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

Intro to Parallel Computing

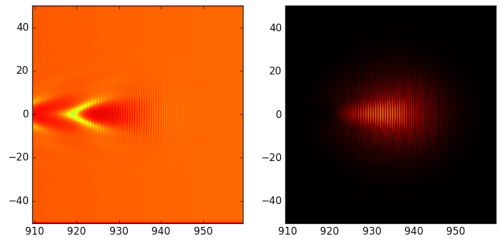
Remi Lehe
Lawrence Berkeley National Laboratory

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.

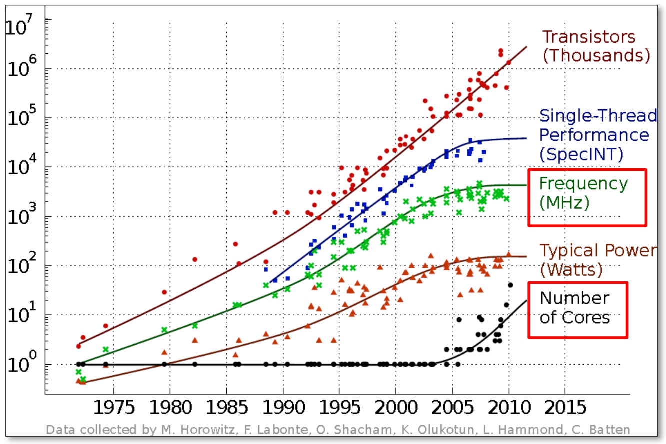


3D grid with 2500 x 200 x 200 grid points
0.2 billion macroparticles
140,000 timesteps (Courant limit!)

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

Why use parallel architectures?

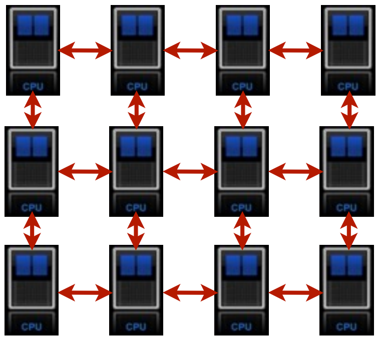
History of CPU performance



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

Parallel clusters

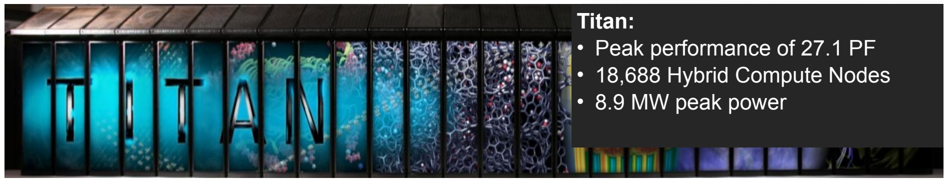
Contain **100,000+** cores



↔ "Fast" network communication (~10 Gb/s)

Individual node

Leadership and Production Computing Facilities



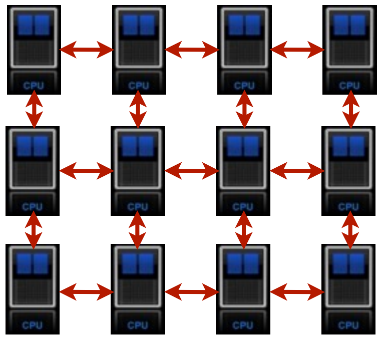
Titan:
- Peak performance of 27.1 PF
- 18,688 Hybrid Compute Nodes
- 8.9 MW peak power

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

dison XC30:
eak performance 2.4 PF
24,608 processing cores
.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.)?

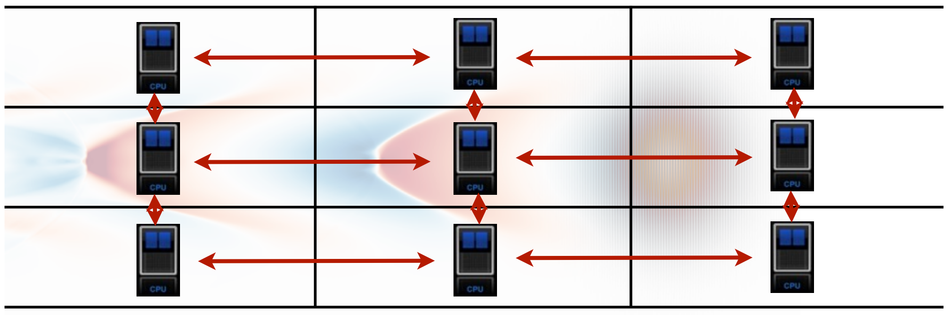
- Do you use GPUs?

Outline

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

Domain-decomposition

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



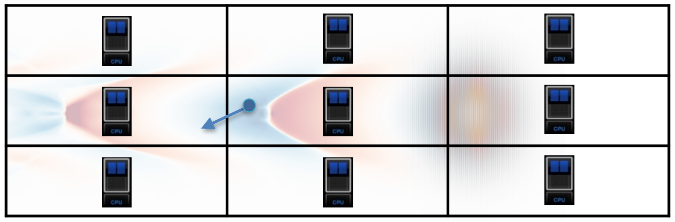
↔ "Fast" network communication

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



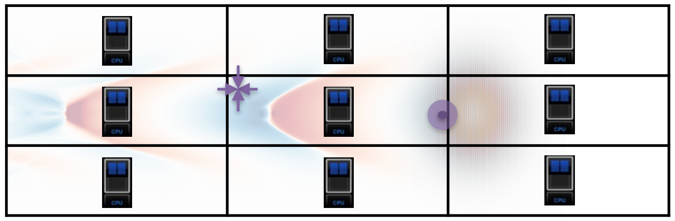
After the particle pusher, the particle data needs to be communicated from one node to the other.

Domain-decomposition: field exchange

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

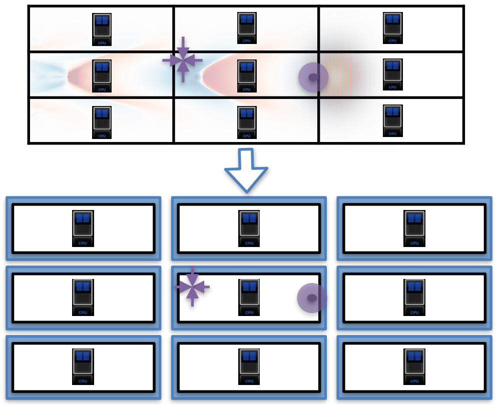
$$\partial_t B_y|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} = -\partial_z E_x|^n_{i+\frac{1}{2},j,k+\frac{1}{2}} + \partial_x E_z|^n_{i+\frac{1}{2},j,k+\frac{1}{2}}$$

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



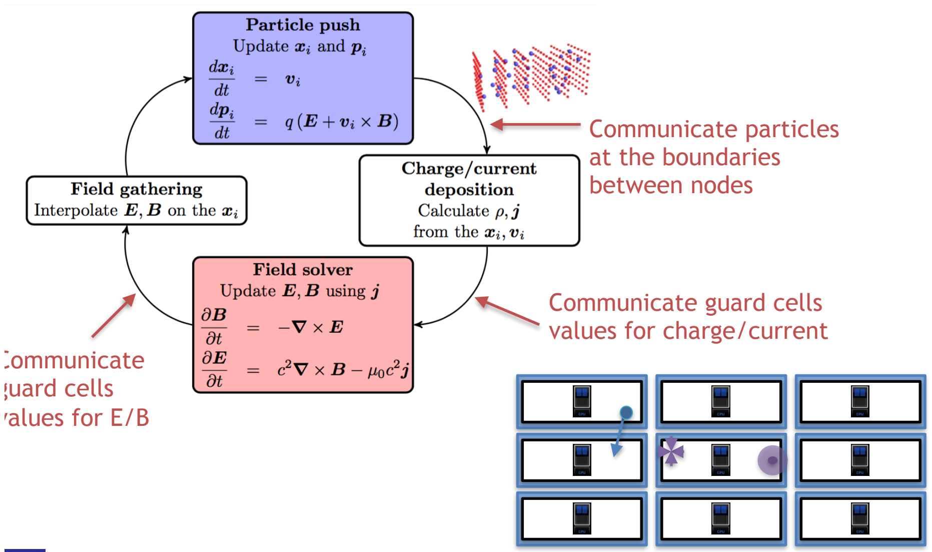
White: physical cells simulated by the node

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



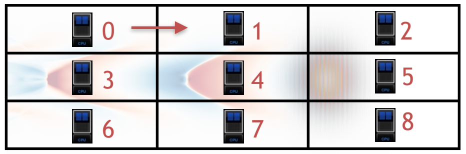
Particle push
Update x_i and p_i
$\frac{dx_i}{dt} = v_i$
$\frac{dp_i}{dt} = q\,(E + v_i \times B)$
Charge/current deposition
Calculate ρ, j from the x_i, v_i
Field solver
Update E, B using j
$\frac{\partial B}{\partial t} = -\nabla \times E$
$\frac{\partial E}{\partial t} = c^2 \nabla \times B - \mu_0 c^2 j$
Field gathering
Interpolate E, B on the 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



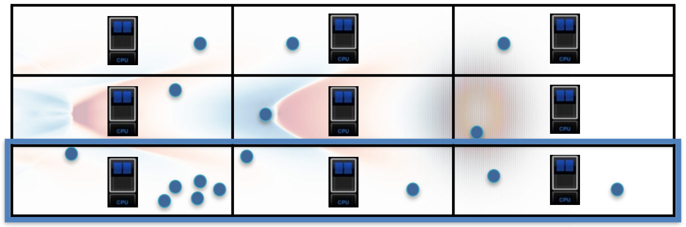
Example in Python:

```
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

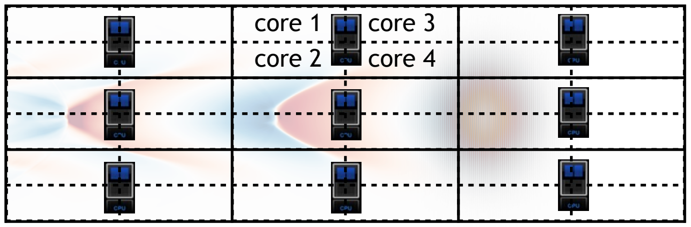
The simulation will always progress at the pace of the slowest node (the one doing the most work)
=> Problematic when the particle distribution is very non-uniform

Outline

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

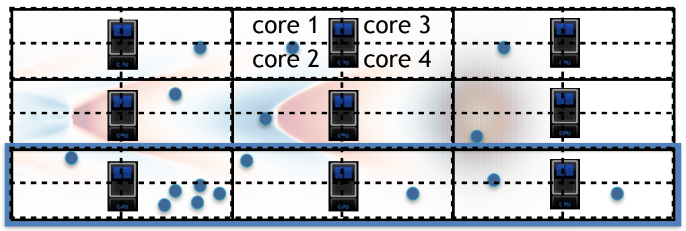
Parallelization within one node: MPI

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).

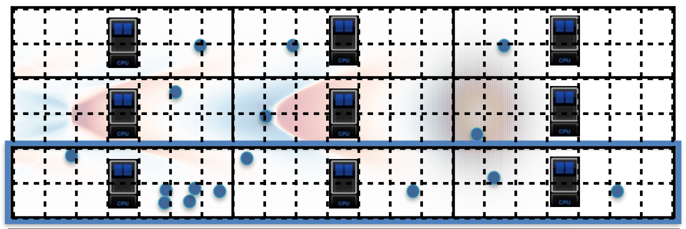
MPI within one node: even worse load balancing



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							

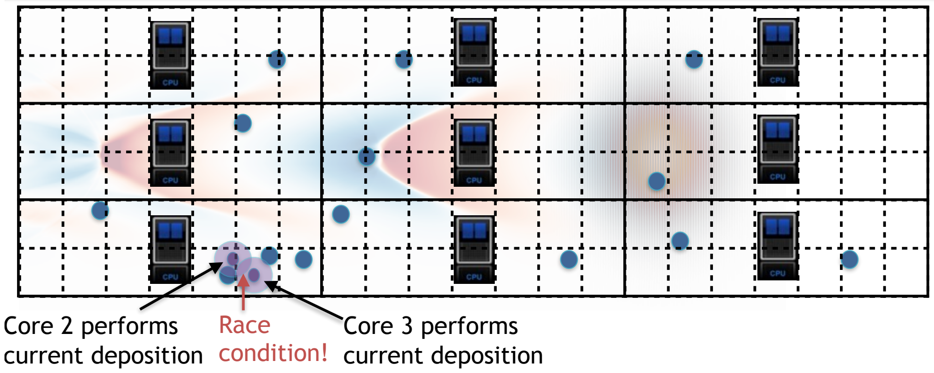
OpenMP within one node: load balancing

- **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


CPU
Core 2 performs current deposition
Race condition!
Core 3 performs current deposition

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

- Potentially, two cores could <u>**simultaneously**</u> 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    (Use OpenMP to do the loop in parallel)
DO it=1,nt            (Loop over "tiles")
    …
    …                 (Perform work on one "tile")
ENDDO
```

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

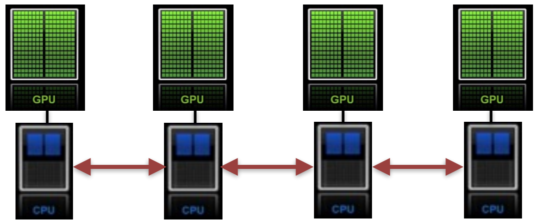
- **But Warp can use PICSAR, which does use OpenMP**
  PICSAR = highly-optimized library for elementary operations, such as particle pusher, current deposition, field gathering, etc.
  PICSAR is soon to be released as open-source.

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.