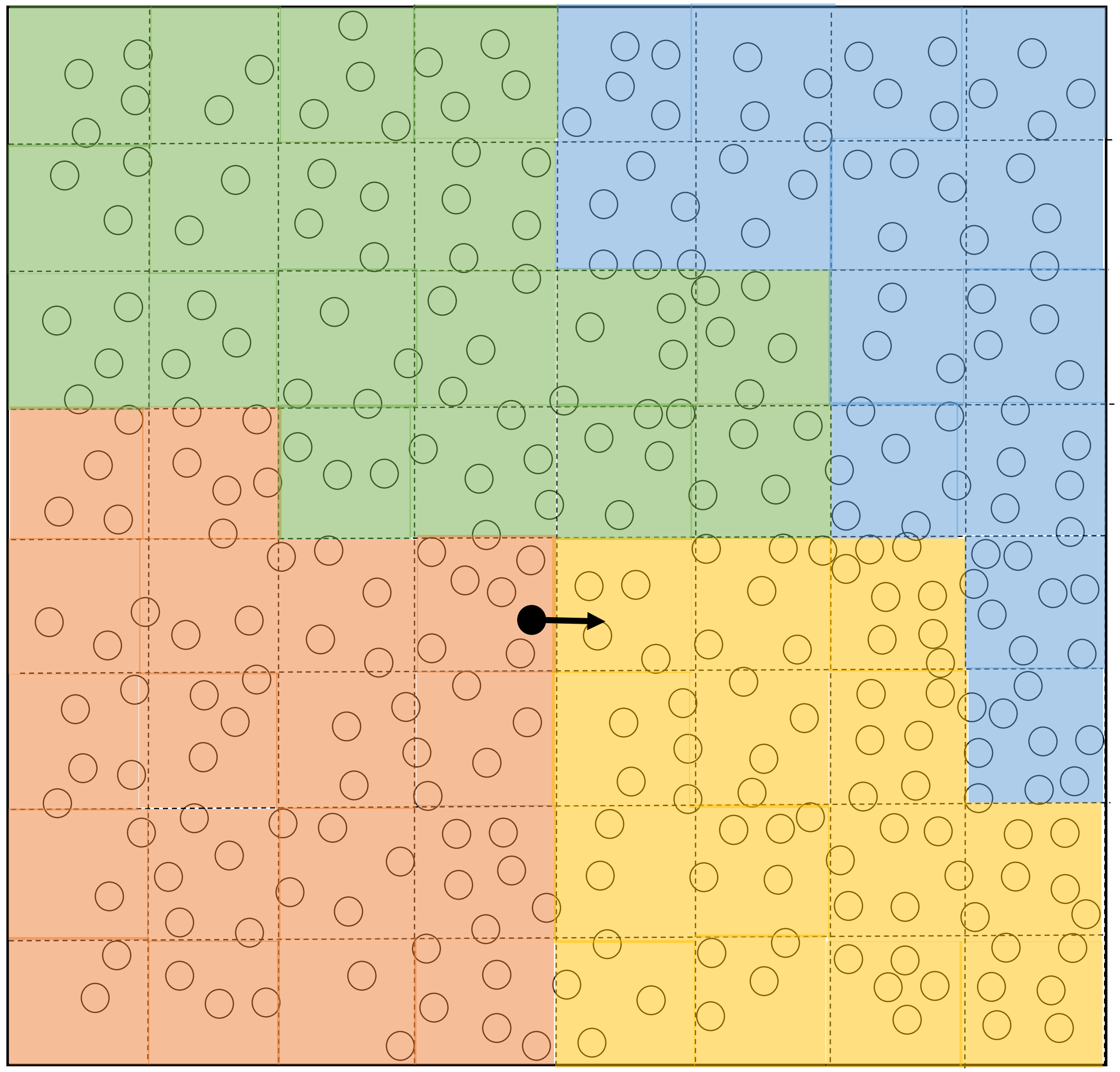
Halo Exchange

- Halo exchange reworked using cells
- Neighbouring cells explicitly known through GlobalCellID
- Identify processes the particles are in and transfer data
- Packing and unpacking algorithms same as previous code



Particle Exchange

- Particles can move out of the cell
- New cell may be in a different process
- Use Cell coordinates to identify edges of the process' domain
- Identify process and cell the particle moves into
- Use same packing/unpacking algorithm
- Process needs to be completed before reordering particle data



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The University of Manchester

Thank you

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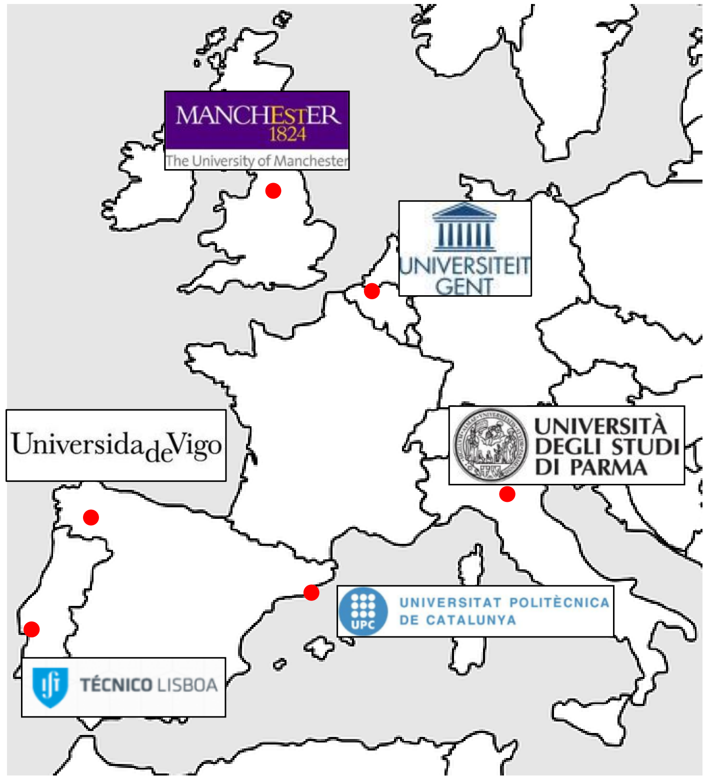
- U-Vigo: Alex Crespo, Moncho Gomez-Gesteira
- U-Parma: Renato Vacondio

@SPH_Manchester

Free open-source **DualSPHysics** code:
http://www.dual.sphysics.org

cpu gpu
DualSPHysics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Additional Models

- Viscosity:

$$\Pi_{ij} = \sum_{j}^{N} \frac{m_j}{\rho_i \rho_j} \left(\mu_j + \mu_i\right) \boldsymbol{u}_{ij} \frac{\boldsymbol{r}_{ij} \cdot \nabla W_{ij}}{\left|\boldsymbol{r}_{ij}\right|^2}$$

- δ-SPH:

$$\left\langle \frac{d\rho}{dt} \right\rangle = \rho_i \sum_{j} \frac{m_j}{\rho_j} \left(\boldsymbol{u}_i - \boldsymbol{u}_j\right) \cdot \nabla_i W_{ij} + D_i \qquad D_i = \delta h c_s \sum_{j}^{N} 2 \frac{m_j}{\rho_j} \left(\rho_j - \rho_i\right) \frac{\boldsymbol{r}_{ij} \cdot \nabla W_{ij}}{\left|\boldsymbol{r}_{ij}\right|^2}$$

- Quintic Wendland kernel:

$$W_{ij} = \alpha_D \left(1 - \frac{q}{2}\right)^4 \left(2q + 1\right) \text{ where } \mathrm{q} = \frac{\boldsymbol{r}_\mathrm{i} - \boldsymbol{r}_j}{h}$$

- Equation of state:

$$P(\rho) = P_0 \left[\left(\frac{\rho}{\rho_0} \right)^{\gamma} - 1 \right]$$

- 2nd order Velocity Verlet time marching scheme