Particle-in-Cell Algorithms for Emerging Computer Architectures: MPI/Open-MP

Viktor K. Decyk and Tajendra V. Singh

UCLA

Particle-in-Cell Codes

Simplest plasma model is electrostatic:

1. Calculate charge density on a mesh from particles:

$$\rho(\boldsymbol{x}) = \sum_i q_i S(\boldsymbol{x} - \boldsymbol{x}_i)$$

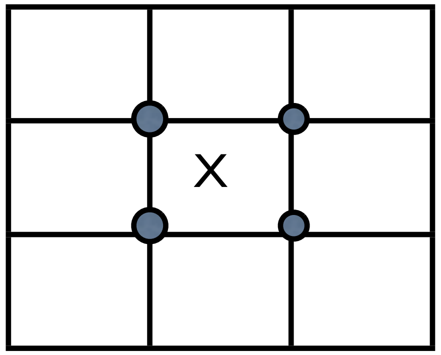
2. Solve Poisson's equation:

$$\nabla \bullet \boldsymbol{E} = 4\pi\rho$$

3. Advance particle's co-ordinates using Newton's Law:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = q_i \int \boldsymbol{E}(\boldsymbol{x}) S(\boldsymbol{x}_i - \boldsymbol{x})\, d\boldsymbol{x} \qquad \frac{d\boldsymbol{x}_i}{dt} = \boldsymbol{v}_i$$

Inverse interpolation (scatter operation) is used in step 1 to distribute a particle's charge onto nearby locations on a grid.



Interpolation (gather operation) is used in step 3 to approximate the electric field from grids near a particle's location.

When running in parallel, data collisions might occur

Distributed Memory Programming (MPI) for PIC

This is dominant technique used on today's supercomputers

Domain decomposition is used to assign which data reside on which processor
- No shared memory, data between nodes sent with message-passing (MPI)
- Most parallel PIC codes are written this way

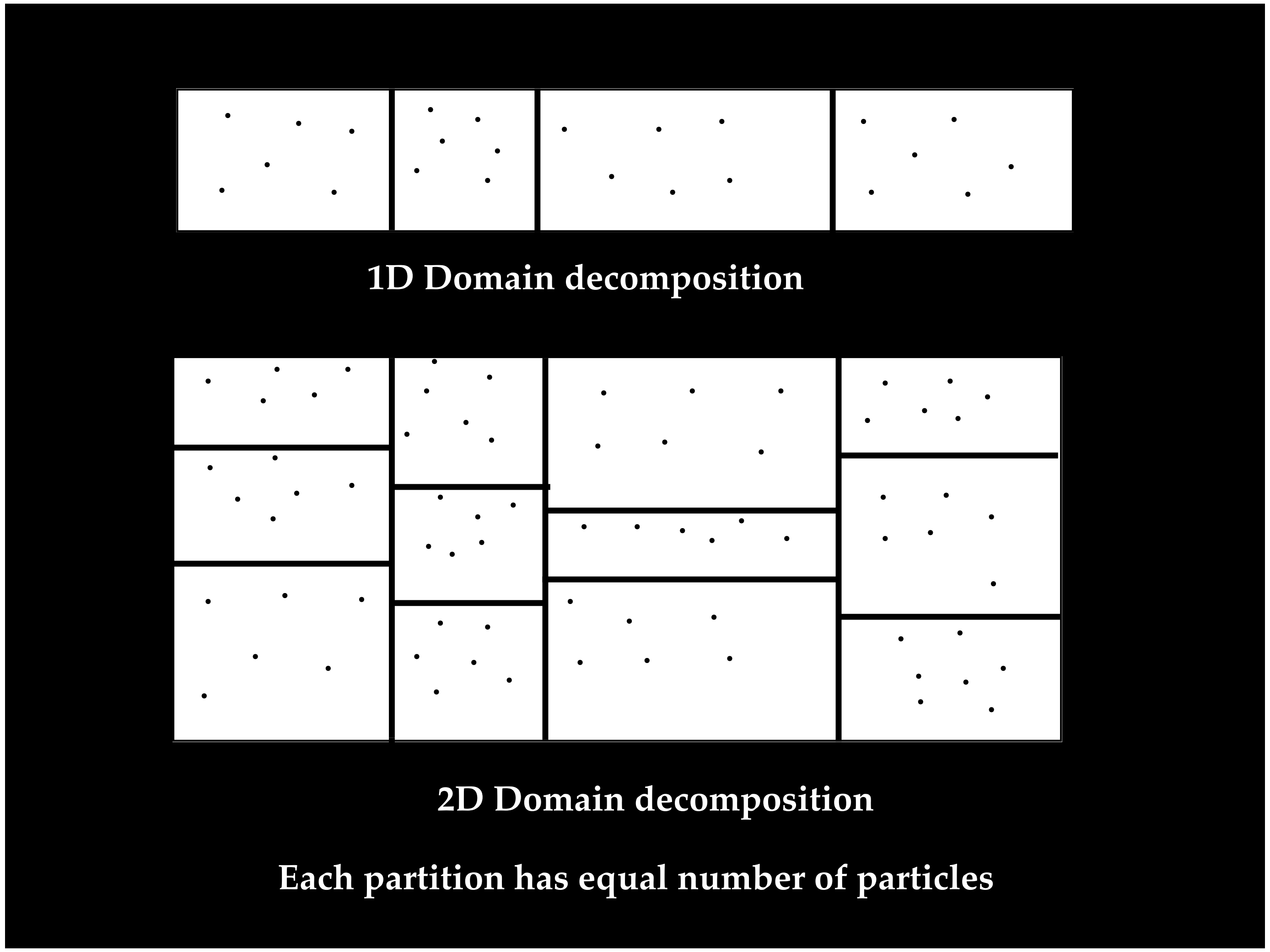
Details can be found at:

P. C. Liewer and V. K. Decyk, "A General Concurrent Algorithm for Plasma Particle-in-Cell Codes," J. Computational Phys. 85, 302 (1989)

Sample codes can be found at:
https://idre.ucla.edu/hpc/parallel-plasma-pic-codes

Distributed Memory Programming for PIC

Domain decomposition with MPI



1D Domain decomposition

2D Domain decomposition

Each partition has equal number of particles

Primary Decomposition has non-uniform partitions to load balance particles

- Sort particles according to spatial location
- Same number of particles in each non-uniform domain
- Scales to many thousands of processors

Particle Manager responsible for moving particles

- Particles can move across multiple nodes

Designing New Particle-in-Cell (PIC) Algorithms for Shared Memory

Most important bottleneck is memory access

- PIC codes have low computational intensity (few flops/memory access)
- Memory access is irregular (gather/scatter)

Memory access can be optimized with a streaming algorithm (global data read only once)

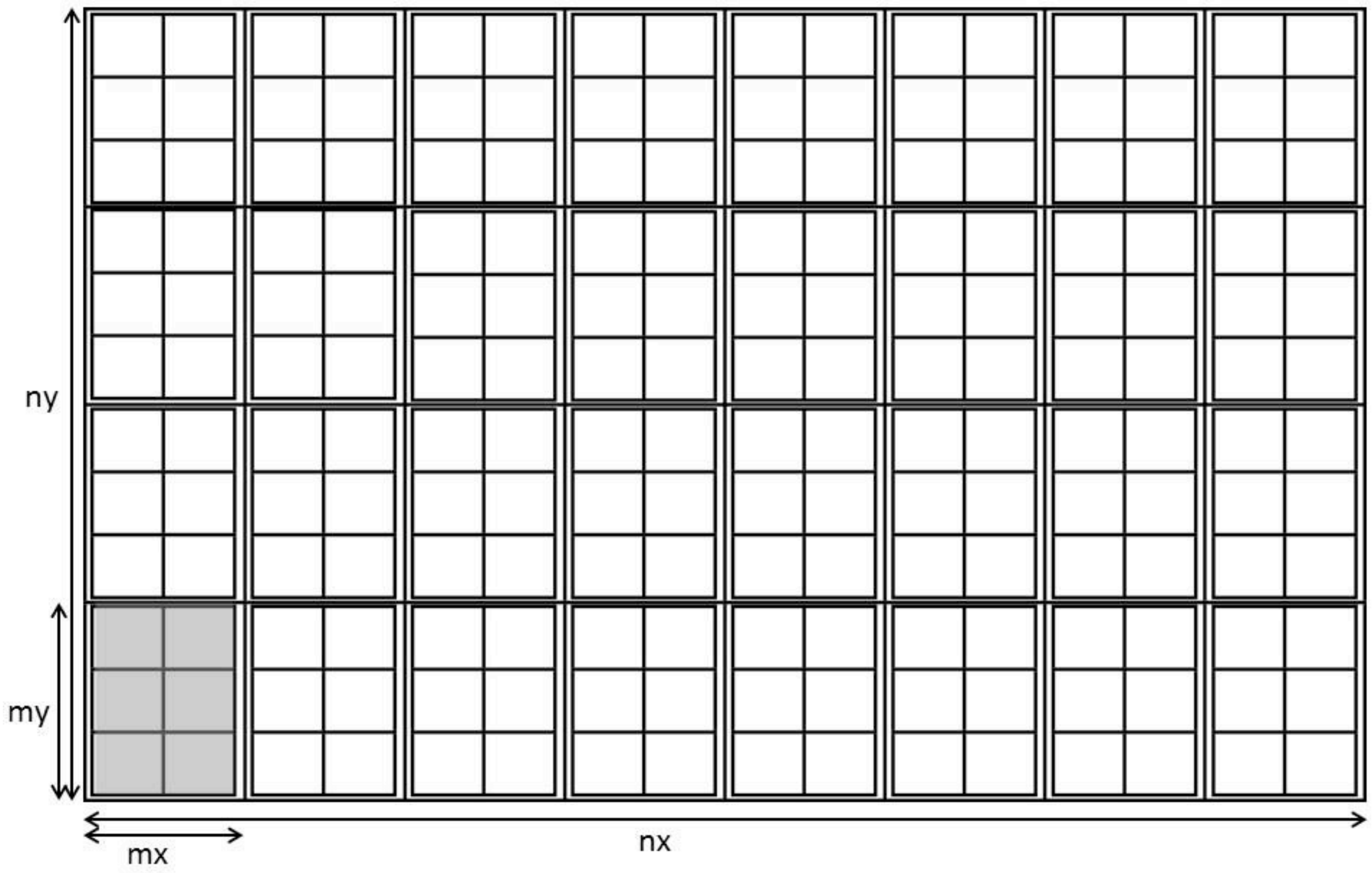
PIC codes can implement a streaming algorithm by keeping particles ordered by small tiles

- Minimizes global memory access since field elements need to be read only once.
- Cache is not needed, gather/scatter can be avoided.
- Deposit and particles update can have optimal stride 1 access.

Designing New Particle-in-Cell (PIC) Algorithms:
Particles ordered by tiles, varying from 2 x 2 to 16 x 16 grid points

We created a new data structure for particles, partitioned among threads blocks:

```
    dimension ppart(idimp,npmax,num_tiles)
```



Designing New Particle-in-Cell (PIC) Algorithms: **Push/Deposit Procedures**:

Within a tile, all particles read or write the same block of fields.
- Before pushing particles, copy fields to fast memory
- After depositing charge to fast memory, write to global memory
- Different tiles can be done in parallel.

Each tile contains data for the grids in the tile, plus guard cells: an extra column of grids on the right, and an extra row of grids on the bottom for linear interpolation.

For push, parallelization is easy, each particle is independent of others, no data hazards
- Similar to MPI code, but with tiny partitions

For deposit, parallelization is relatively easy if each tile is controlled by one thread
- Care has to be taken in adding fast tile memory to global memory for the guard cells
- Atomic updates (which treat an update as an uninterruptible operation) are one approach

Designing New Particle-in-Cell (PIC) Algorithms: **Maintaining Particle Order**

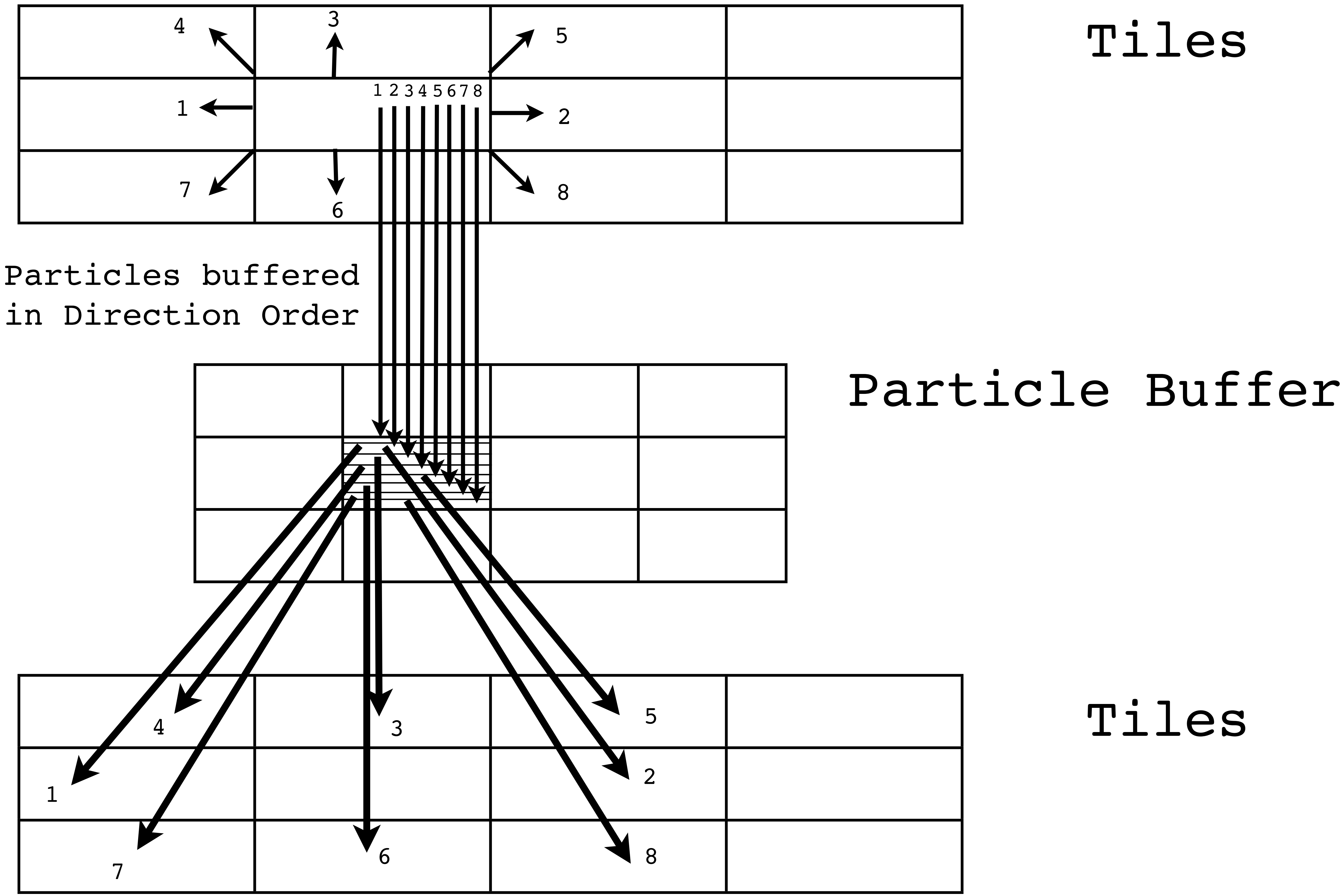
Three steps:
1. Create a list of particles which are leaving a tile, and where they are going
2. Using list, each thread places outgoing particles into an ordered buffer it controls
3. Using lists, each tile copies incoming particles from buffers into particle array

- Less than a full sort, low overhead if particles already in correct tile
- Can be done in parallel
- Essentially message-passing, except buffer contains multiple destinations

In the end, the particle array belonging to a tile has no gaps

- Incoming particles are moved to any existing holes created by departing particles
- If holes still remain, they are filled with particles from the end of the array

Particle Reordering



Tiles

Particles buffered in Direction Order

Particle Buffer

Tiles

Evaluating New Particle-in-Cell (PIC) Shared Memory Algorithms: **Electromagnetic Case**

2-1/2D EM Benchmark with 2048x2048 grid, 150,994,944 particles, 36 particles/cell
optimal block size = 128, optimal tile size = 16x16. Single precision

```
Hot Plasma results with dt = 0.04, c/vth = 10, relativistic
              CPU:Intel i7    OpenMP(12 cores)
Push             66.5 ns.        5.645 ns.
Deposit          36.7 ns.        3.362 ns.
Reorder           0.4 ns.        0.056 ns.
Total Particle  103.6 ns.        9.062 ns.

The time reported is per particle/time step.
```

Designing New Particle-in-Cell (PIC) Algorithms: **Multiple Shared Memorys**

Multiple Shared Memorys can be controlled with MPI

- Merge MPI and OpenMP algorithms

We started with existing 2D MPI codes from UPIC Framework

- Replacing MPI push/deposit with OpenMP version was no major challenge

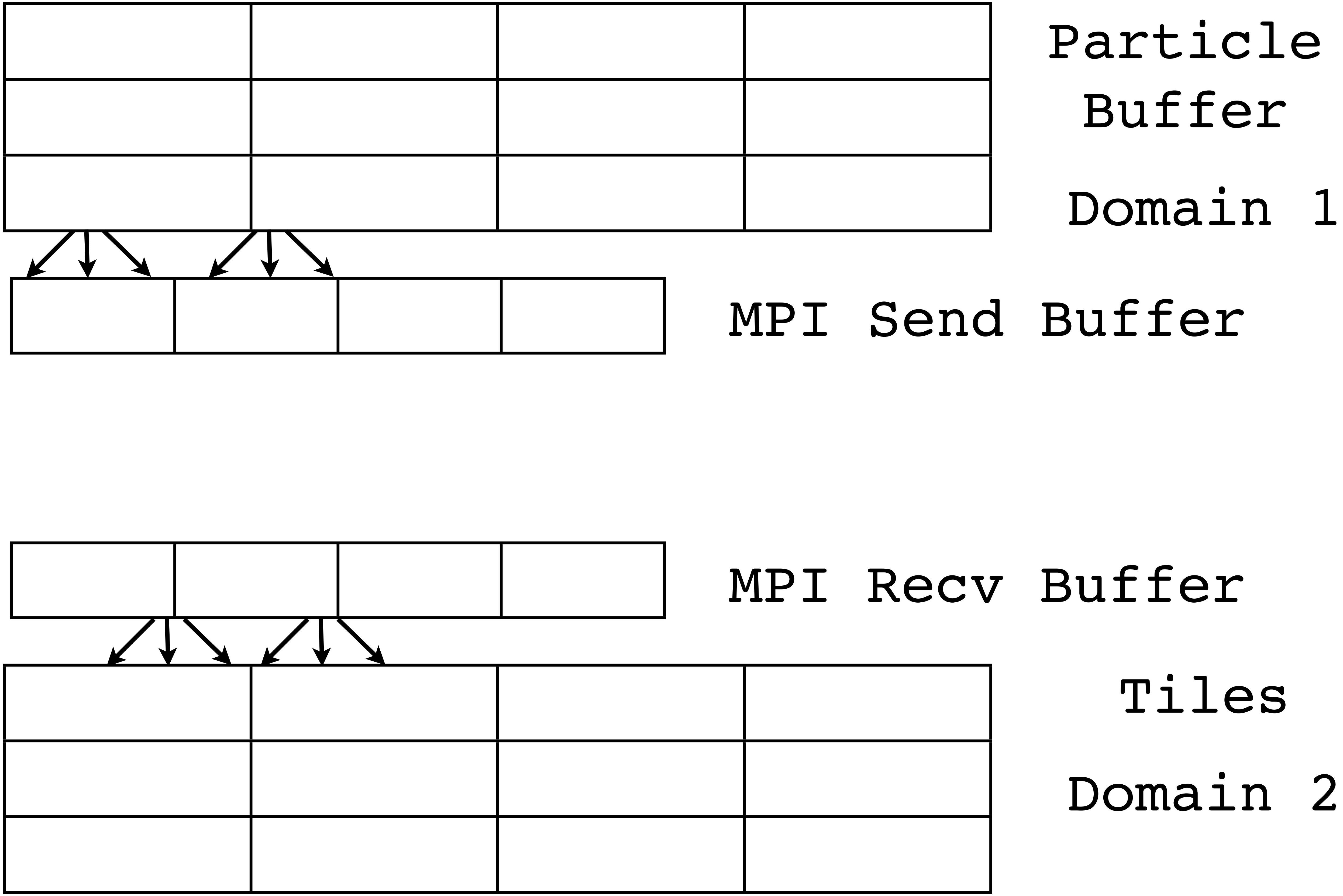
With multiple Shared Memorys, need to integrate two different particle partitions

- MPI and OpenMP each have their own particle managers to maintain particle order

Only first/last row or column of tiles on Shared Memory interacts with neighboring MPI node

- Particles in row/column of tiles collected in MPI send buffer
- Table of outgoing particles are also sent
- Table is used to determine where incoming particles must be placed

OpenMP-MPI Particle Reordering



Particle Buffer

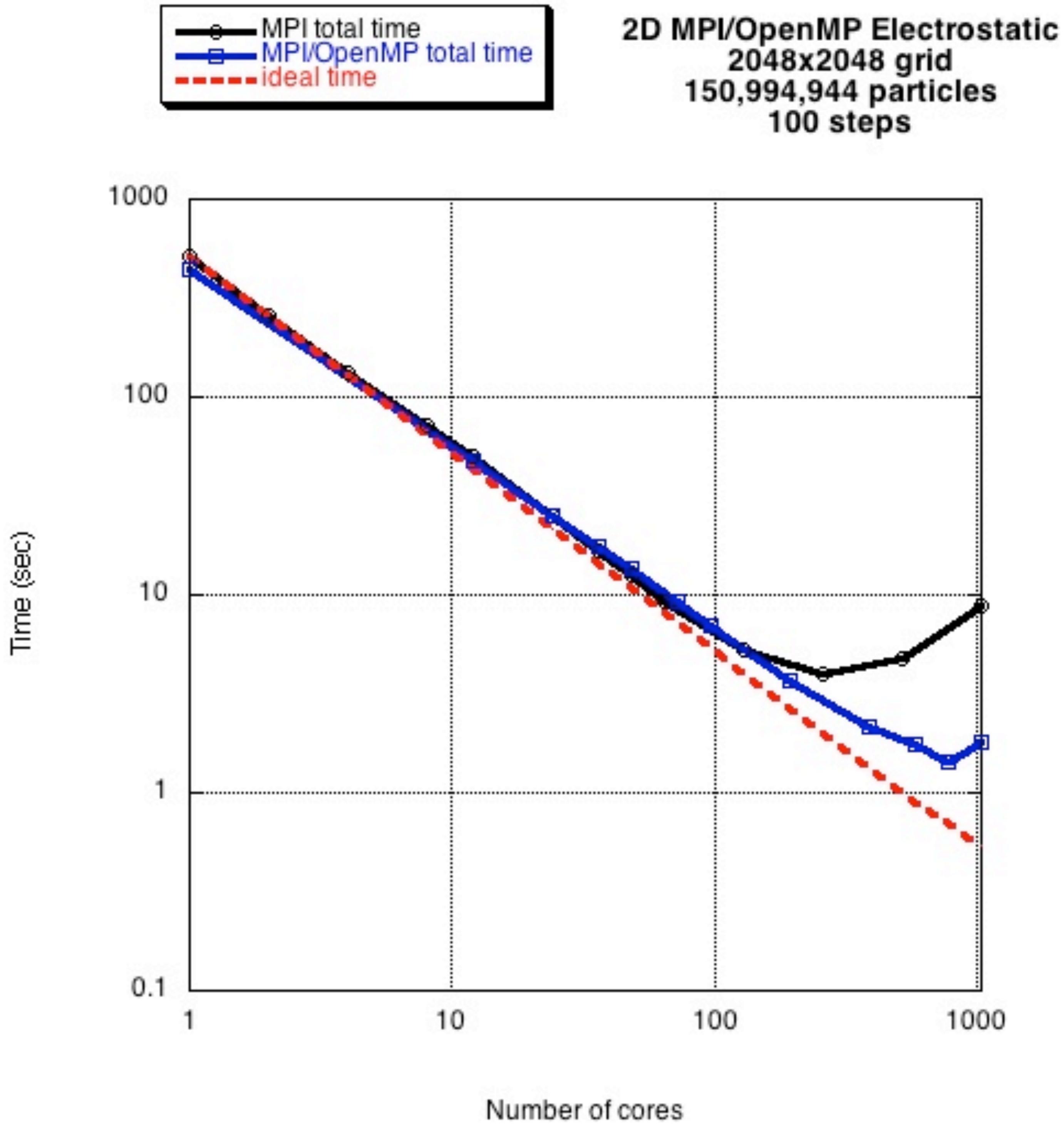
Domain 1

MPI Send Buffer

MPI Recv Buffer

Tiles

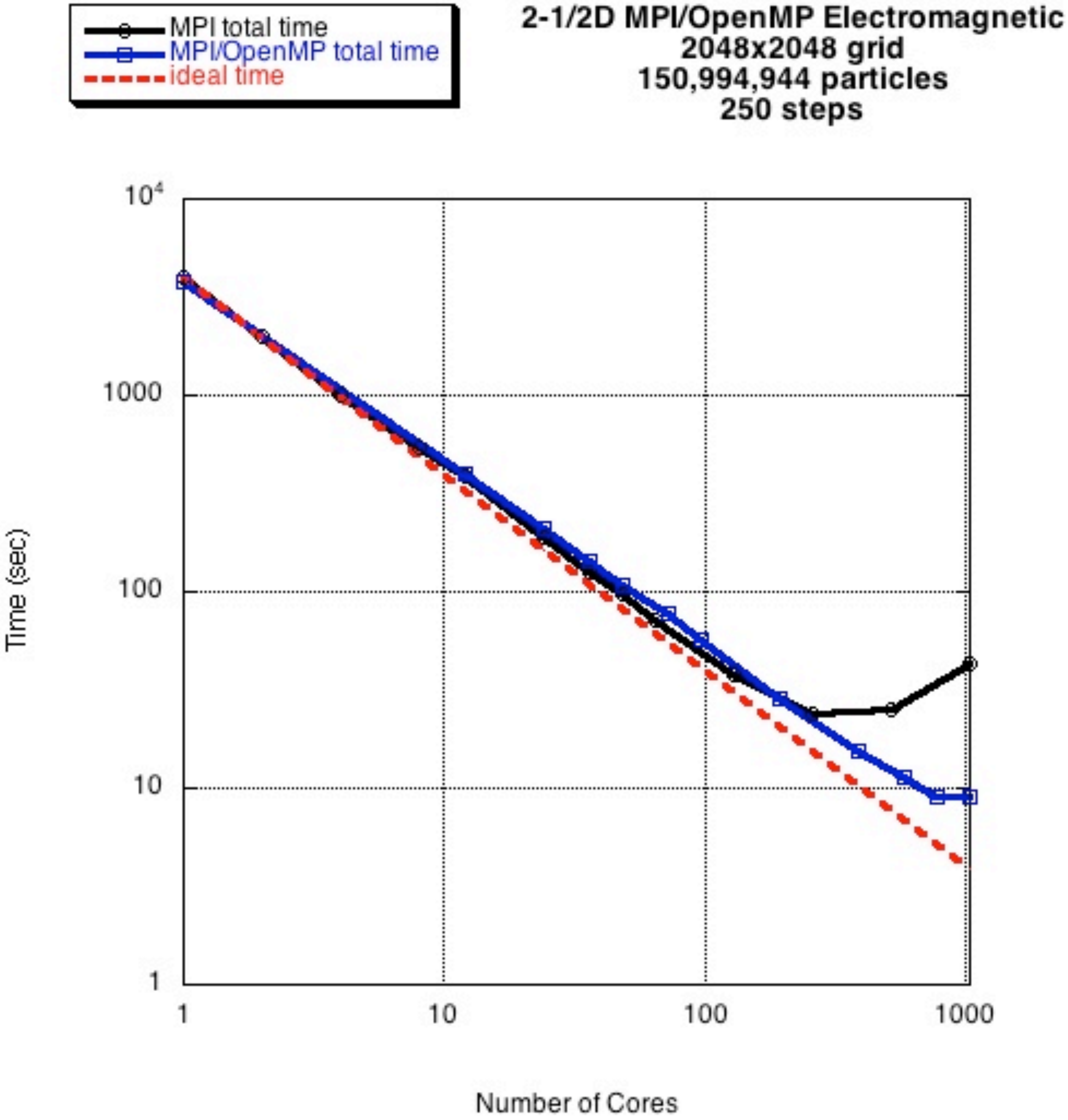
Domain 2



Electrostatic code

Mixed MPI/OpenMP spectral code scales better than MPI alone

- Due to reduced number of messages for transpose in FFT



Electromagnetic code

Mixed MPI/OpenMP spectral code scales better than MPI alone

- Due to reduced number of messages for transpose in FFT

Further information available at:

V. K. Decyk and T. V. Singh, "Particle-in-Cell Algorithms for Emerging Computer Architectures," Computer Physics Communications, 185, 708, (2014), available at http://dx.doi.org/10.1016/j.cpc.2013.10.013.

http://www.idre.ucla.edu/hpc/research/

Source codes available at:
https://idre.ucla.edu/hpc/parallel-plasma-pic-codes/