NEPTUNE: PARTICLES

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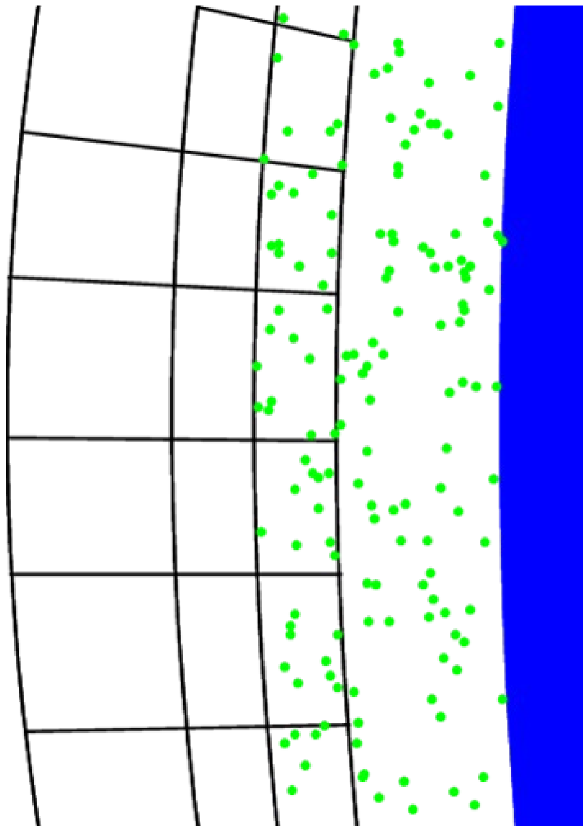
NEPTUNE Particle Use Cases

- Kinetic representations (I.e. distribution functions are not Maxwellian).
- Plasma
  1. Tritium, Deuterium fuel
  2. Alpha particles
  3. Ionised impurities
- Neutrals
  1. Injected (diagnostics)
  2. Recombined plasma (cooler regions)
  3. Sputtering from wall (molecules ejected from wall)
  4. Impurities
- Boundary conditions

- Less interested in molecular dynamics style operations – e.g. pairwise interactions.
- Small quantities of impurities important due to strong localised radiation.



NEPTUNE Particle Usage

- Domain Specialists desire a high-level interface
    1. Varying levels of interface to match desired level of control.
    2. e.g. Create a set of particles from an existing species and distribution.
    3. e.g. Per-particle control of properties and particle creation/deletion.

- Computational scientists
    1. Abstraction for particle data
    2. Abstraction for particle operations
    3. Works for both plasma and neutral species

- Both parties want efficiency across architectures without re-write (performance-portability).

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Core Components

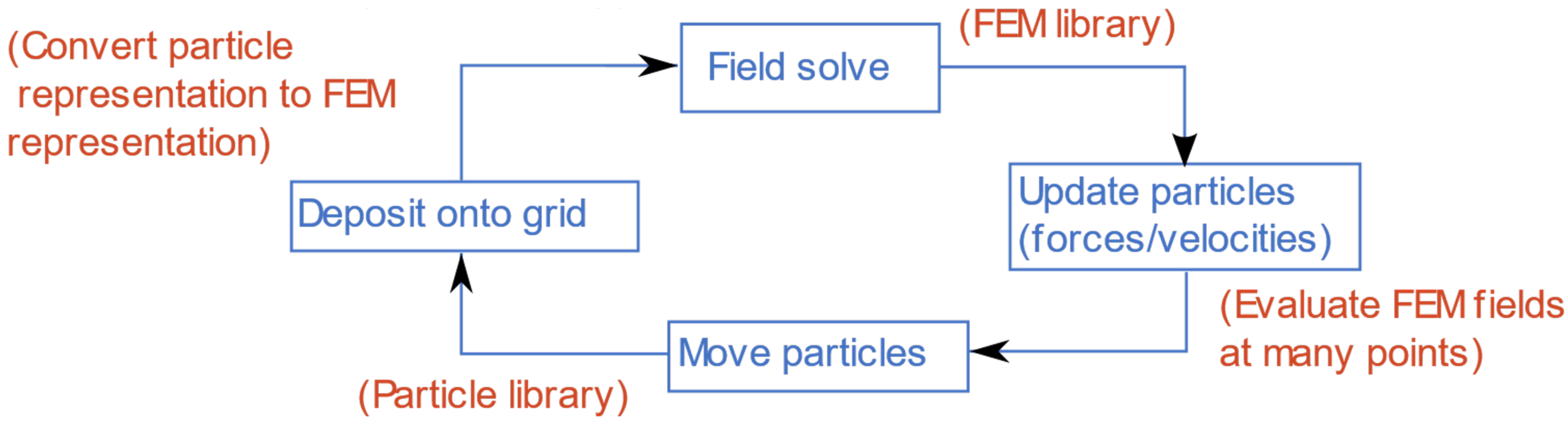
- Particle data communication
    1. Highly directional plasma flow (along field lines)
    2. Fast neutral flow (typically global and omnidirectional)
    3. Unstructured high-order mesh

- Particle current deposition / field evaluation
    1. Compute FEM fields for the deposition stage
    2. Evaluate FEM fields for particle push

- Particle Based Operations/Data structures
    1. Particle properties – position, velocity, charge, id...
    2. Loops over particles
    3. Degrees of Freedom (DOF) – Particle Loops
    4. Particle – Particle Loops

PIC Loop

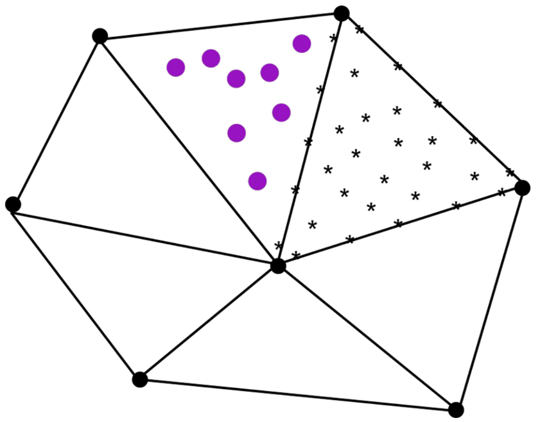
Overview



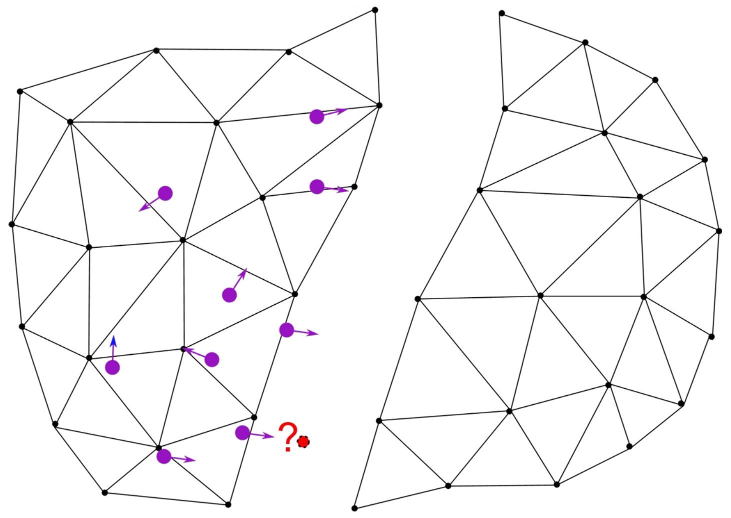
- Rough overview – More involved (and useful) schemes may combine steps.
- PIC schemes which exist to conserve quantities of interest, e.g. charge(mass), energy and momentum.
- Loop till convergence/end time.

Efficient Particle Implementation

Functional Requirements



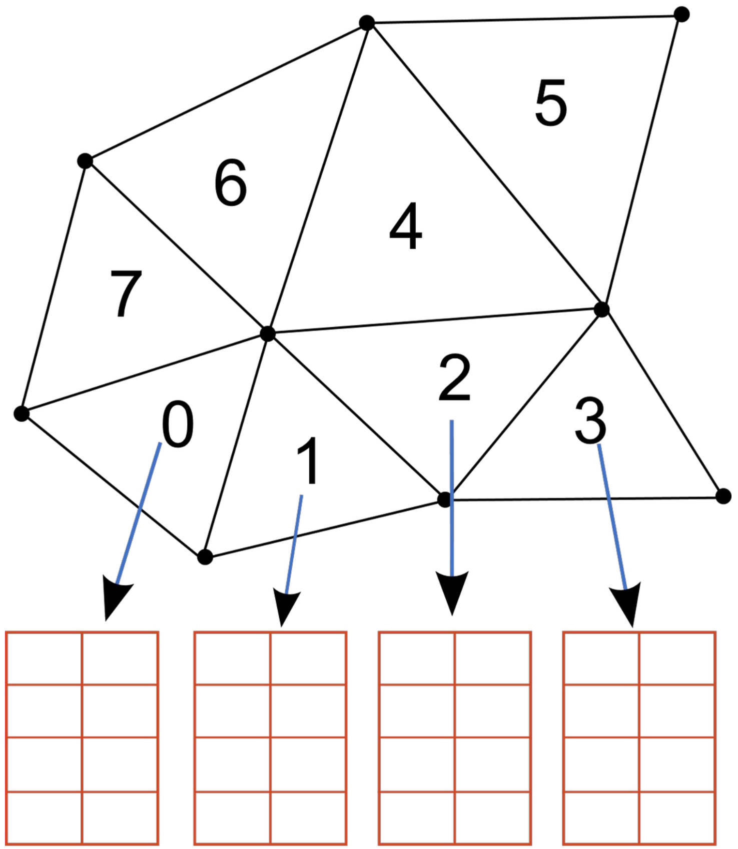
- Enable efficient particle – grid operations.
    1. Hybrid/dual representations as particle and continuum.
    2. Continuum evaluation at many points
    3. Motivates close coupling between mesh and particles.



- Efficient and scalable particle movement.
    1. Fast (essentially global) movement of neutrals
    2. Anisotropic flow
- Target implementation for a DSL.
    1. Generate looping operations/tasks

Data – Each mesh cell

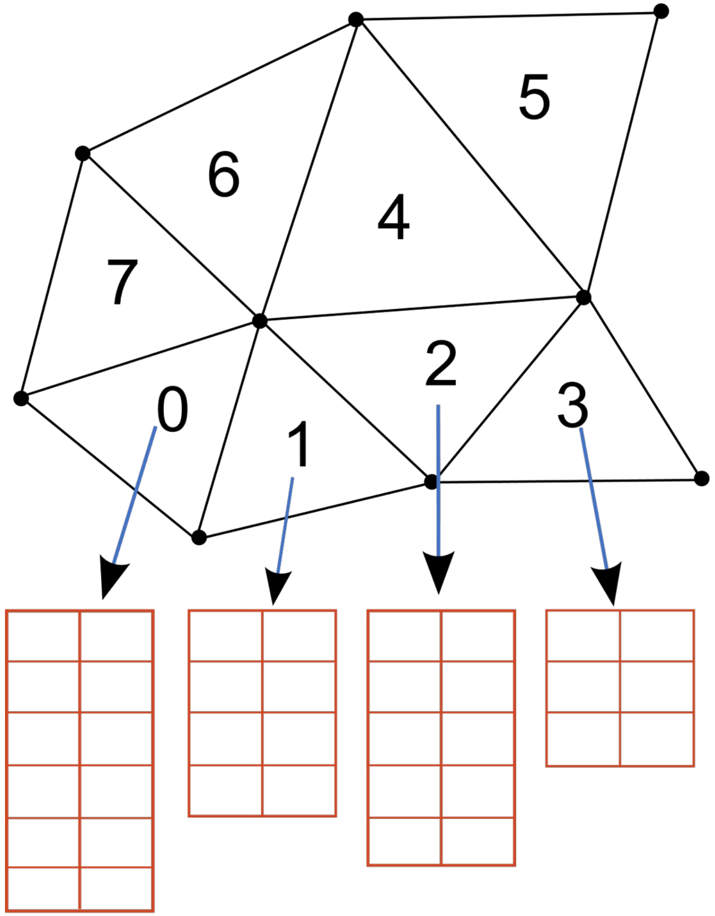
CellDatConst



- Datatype, Column count and Row count (per cell) fixed at construction
- Device allocated (*sycl*::malloc_device)
- DOF Data
- Expansion coefficients
- Geometry/domain information
- Lookup indices

Data – Variable Row Count

CellDat

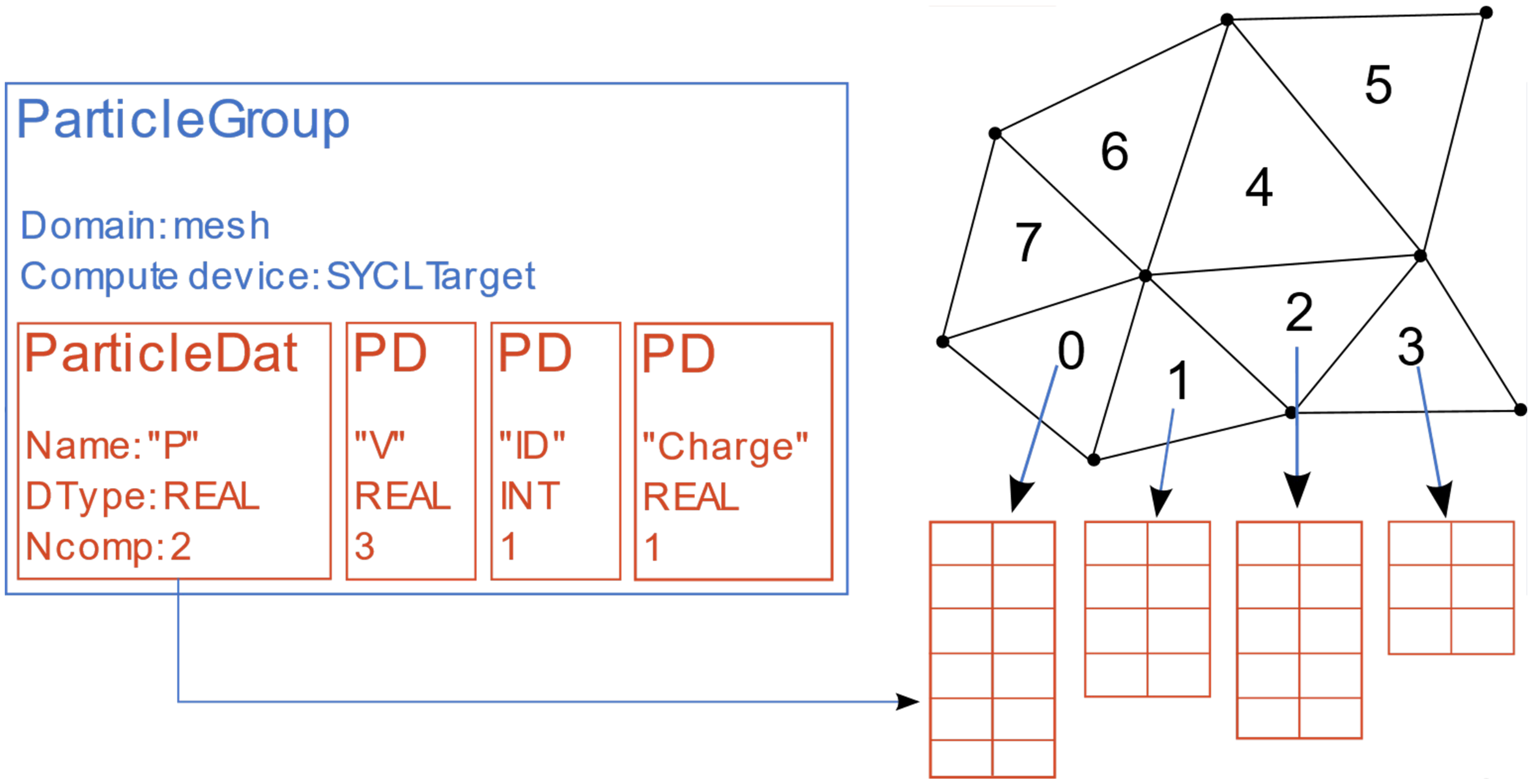


- Datatype and Column count (per cell) fixed at construction
- Variable number of rows (per cell)
- Device allocated (*sycl*::malloc_device)
- Base container for particle data, e.g. A floating point CellDat with 2 columns could store 2D positions.
- Per cell storage is advantageous for particle – grid operations

Particle Data

ParticleGroup, ParticleDat

- Combines the: mesh, compute device and particle data.
- Implements particle bookkeeping – cells and MPI ranks.
- General particle properties, e.g. charge, mass, weight, velocity.



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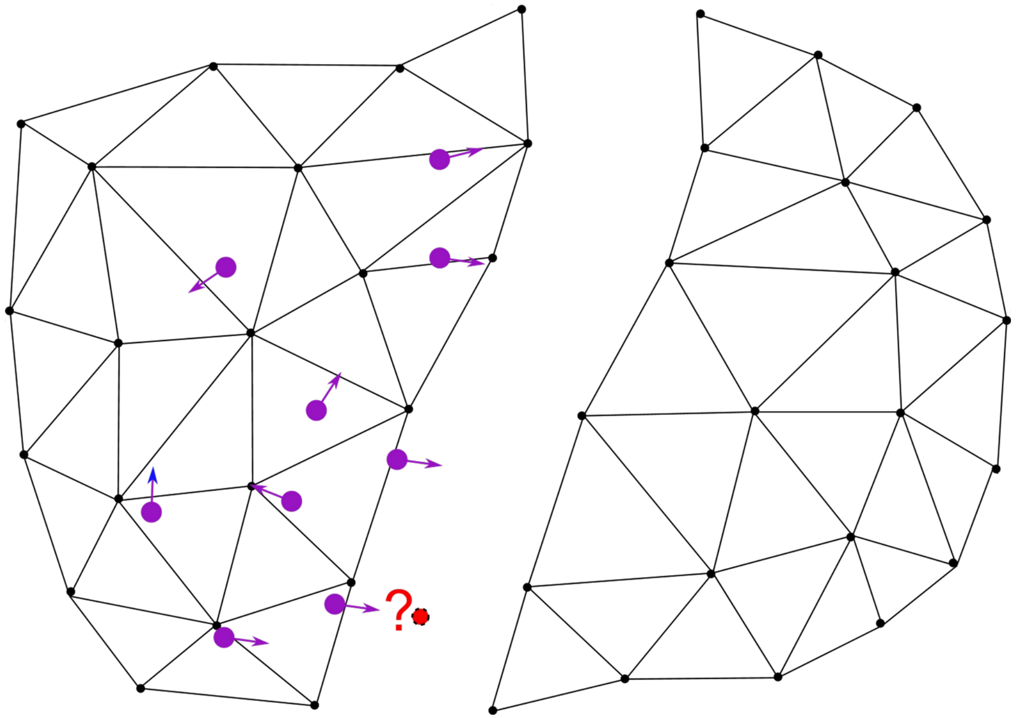
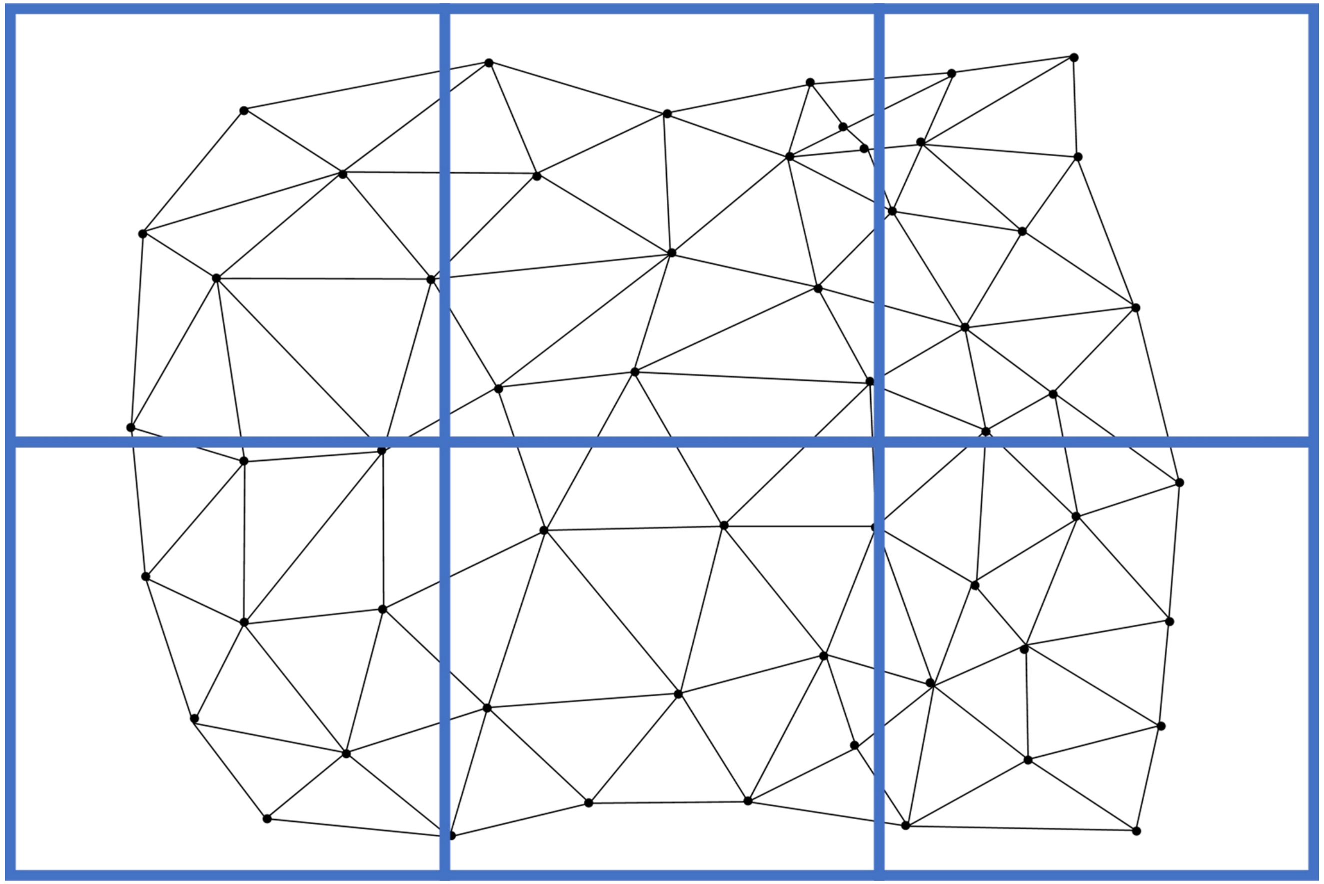
Global Particle Movement



- Efficiently transfer particle ownership – domain decomposition
- Fast moving particles – essentially global
- Want local communication patterns where possible
- Minimise number of non-linear solves (high-order mesh)

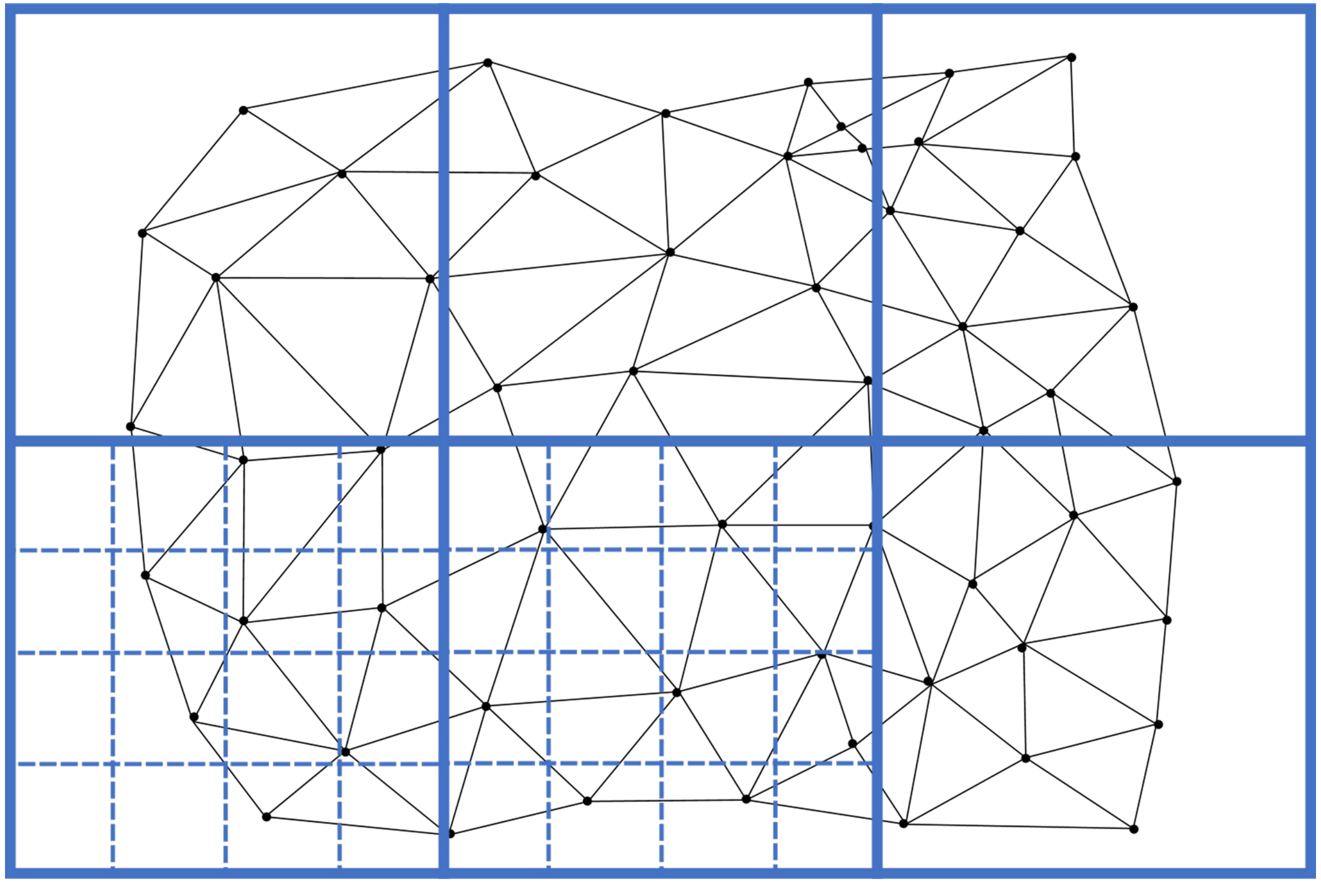
Solution

Overlay Coarse Grid of squares/cubes



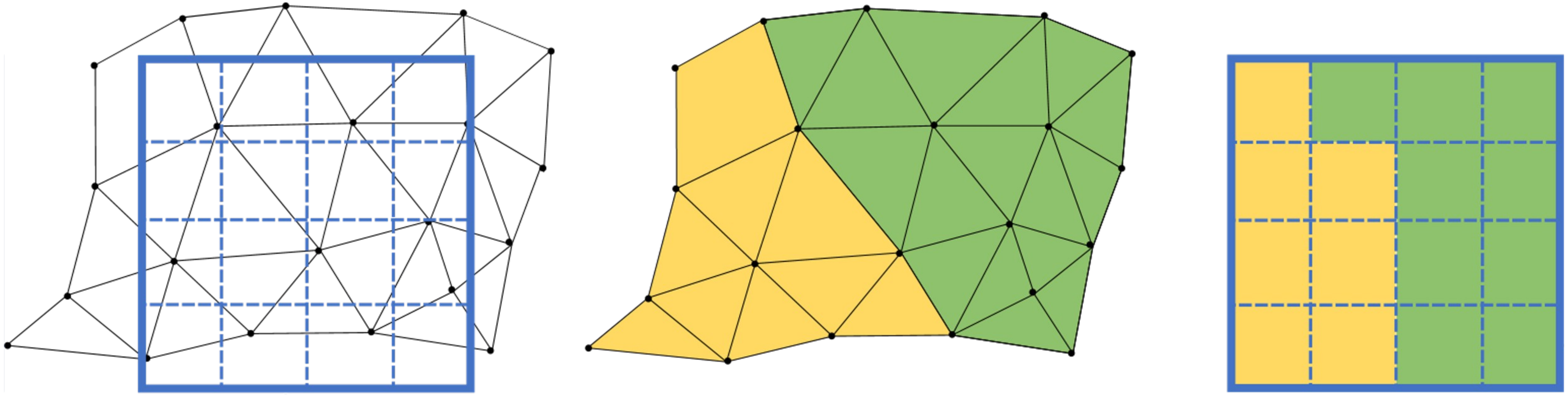
Solution

Subdivide coarse mesh cells



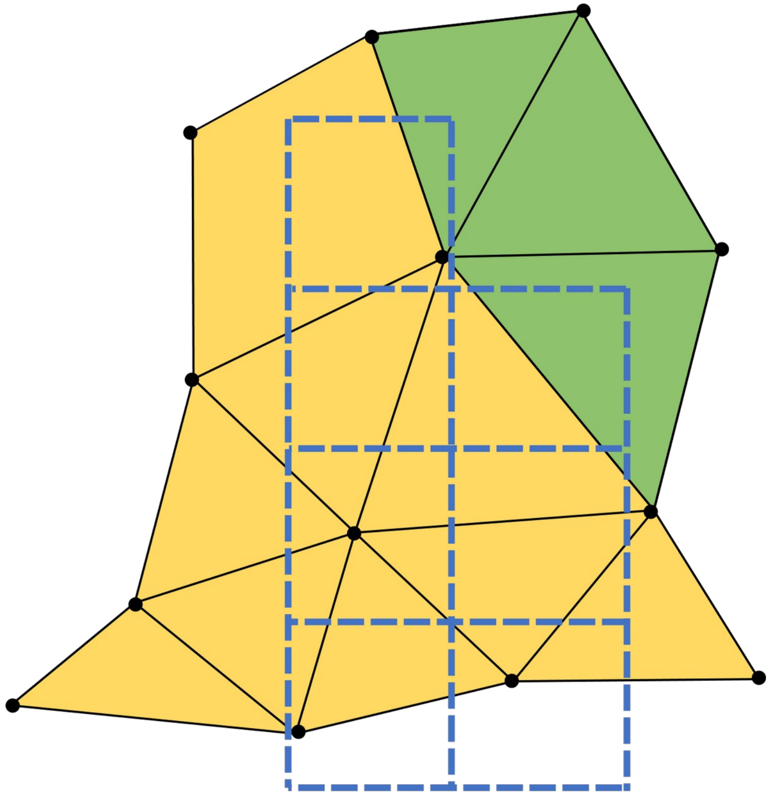
Decompose Fine Mesh

Assign MPI owners to fine mesh cells



Build Halo Regions

Duplicate Geometry Objects



- Duplicate remotely owned geometry to cover owned coarse mesh cells.
- Store owning rank and local id of copied geometry.
- Particles in the coarse mesh cells can be mapped to geometry objects and owning ranks.
- Setup point-to-point communication patterns between neighbours.
- Halo width is tuneable – increase local communication.

Hybrid Particle Transfer

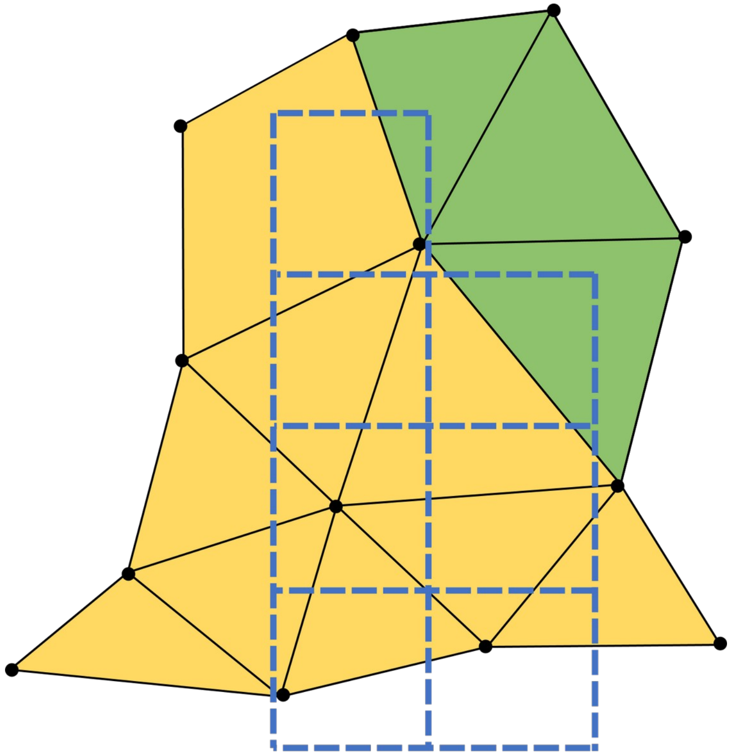
Global + Local Transfer

For each particle:
  Attempt to bin into local mesh cell (either owned or halo)

For "far moving" particles (not binned into owned or halo cells):
  Transfer to MPI rank owning overlayed cartesian cell
  (global transfer)

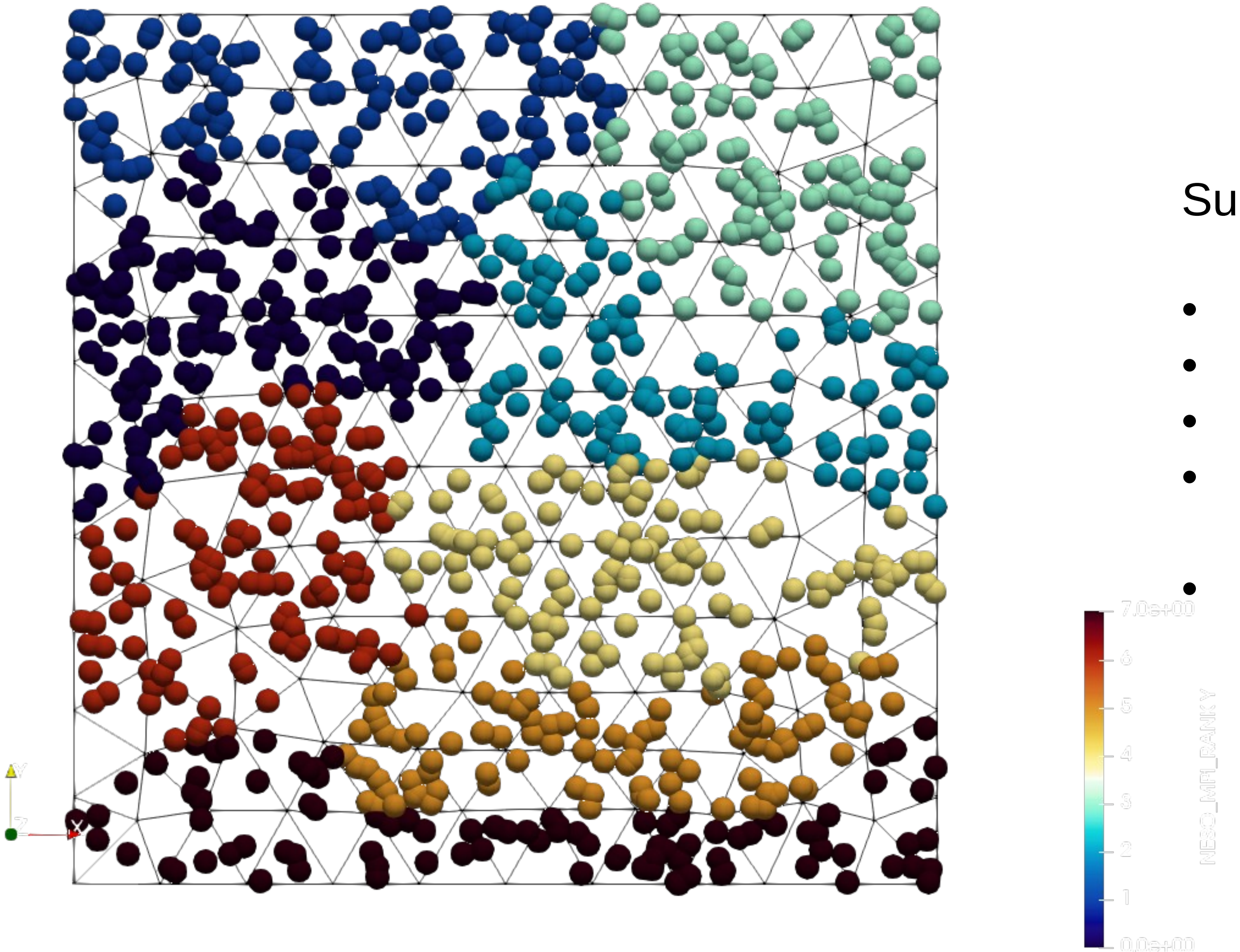
For each particle received in global transfer:
  Bin into local mesh cell (either owned or halo)

For "locally moving" particles:
  Transfer to neighbour using local communication pattern.



Trajectory Snapshot

Colour – owning MPI rank



Summary:

- On device particle state and computation[1].
- Performance oriented data structures.
- Base implementation for DSL.
- MPI domain decomposition with hybrid (global + local) move.
- Particle transport on 2D linear Nektar++ meshes[2].

[1] https://github.com/ExCALIBUR-NEPTUNE/NESO-Particles
[2] https://github.com/ExCALIBUR-NEPTUNE/NESO

The End

UKAEA NEPTUNE:

Rob Akers
Wayne Arter
Matthew Barton
James Cook
Joseph Parker
Owen Parry
Will Saunders
Ed Threlfall

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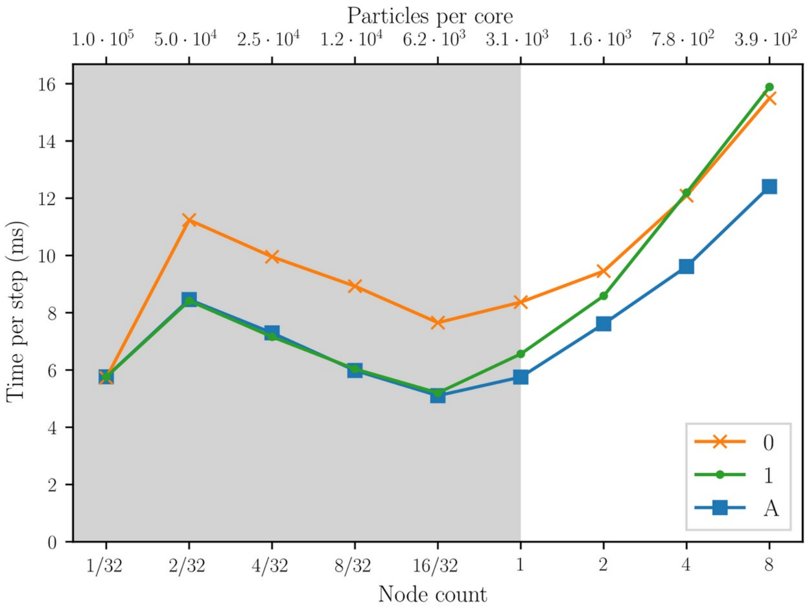
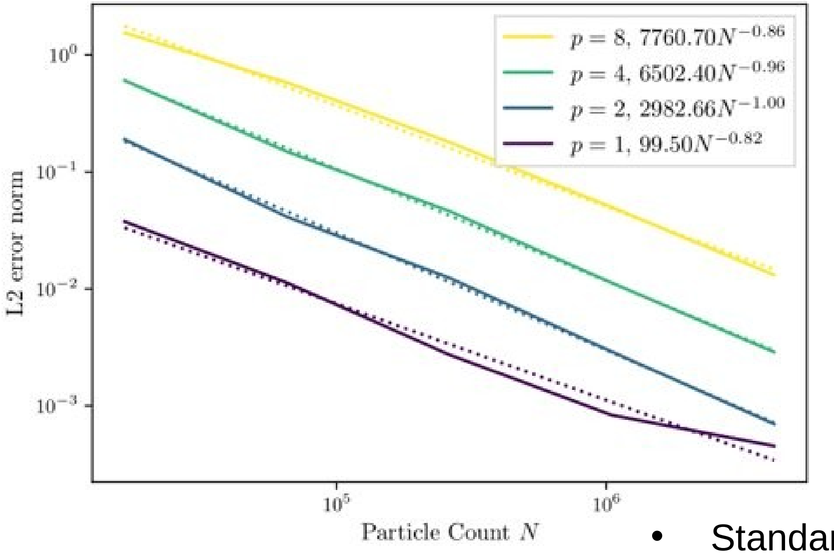
Core Components – Exploratory Ideas and Progress

- Particle data communication
  1. Combine coarse grid/octree with halo cells
  2. Majority of transport using local communication patterns through halos
  3. Global communication where needed (MPI RMA)



0: Halo width 0
1: Halo width 1
A: Adaptive halo width

- Particle current deposition / field evaluation
  1. L2 Galerkin projection inspired (for deposition)
  2. Cell-wise data representation: DOFs/Coefficients
  3. Cell-wise loops between particles and DOFs



- Standard L2 error computed against reference 2D Gaussian
- Higher FEM order captures more particle noise

Particle DSL - Exploratory Ideas and Progress

- User/Developer facing
- Separation of Concerns

- Abstraction:
  - Data Structures: Particle/FEM DOFs
  - Looping operations: Iteration set + kernel + access descriptors
    1. Loops over particles
    2. Cell-wise loops over particles and DOFs
    3. Pairwise particle loops (for particle-particle interactions)

- Implementation
  1. SYCL – low level target language
  2. Python code generation framework
  3. DSL embedded in Python
  4. PPMD/pyOP2 inspired

```
advection = ParticleLoop(
    target_device, # where to execute
    Kernel(
        "advection_kernel",
        """
        P[ix, 1] += V[ix, 1] * $dt
        P[ix, 2] += V[ix, 2] * $dt
        P[ix, 3] += V[ix, 3] * $dt
        global[1] += 1
        """
    ),
    Dict( # map from kernel symbols to data
structures
         "P" => (particle_group["P"], WRITE),
         "V" => (particle_group["V"], READ),
         "global" => (global_data, INC),
    )
)
execute(advection)
```