U.S. Particle Accelerator School
Education in Beam Physics and Accelerator Technology

Intro to Parallel Computing

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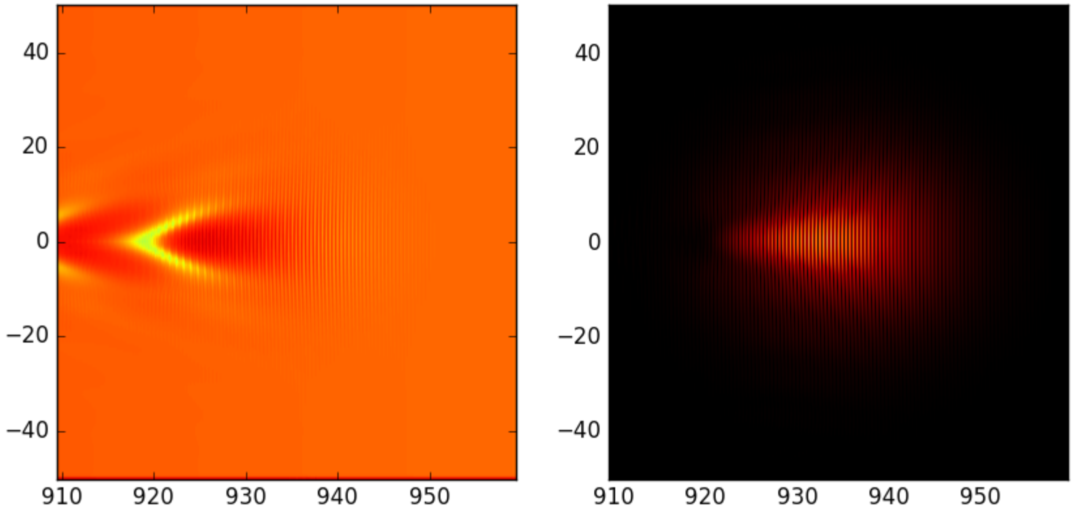
Outline

- Modern parallel architectures
- Parallelization between nodes: MPI
- Parallelization within one node: OpenMP

Why use parallel architecture?

- **Example:** Laser-wakefield simulation to interpret experiments at LBNL.

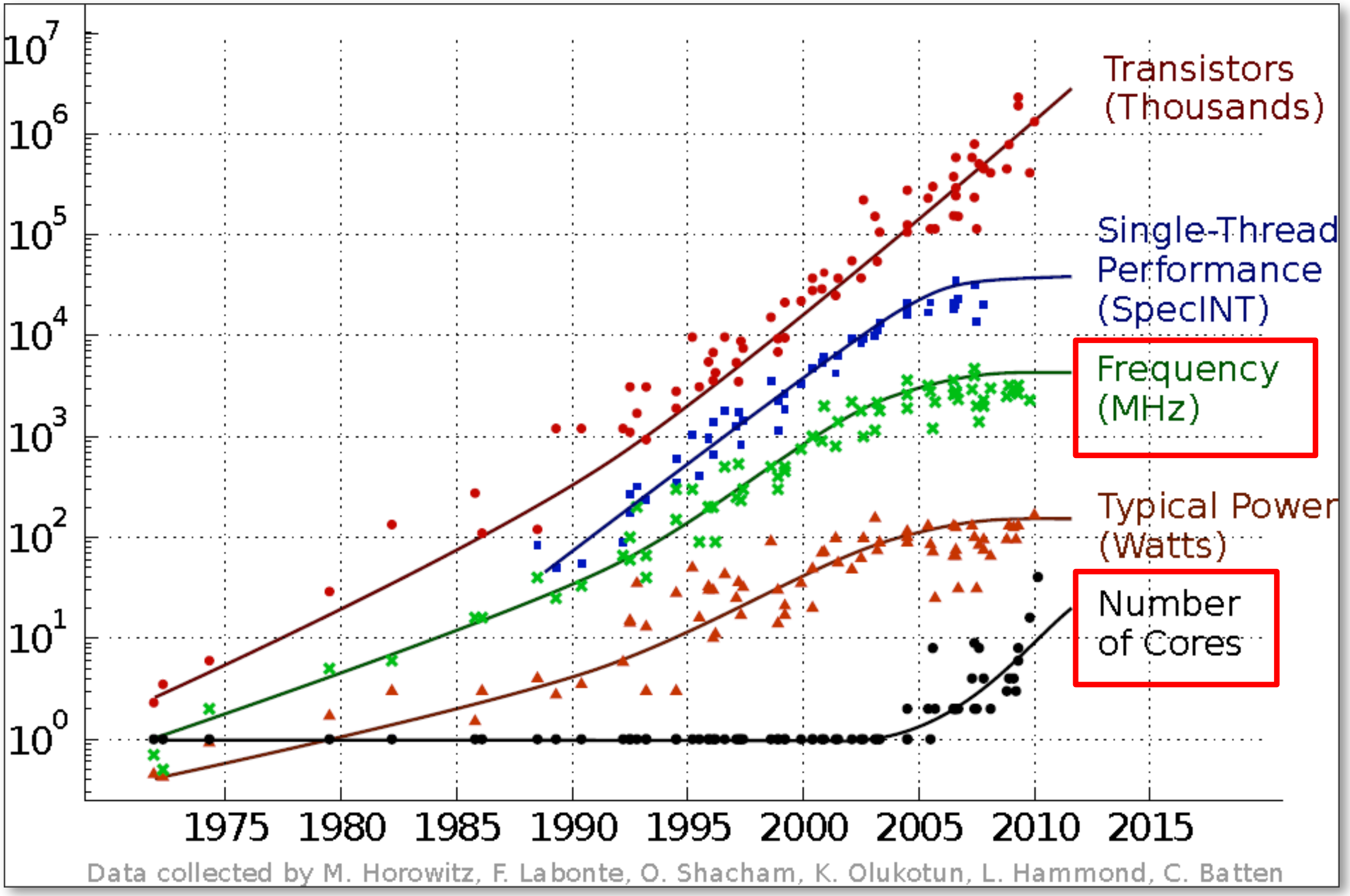


3D grid with 2500 x 200 x 200 grid points
0.2 billion macroparticles
140,000 timesteps (Courant limit!)

~60,000 hours on 1 core = 7 years!
=> Need either faster cores or more cores in parallel

Why use parallel architectures?

History of CPU performance



Data collected by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, C. Batten

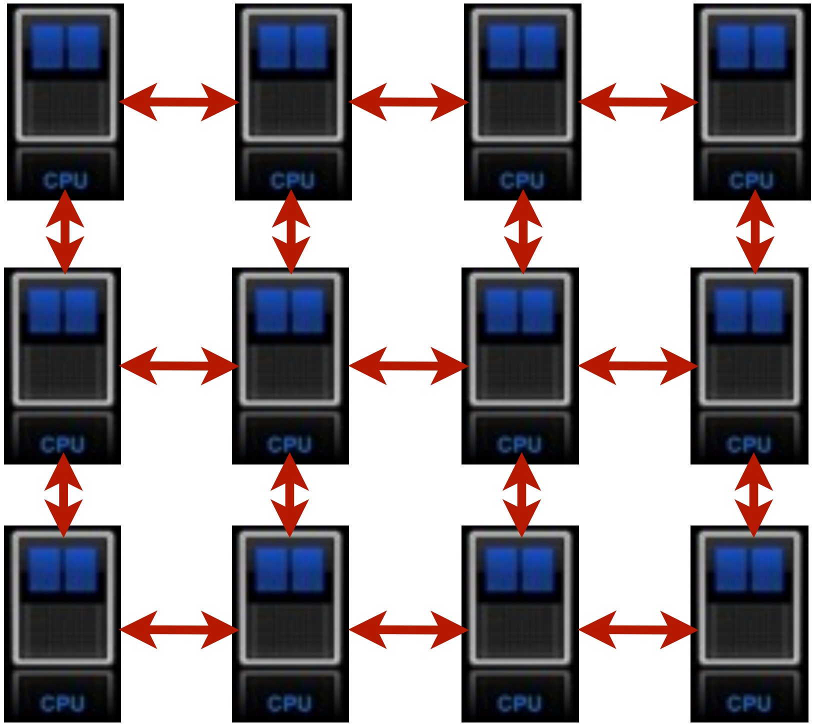
Nowadays, individual cores do not get faster.
We need to use **many cores in parallel**.

Parallel clusters

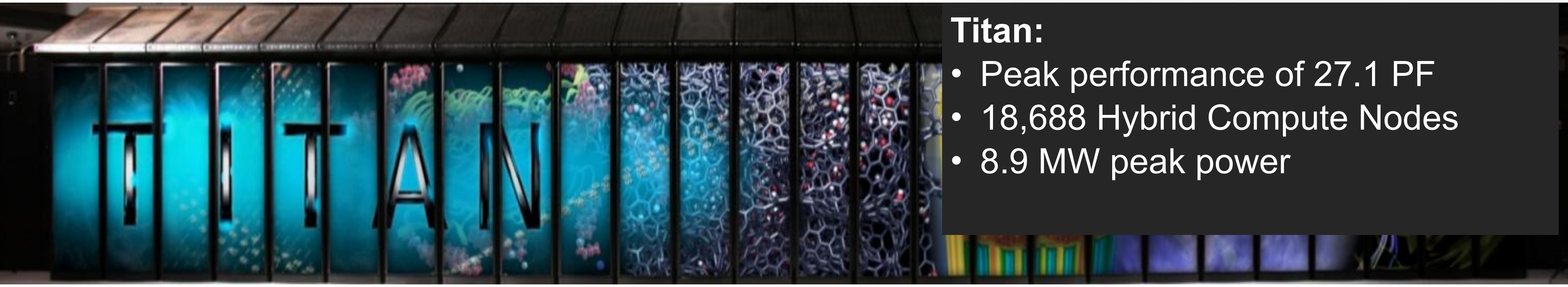
Contain **100,000+** cores

↔ “Fast” network communication (~10 Gb/s)

Individual node



Leadership and Production Computing Facilities



Titan:

- Peak performance of 27.1 PF
- 18,688 Hybrid Compute Nodes
- 8.9 MW peak power

Mira:

- Peak performance of 10 PF
- 49,152 Compute Nodes
- 4.8 MW peak power

Edison XC30:

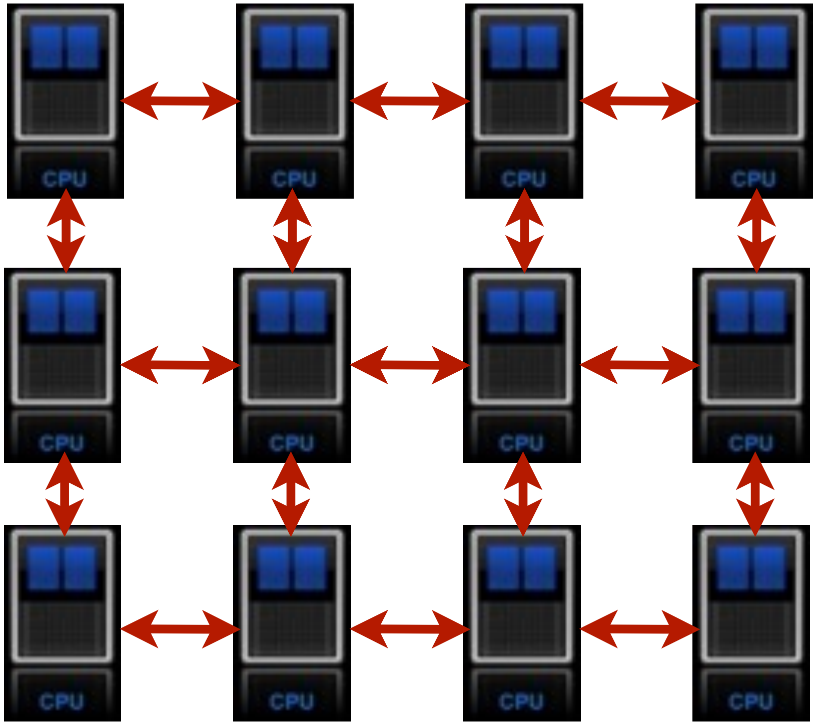
•Peak performance 2.4 PF

•124,608 processing cores

•2.1 MW peak power

Courtesy Steve Binkley, BESAC 2016

Parallel clusters



Individual nodes have several cores (i.e. computing units):

- "Traditional" CPUs: ~10 cores

- Xeon Phi: 68 cores

- GPUs: ~1000 (slow) cores

Cores within one node <u>share memory</u>.
Cores from different nodes do not.

- How to use this architecture to make a PIC code faster?
- How to use the two levels of parallelism?
(within one node and between nodes)

Class discussion

- Is the code that you use parallelized?
  Do you know what technology it uses (MPI, OpenMP, etc.)?

- Do you ever use ~100 nodes, ~1000 nodes?
  Did you experience difficulties associated with it (scaling, etc.)?

- Do you use GPUs?

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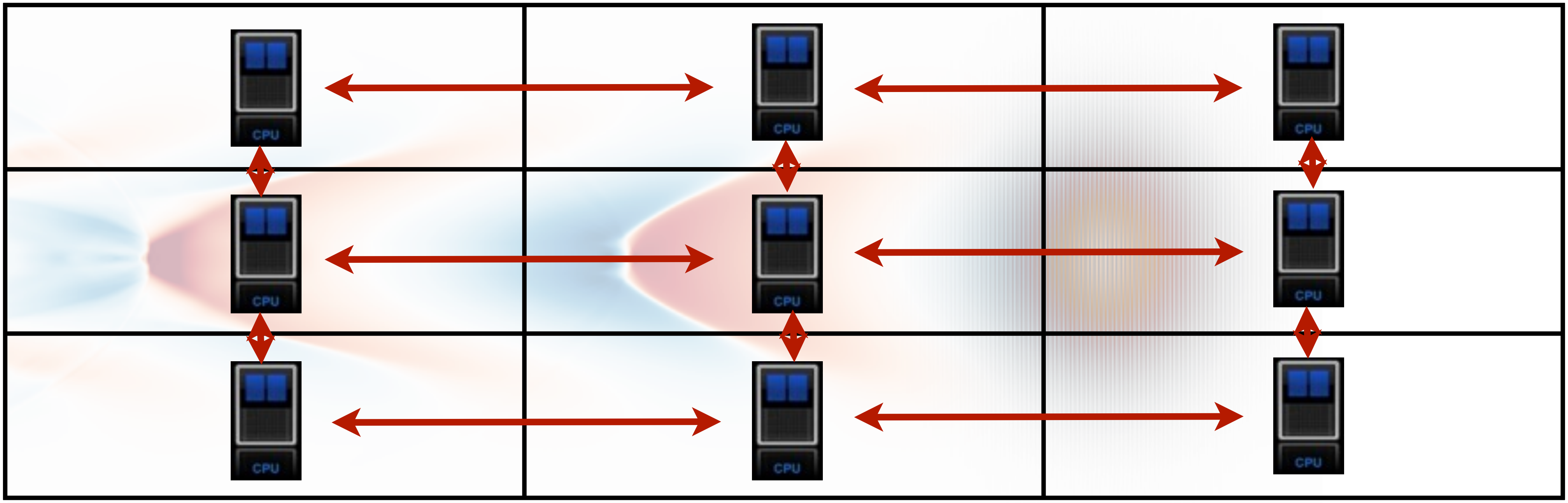
Domain-decomposition

Each node deals with a fixed chunk of the simulation box
(which includes fields on the grid + macroparticles)



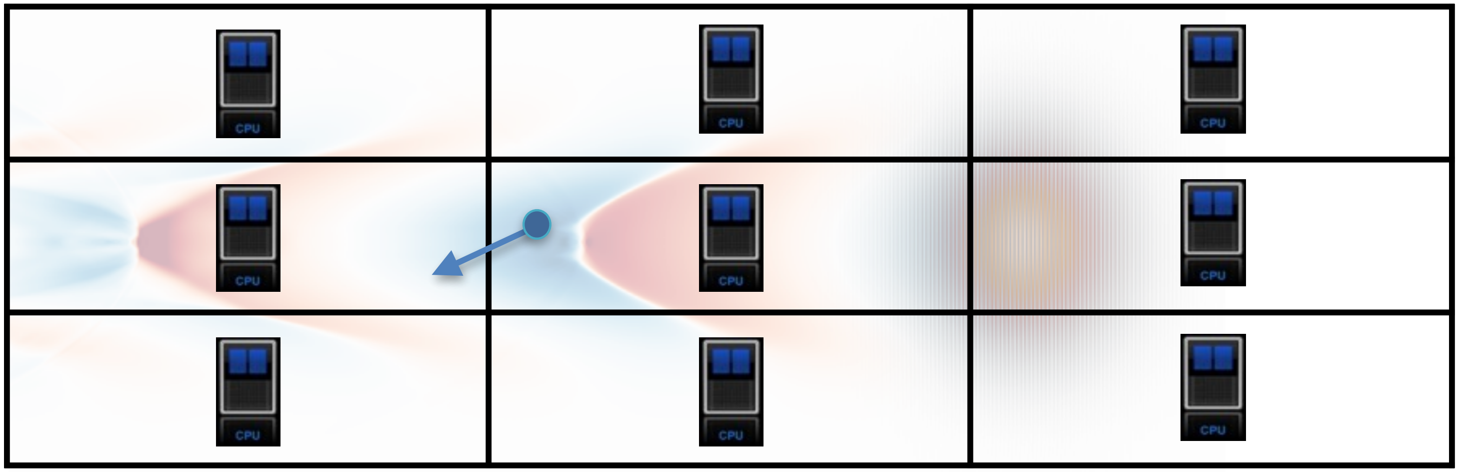
↔ “Fast” network communication

The nodes are not independent:
They need to exchange information with other nodes via the **network.**

Domain-decomposition minimizes this: communications only with a few neighbors

Domain-decomposition: particle exchange

Particle pusher: macroparticles may cross domain boundaries



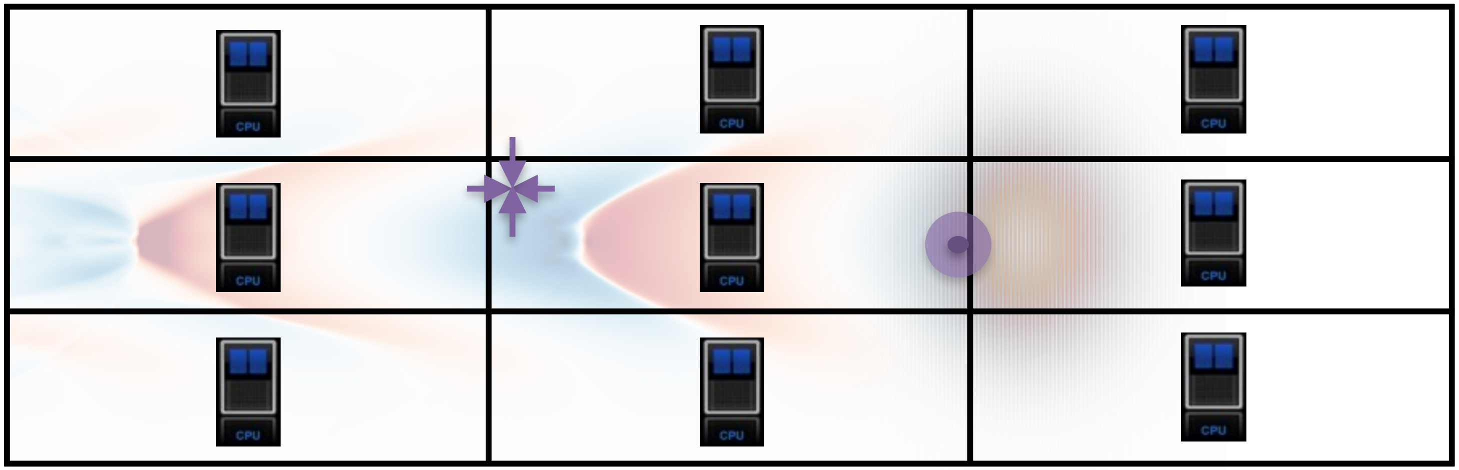
After the particle pusher, the particle data needs to be communicated from one node to the other.

Domain-decomposition: field exchange

Field update: each node needs values from neighboring nodes to calculate the spatial derivatives at the boundary

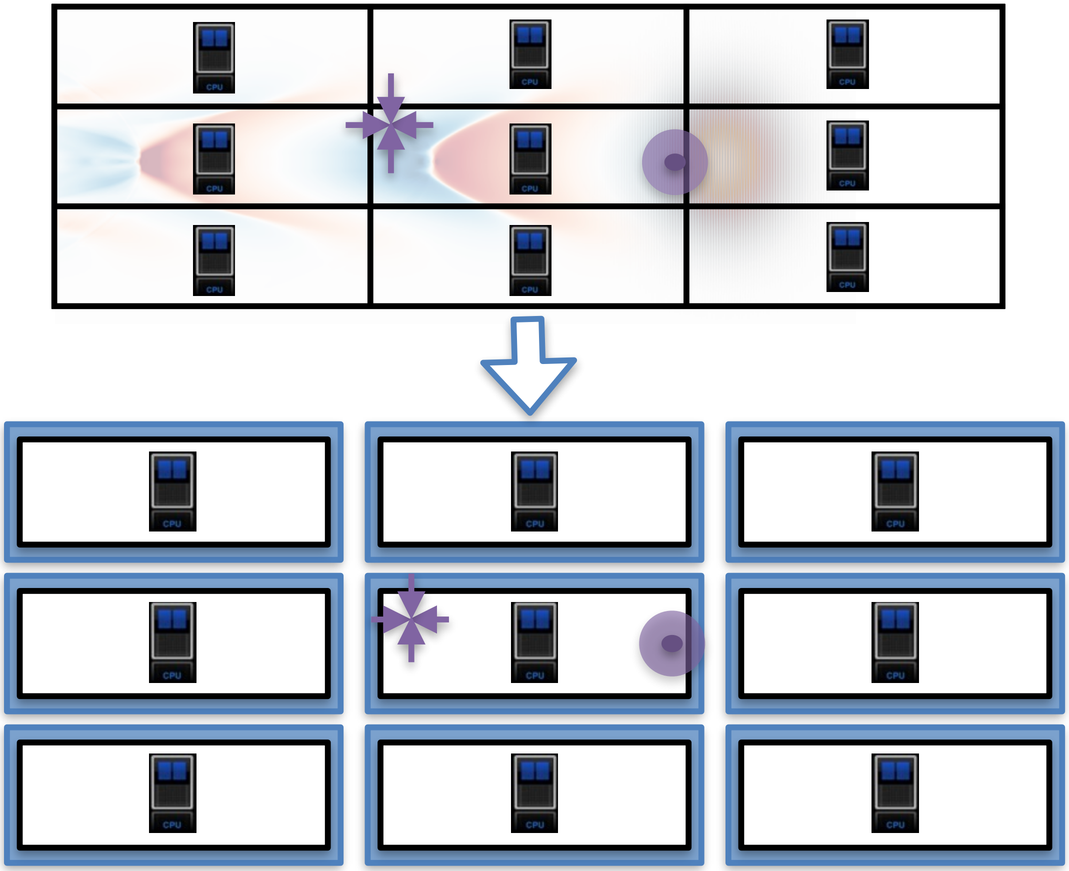
$$\partial_t B_y|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} = -\partial_z E_x|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} + \partial_x E_z|^n_{i+\frac{1}{2},j,k+\frac{1}{2}}$$

Field gathering/Current deposition: with wide shape factor, particles gather field values **from** other nodes and deposit some current/charge **to** other nodes



But the cores from different nodes do not share memory!
(i.e. the required data is not readily available)

Domain-decomposition: guard cells



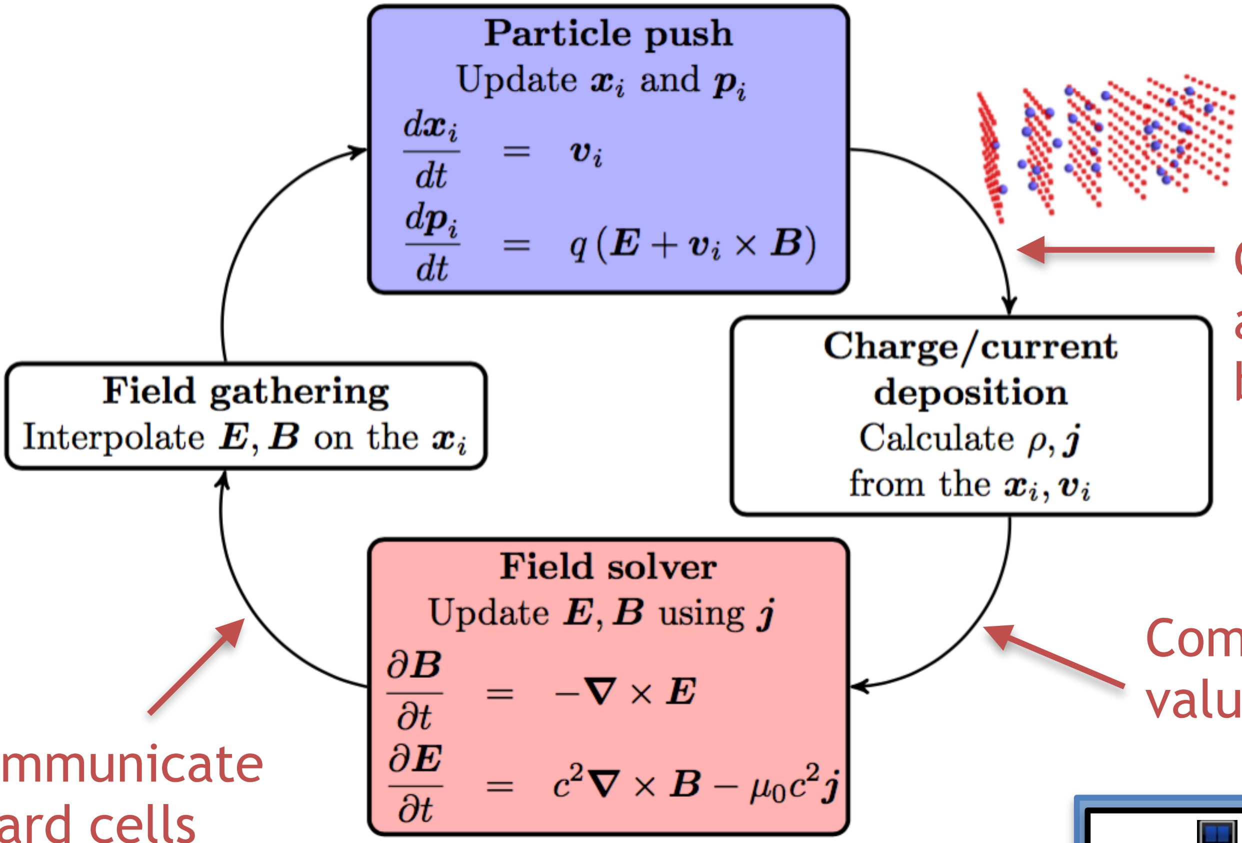
White: physical cells simulated by the node

Blue: guard cells

Each node has **guard cells** i.e.
cells that are a **local copy** of the **physical cells** from neighbor nodes
and make these values **readily available.**

The guard cells need to be “synced”, whenever their value is updated.

Sum up: the PIC loop



Particle push

Update $\boldsymbol{x}_i$ and $\boldsymbol{p}_i$

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

$$\frac{d\boldsymbol{p}_i}{dt} = q\,(\boldsymbol{E} + \boldsymbol{v}_i \times \boldsymbol{B})$$

Charge/current deposition

Calculate $\rho, \boldsymbol{j}$ from the $\boldsymbol{x}_i, \boldsymbol{v}_i$

Field solver

Update $\boldsymbol{E}, \boldsymbol{B}$ using $\boldsymbol{j}$

$$\frac{\partial \boldsymbol{B}}{\partial t} = -\boldsymbol{\nabla} \times \boldsymbol{E}$$

$$\frac{\partial \boldsymbol{E}}{\partial t} = c^2 \boldsymbol{\nabla} \times \boldsymbol{B} - \mu_0 c^2 \boldsymbol{j}$$

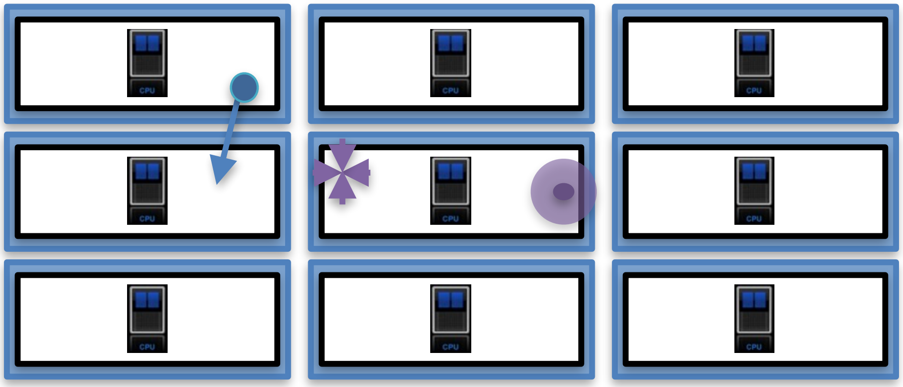
Field gathering

Interpolate $\boldsymbol{E}, \boldsymbol{B}$ on the $\boldsymbol{x}_i$

Communicate particles at the boundaries between nodes

Communicate guard cells values for charge/current

Communicate guard cells values for E/B

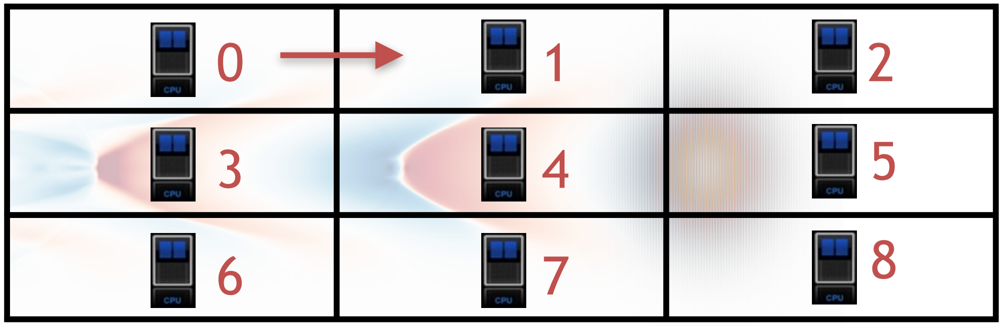


Exchanging information: MPI

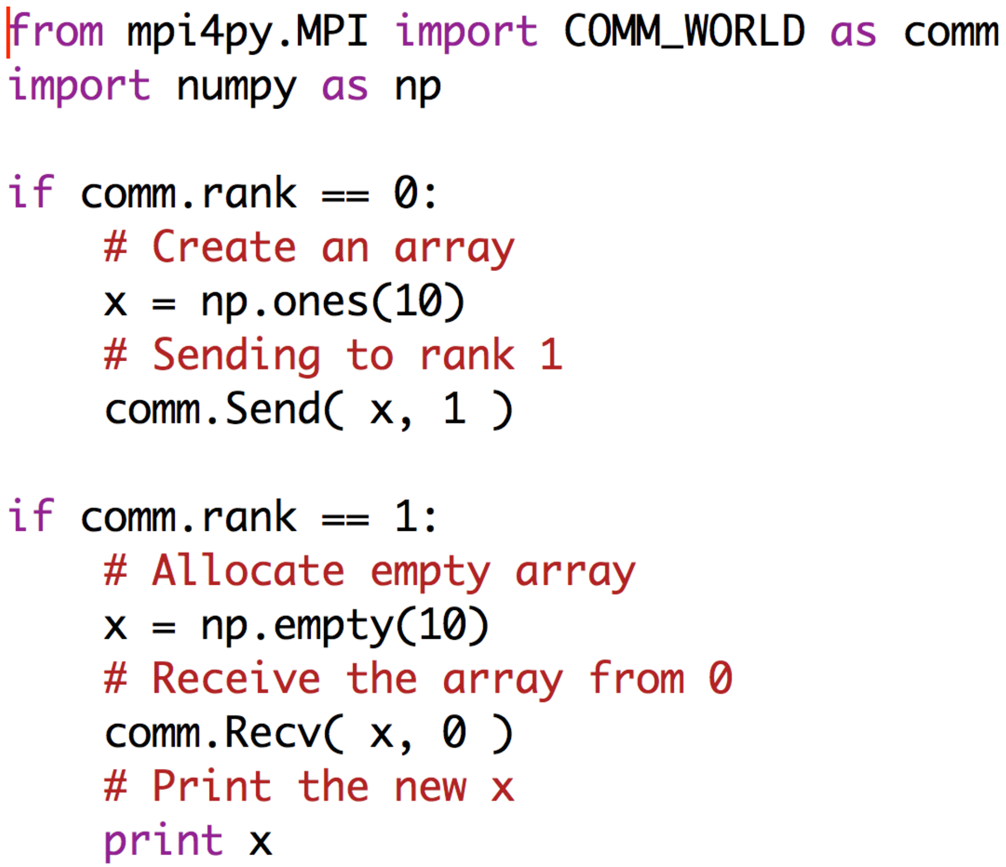
MPI: Message Passing Interface

Library that allows to **send/receive information** between processes:

- Each process has an **id** (or “rank”)
- Each process executes the **same source code**
- Call sending/receiving commands based on id



Example in Python:

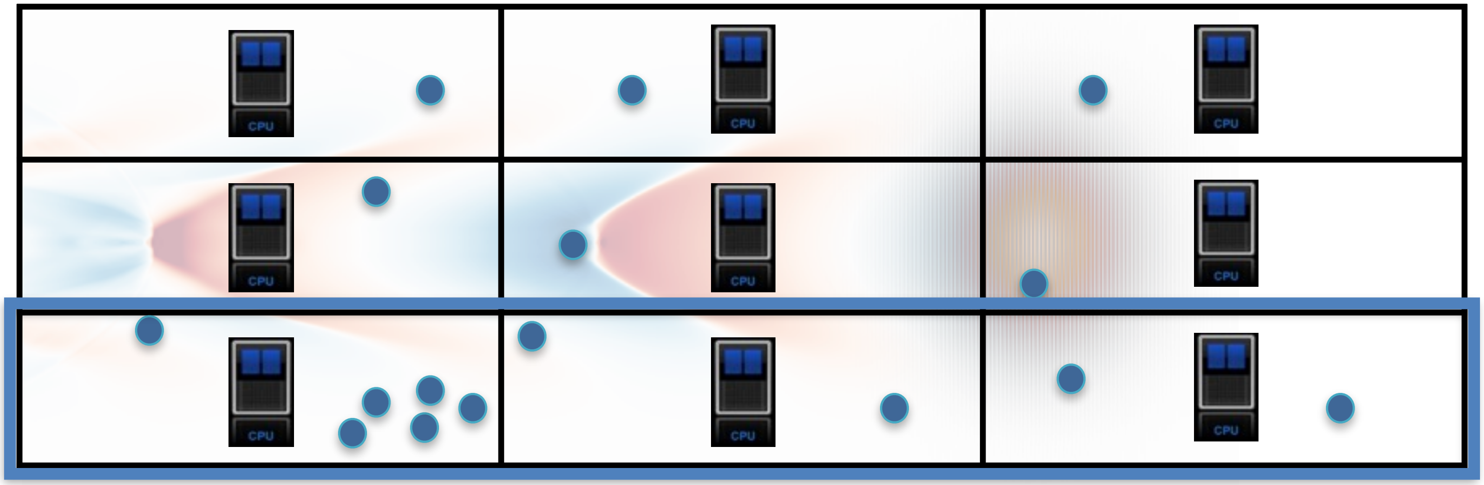


```
from mpi4py.MPI import COMM_WORLD as comm
import numpy as np

if comm.rank == 0:
    # Create an array
    x = np.ones(10)
    # Sending to rank 1
    comm.Send( x, 1 )

if comm.rank == 1:
    # Allocate empty array
    x = np.empty(10)
    # Receive the array from 0
    comm.Recv( x, 0 )
    # Print the new x
    print x
```

Problem: load balancing



Example:
particle pusher,
schematic view

Push particle 1	Push particle 1	Push particle 1
Push particle 2	Push particle 2	Push particle 2
Push particle 3	Exchange particles ↔	Exchange particles
Push particle 4	Wait	...
Push particle 5	Wait	
Push particle 6	Wait	
Exchange particles ↔	Exchange particles	

Compute time

The simulation will always progress at the pace of the slowest node (the one doing the most work)

=> Problematic when the particle distribution is very non-uniform

Outline

- Modern parallel architectures

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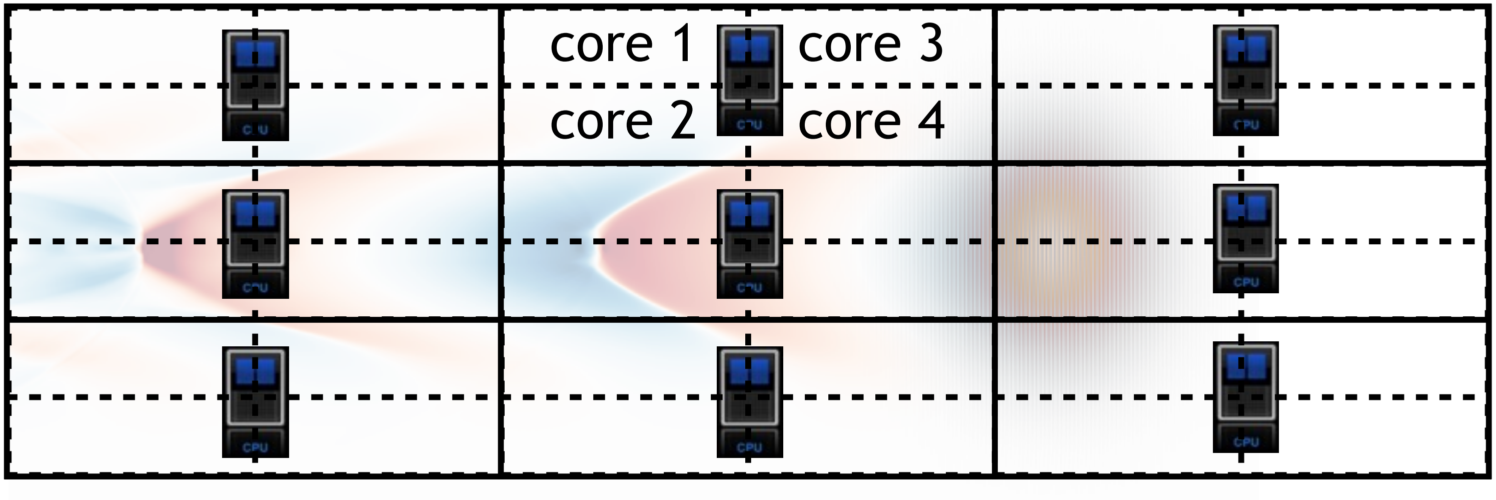
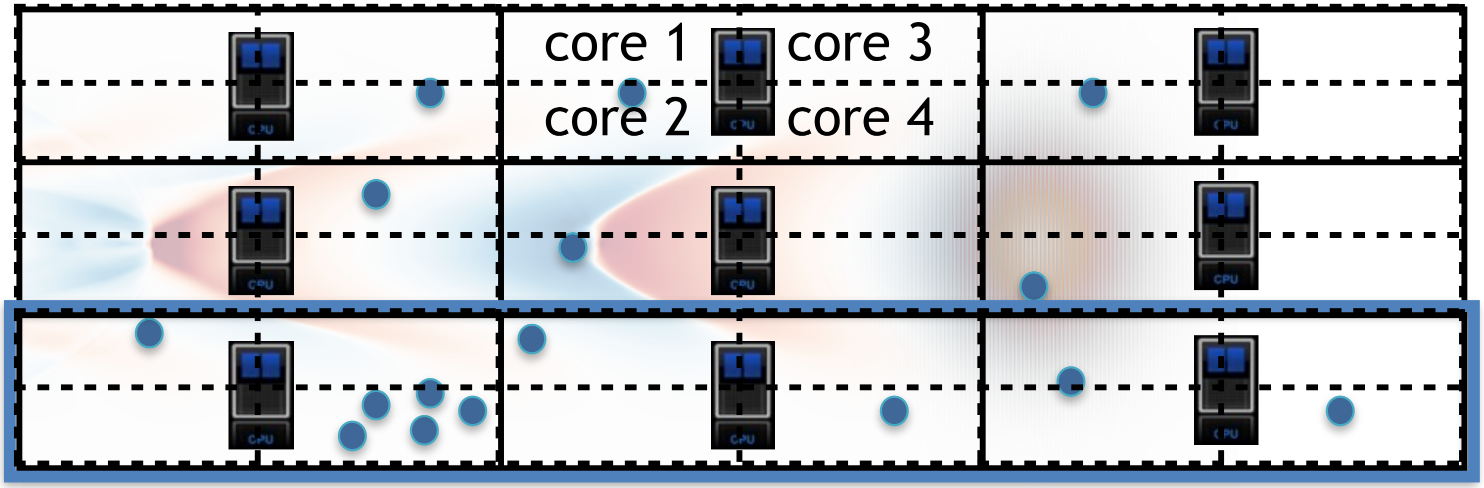
Parallelization within one node: MPI

Parallelization within one node can be done with MPI:
Divide each nodes's sub-domain into smaller sub-domain.
Each core is **tied** to one of the smaller sub-domain.



The smaller sub-domains have guard cells and exchange information via **MPI send/receive**, within one node. (but in this case the information does not go through the network).

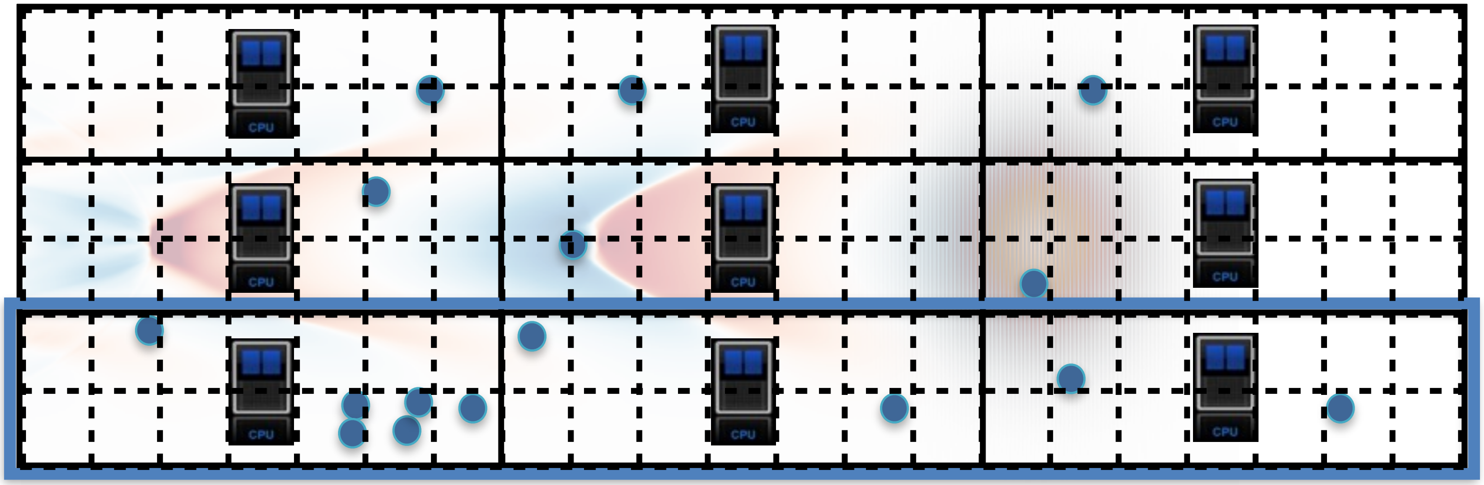
MPI within one node: even worse load balancing!



core1	core2	core3	core4	core1	core2	core3	core4	core1	core2	core3	core4
push			push	push			push	push			push
			push	Exchange particles ↔				Exchange particles			
			push								
			push								
			push								
Exchange particles ↔				Exchange particles							

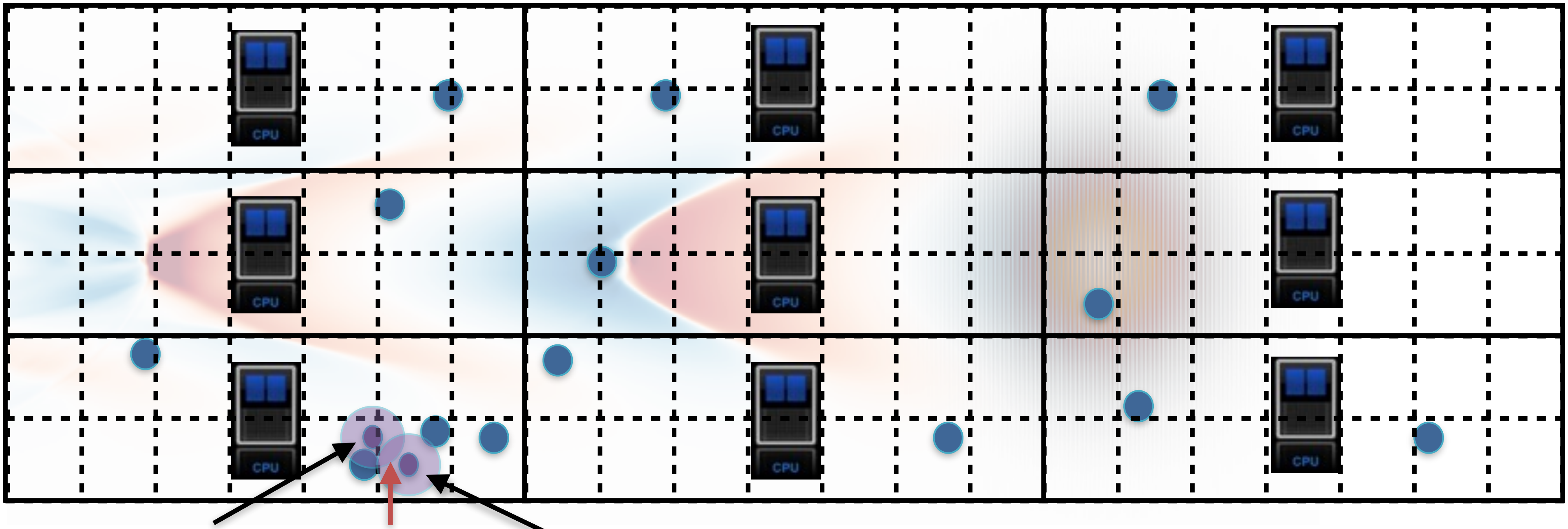
OpenMP within one node: load balancing

- **Create more subdomains than cores**
  (here 4 cores per node but 14 subdomains or "tiles")
- **With OpenMP, cores are not tied to one subdomain**
  Cores can work one subdomain and then **switch** to another depending on the work that remains to be done.
  Only possible **within one node**, because memory is **shared**
- **No need for guard cells within one node.**



core1	core2	core3	core4	core1	core2	core3	core4	core1	core2	core3	core4
push	push	push	push	push			push	push			push
	push	push		Exchange particles ⟷				Exchange particles			
Exchange particles ⟷				Exchange particles							

OpenMP's dangers: race condition



Core 2 performs current deposition

Race condition!

Core 3 performs current deposition

- The cores do not exchange information via **MPI send/receive**. Instead they **directly** modify the value of the current **in shared memory**, without notifying the other cores.

- Potentially, two cores could **simultaneously** try to modify the value of the current in a given cell (leads to inconsistencies). This can be avoided with proper care (e.g. "atomic operations").

OpenMP: practical consideration

- **On the developer side:**
  Not available in Python, but available in **C** and **Fortran**
  Requires to use “**pragmas**” in the code.

  Example in Fortran:

```
!!$OMP PARALLEL DO
DO it=1,nt
    …
    …
ENDDO
```

(Use OpenMP to do the loop in parallel)
(Loop over “tiles”)

(Perform work on one “tile”)

- **Warp does not use OpenMP for the moment**

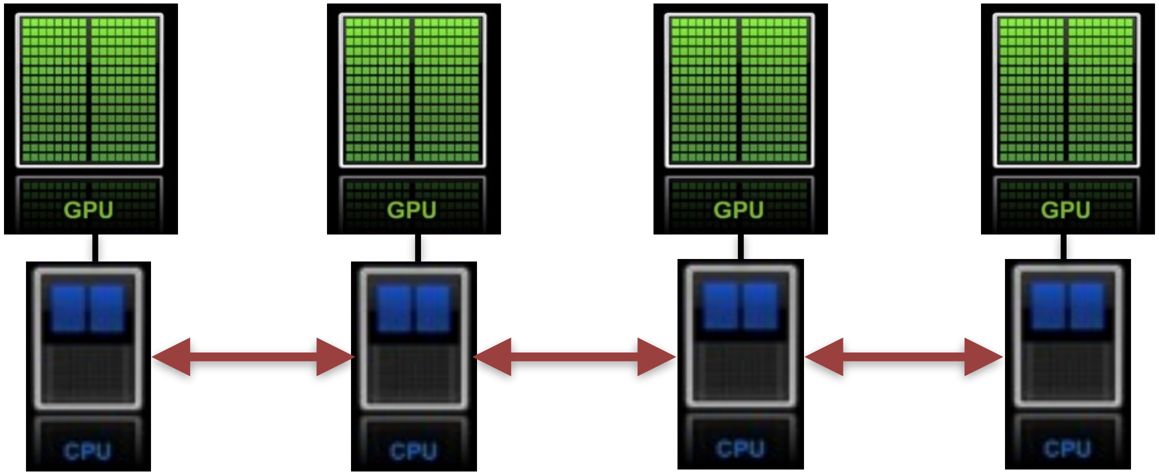
- **But Warp can use PICSAR, which does use OpenMP**
  PICSAR = highly-optimized library for elementary operations, such as particle pusher, current deposition, field gathering, etc.
  PICSAR is soon to be released as open-source.

GPU programming

- **Conceptual similarities with OpenMP programming:**
  load balancing by tiling, race conditions

- **But also differences:**
  ~1000s (slow) cores instead of 10-60 cores
  Only connected to the network through an associated CPU
  GPU programming uses **<u>specific language</u>** (CUDA, OpenCL, …)

- **The trend for the future is to bridge the difference between many-core CPUs and GPU:**
  hardware (more cores on CPU, GPUs to be integrated with CPUs)
  language (OpenMP starts targeting GPUs)



Summary

- Parallel architectures are organized around (at least) **two levels of parallelization**:
  - Inter-nodes (uses network)
  - Intra-node (uses shared memory)

- The "traditional" paradigm (in the PIC community) is to use MPI at both levels. This is limited, esp. due to load-balancing.

- "Novel" paradigms are becoming more and more common: MPI+OpenMP (with tiles), MPI+GPU, etc.