The Abdus Salam
International Centre
for Theoretical Physics

Overview on Parallel Programming Paradigms

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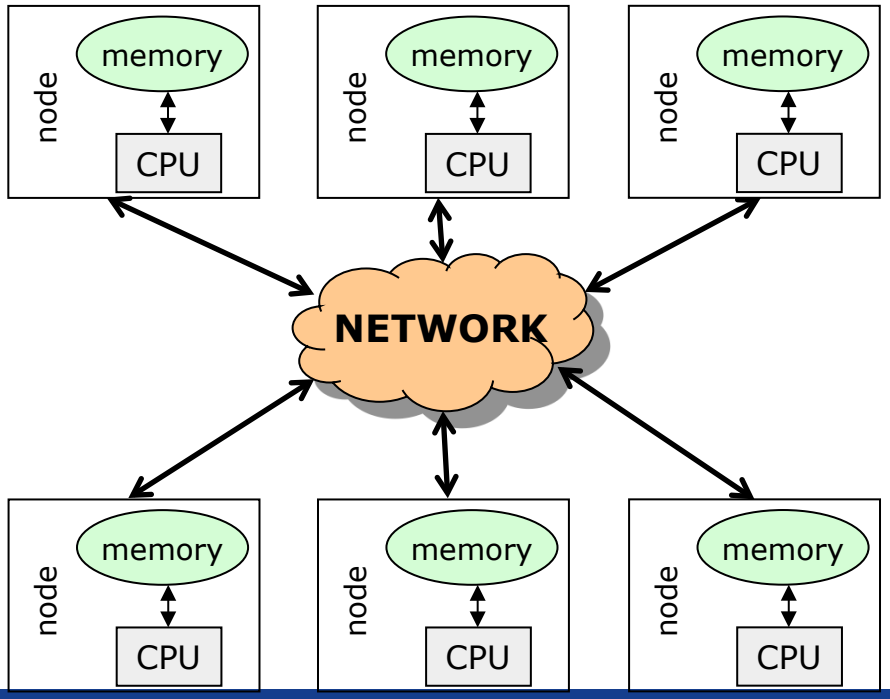
What Determines Performance?

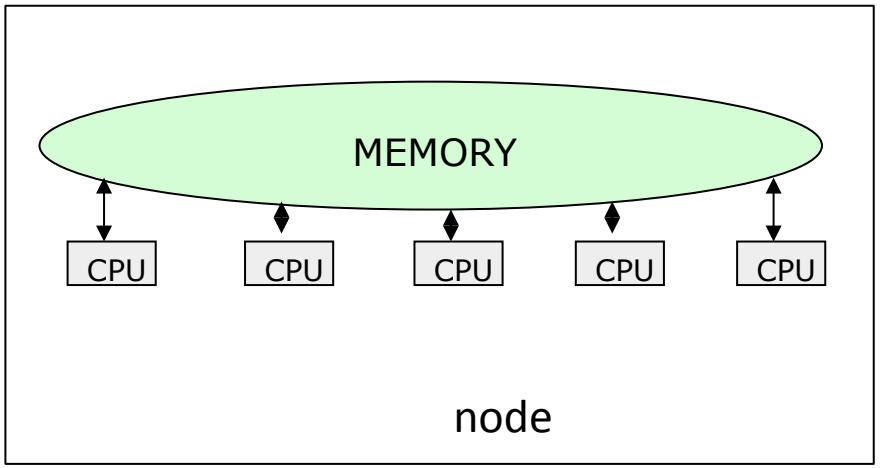
- How fast is my CPU?
- How fast can I move data around?
- How well can I split work into pieces?
  - Very application specific: never assume that a good solution for one problem is as good a solution for another
  - always run benchmarks to understand requirements of your applications and properties of your hardware
  - respect Amdahl's law

Parallel Architectures

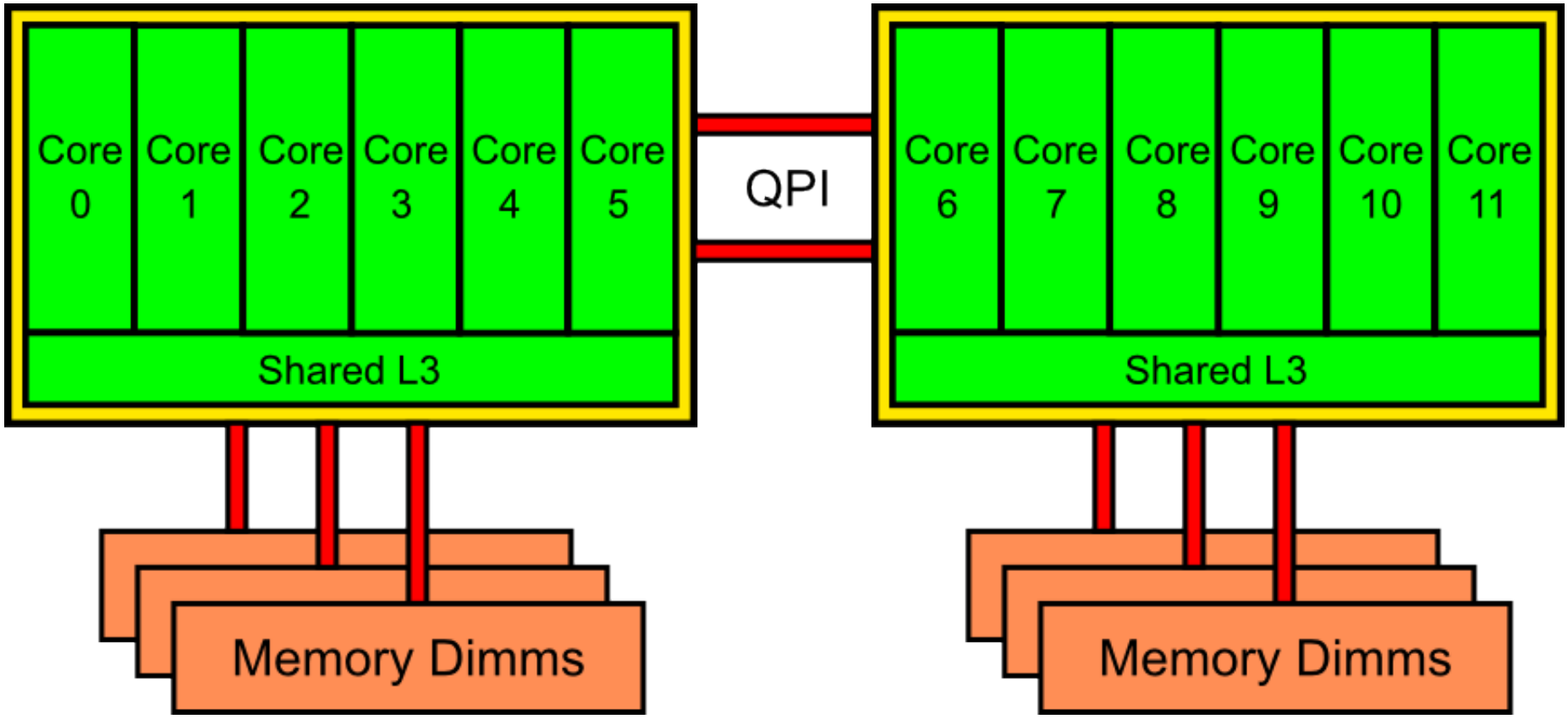
- Distributed Memory



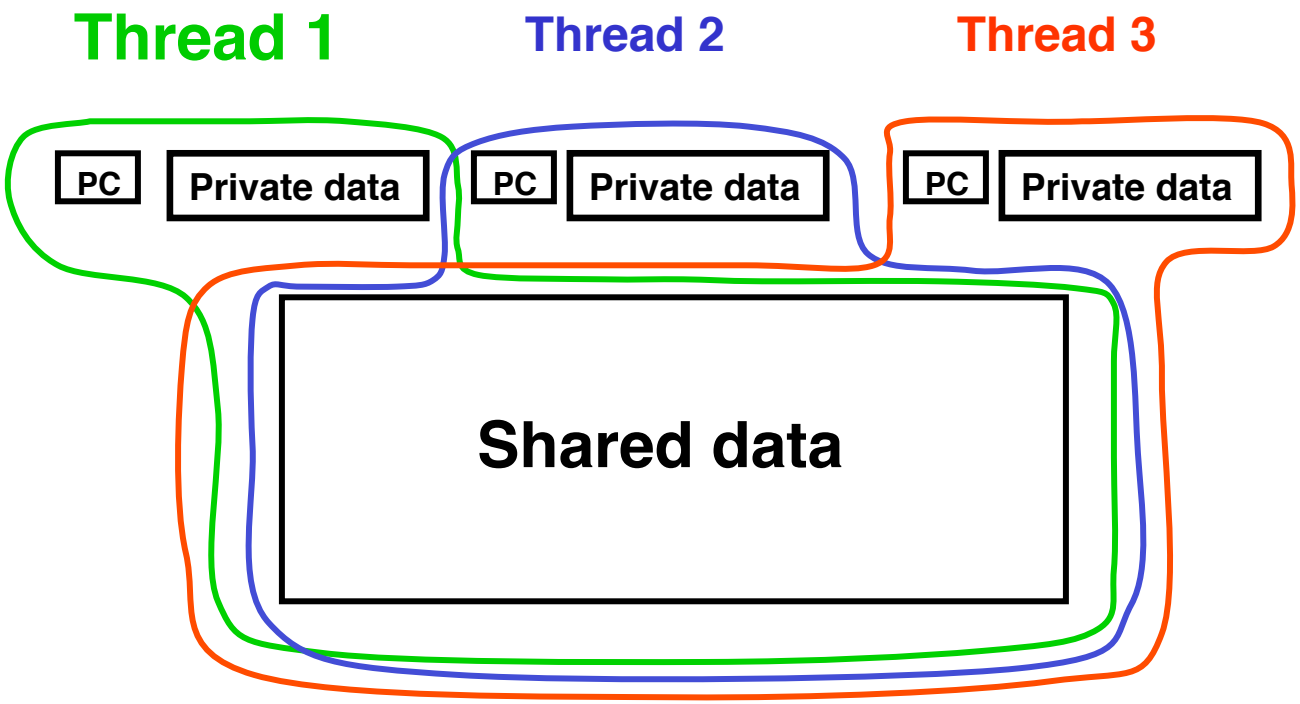
- Shared Memory



Multiple Socket CPUs



Paradigm at Shared Memory /1



Paradigm at Shared Memory /2

- Usually indicated as Multithreading Programming
- Commonly implemented in scientific computing using the OpenMP standard (directive based)
- Thread management overhead
- Limited scalability
- Write access to shared data can easily lead to race conditions and incorrect data

Parallel Programming Paradigms

- MPI (Message Passing Interface)
  - A standard defined for portable message passing
  - It available in the form of library which includes interfaces for expressing the data exchange among processes
  - A framework is provided for spawning the independent processes (i.e., mpirun)
  - Processes communication is via network
  - It works on either shared and distributed mem. architecture
  - ideal for distributing memory among compute nodes

MPI Program Design

- Multiple and separate processes (can be local and remote) concurrently that are coordinated and exchange data through “messages” => a “share nothing” parallelization
- Best for coarse grained parallelization Distribute large data sets; replicate small data
- Minimize communication or overlap communication and computing for efficiency => Amdahl's law

What is MPI?

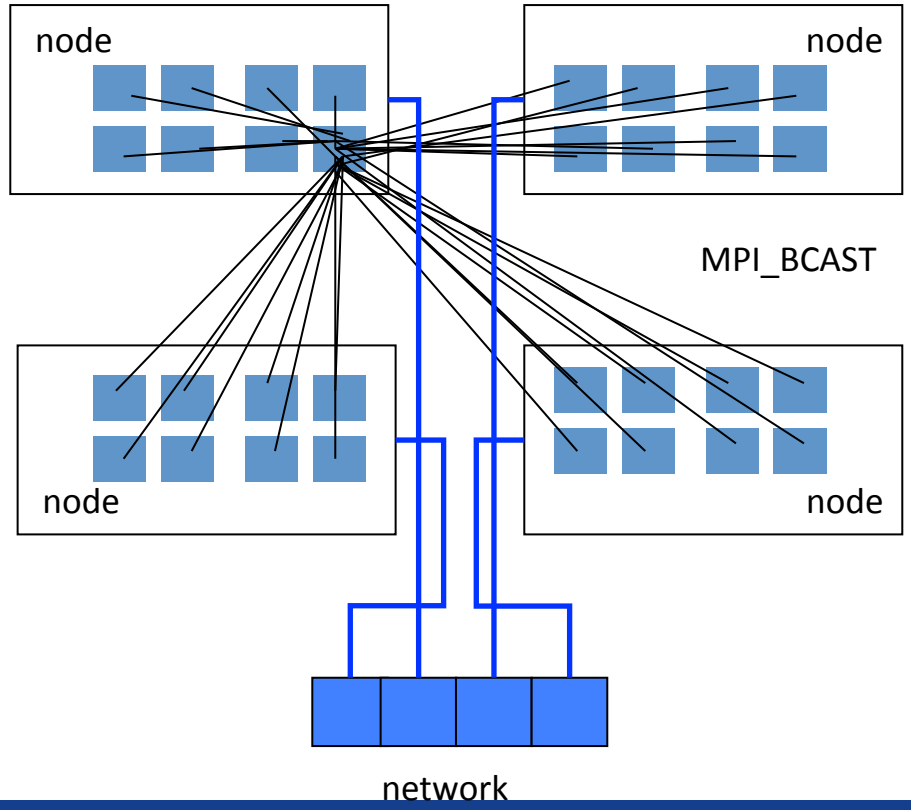
- A standard, i.e. there is a document describing how the API (constants & subroutines) are named and should behave; multiple "levels", MPI-1 (basic), MPI-2 (advanced), MPI-3 (new)
- A library or API to hide the details of low-level communication hardware and how to use it
- Implemented by multiple vendors
- Open source and commercial versions
- Vendor specific versions for certain hardware
- Not binary compatible between implementations

Programming Parallel Paradigms

- Are the tools we use to express the parallelism for on a given architecture
- They differ in how programmers can manage and define key features like:
  - parallel regions
  - concurrency
  - process communication
  - synchronism

MPI inter process communications

MPI on Multi core CPU



1 MPI proces / core
Stress network
Stress OS

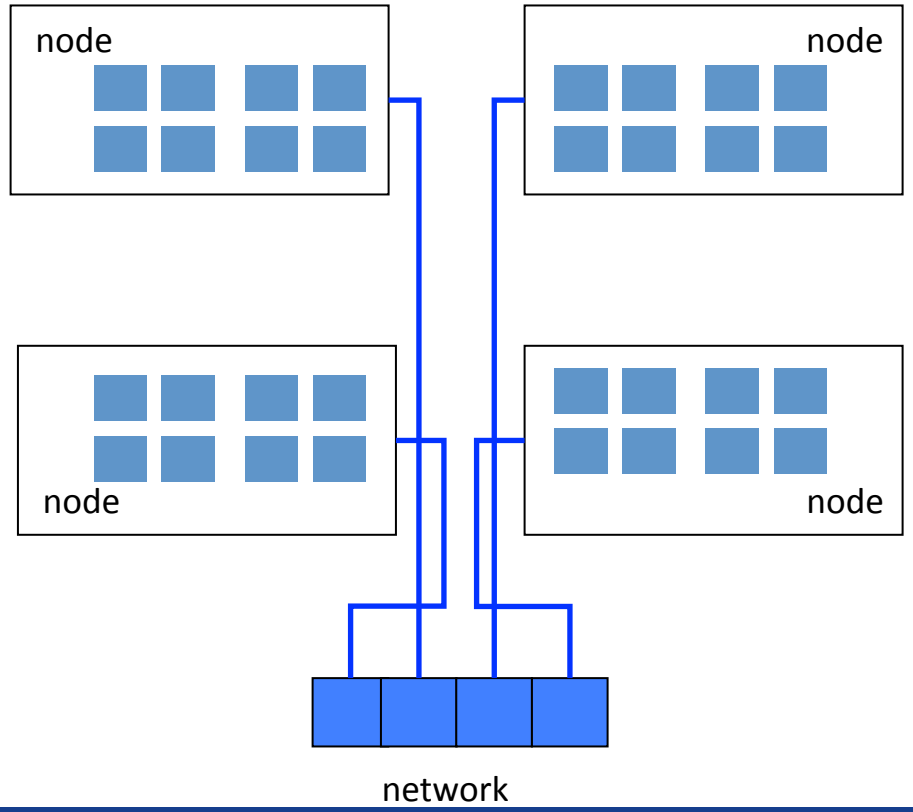
Many MPI codes (QE) based on ALLTOALL
Messages = processes * processes

We need to exploit the hierarchy

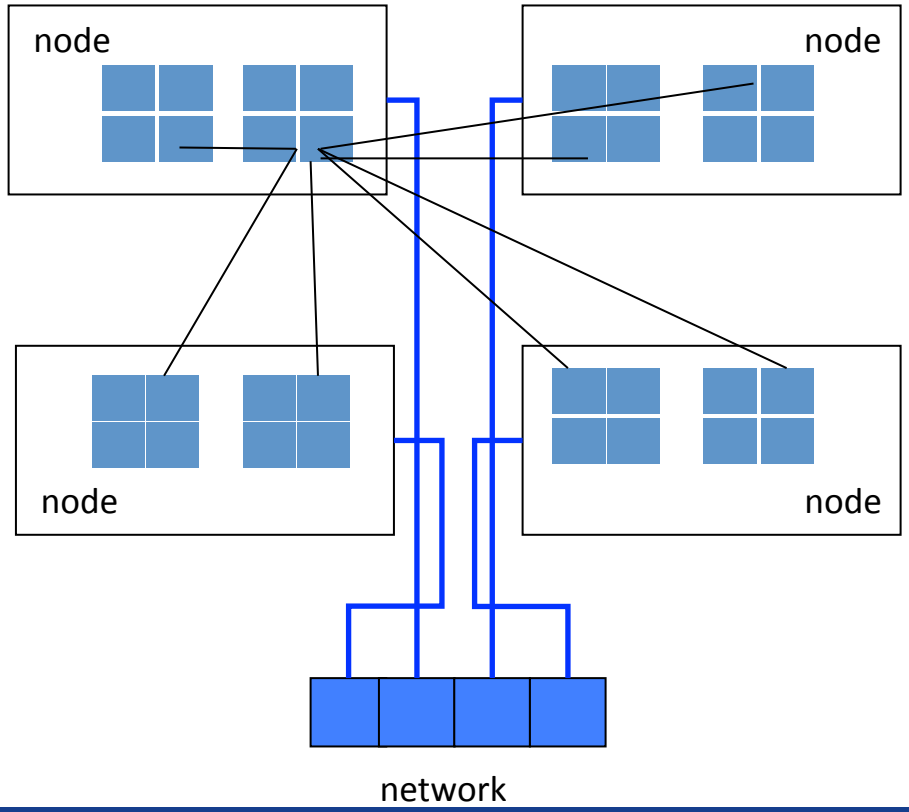
Re-design applications

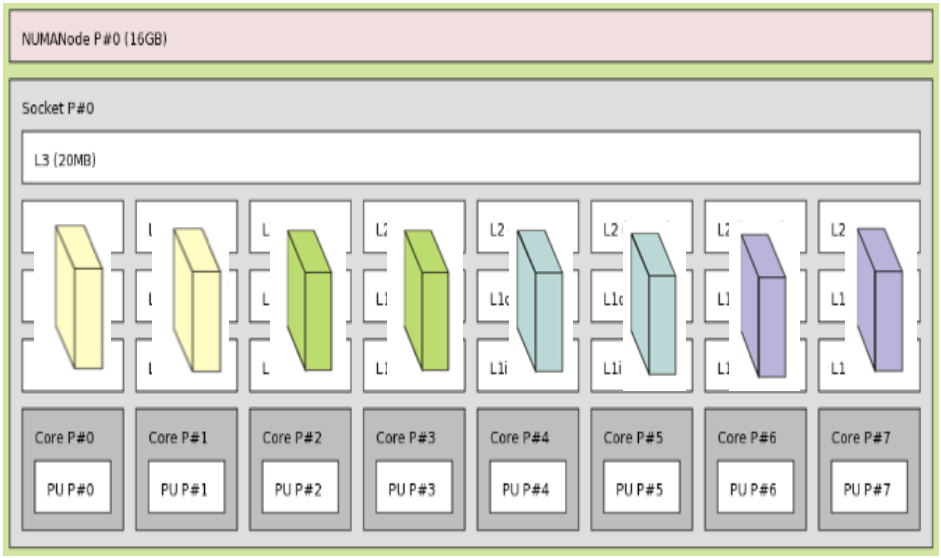
Mix message passing And multi-threading

The Hybrid Mode

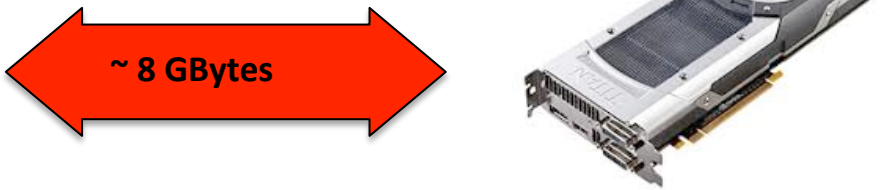


The Hybrid Mode

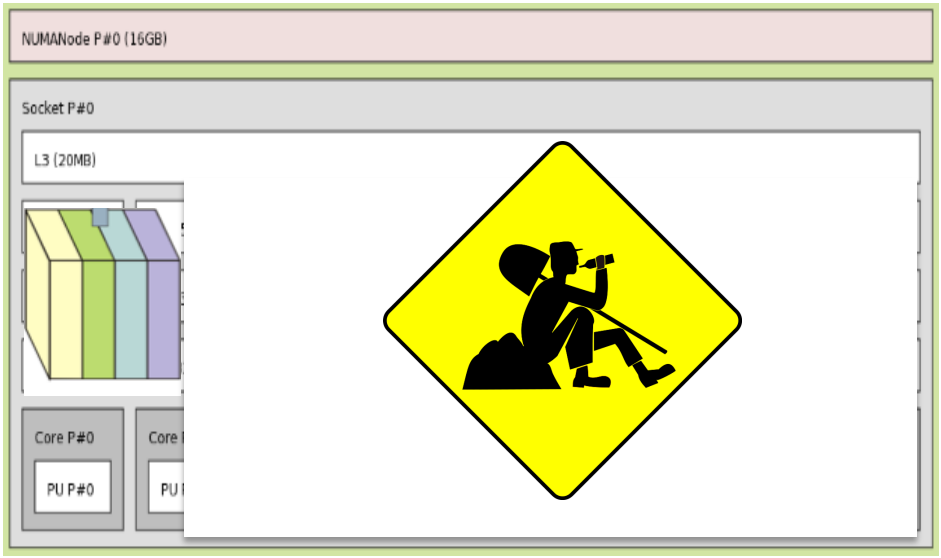




The Intel Xeon E5-2665
Sandy Bridge-EP 2.4GHz




```
mpirun -np 8 pw-gpu.x -inp input file
```



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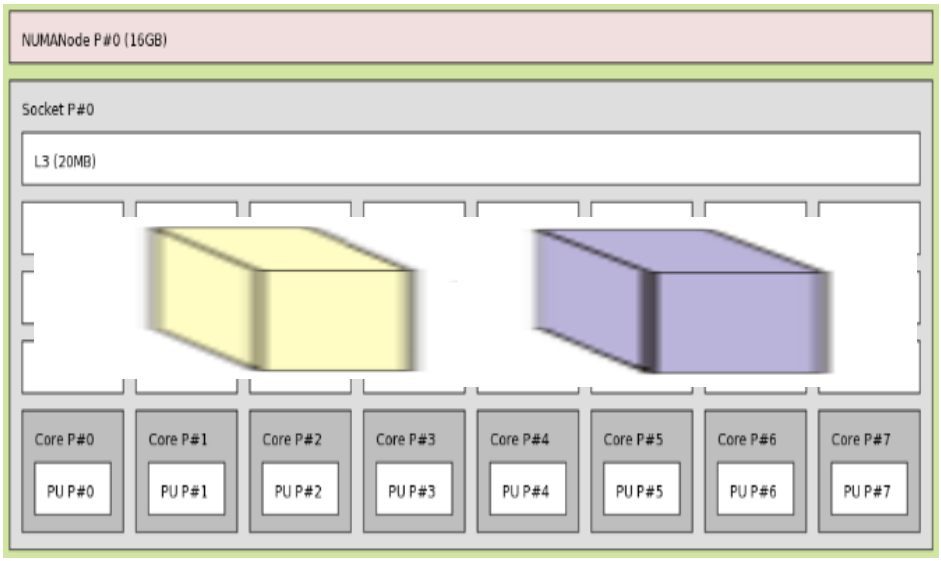

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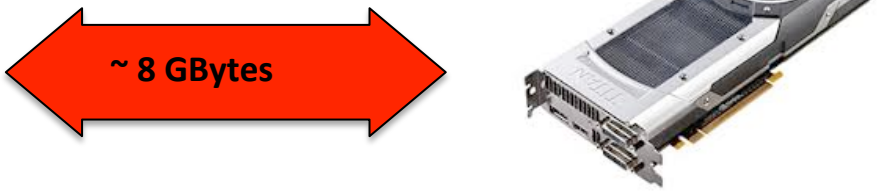
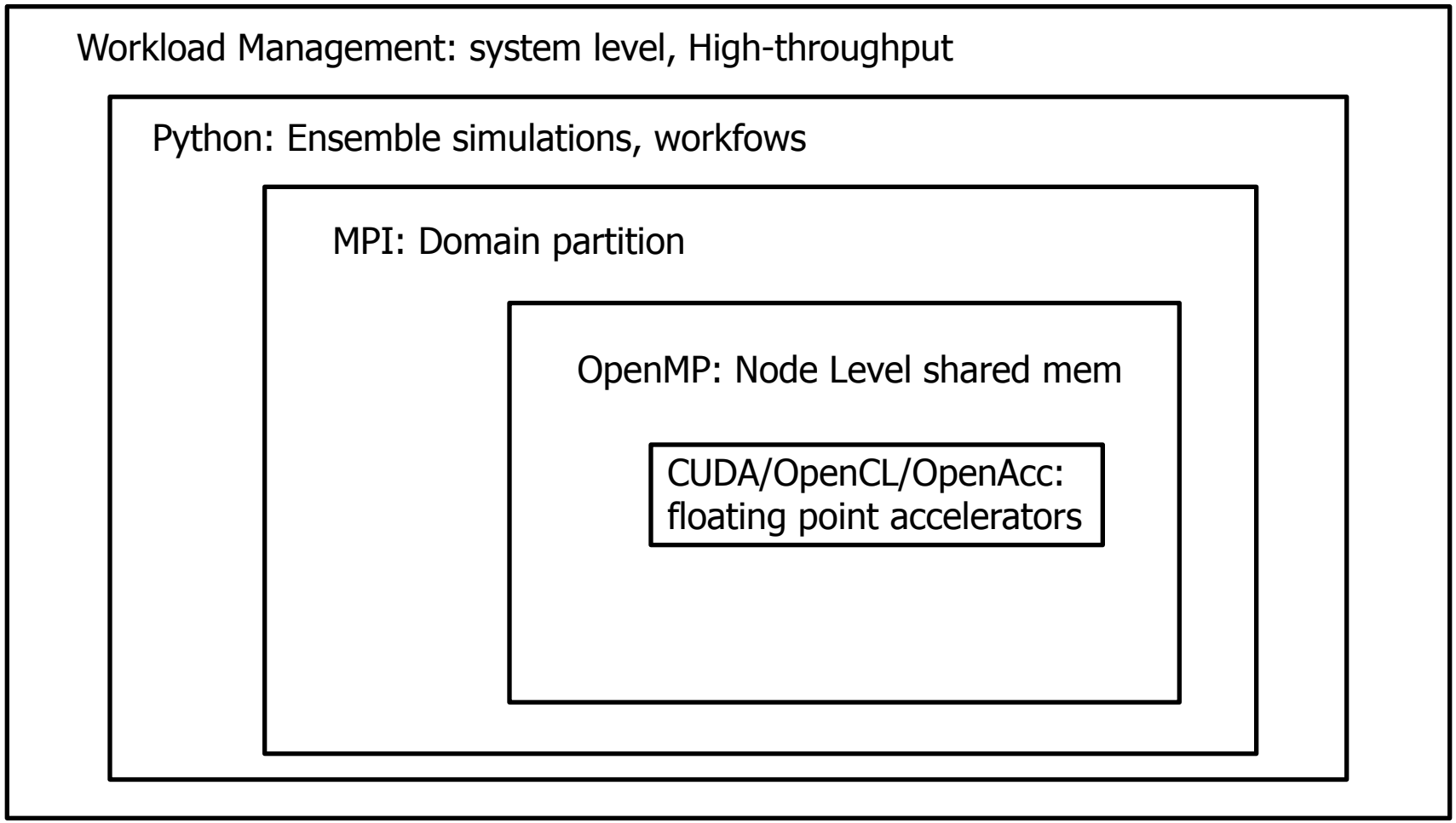



```
export OMP_NUM_THREADS=4
export OPENBLAS_NUM_THREADS=$OMP_NUM_THREADS
mpirun -np 2 pw-gpu.x -inp input file
```


Workload Management: system level, High-throughput
Python: Ensemble simulations, workfows
MPI: Domain partition
OpenMP: Node Level shared mem
CUDA/OpenCL/OpenAcc:
floating point accelerators

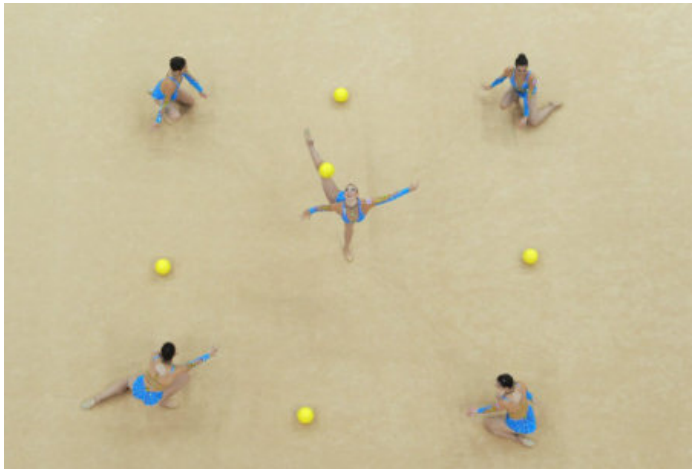
Type of Parallelism

- **Functional (or task) parallelism**: different people are performing different task at the same time

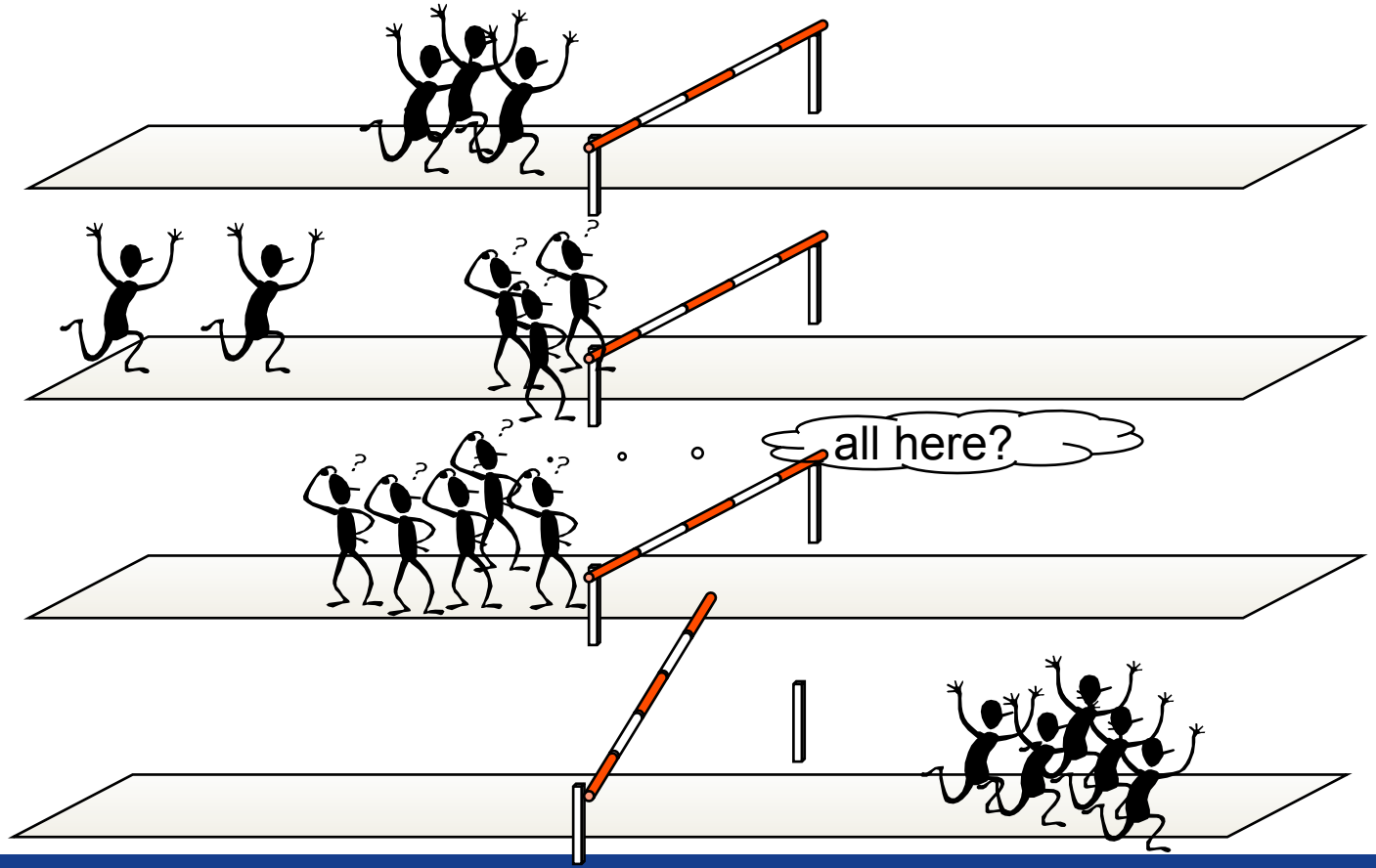
- **Data Parallelism**: different people are performing the same task, but on different equivalent and independent objects

Process Interactions

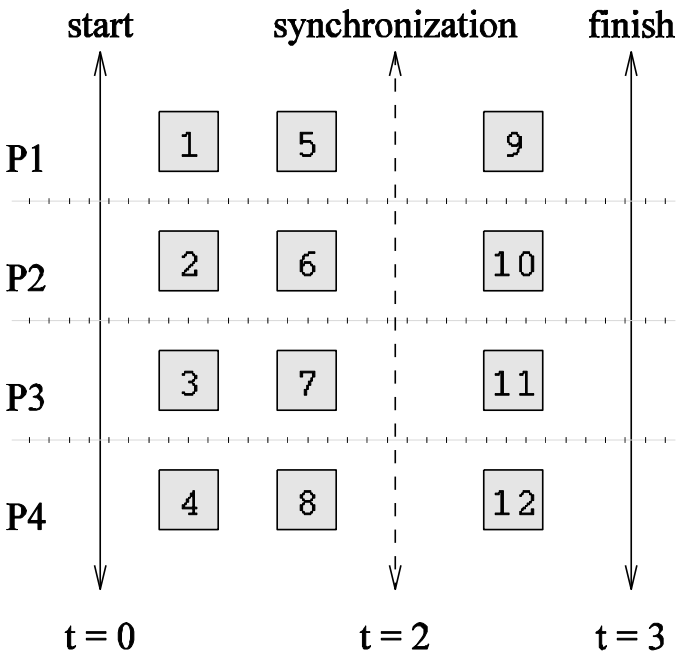
- The effective speed-up obtained by the parallelization depend by the amount of overhead we introduce making the algorithm parallel
- There are mainly two key sources of overhead:
  1. Time spent in inter-process interactions (**communication**)
  2. Time some process may spent being idle (**synchronization**)



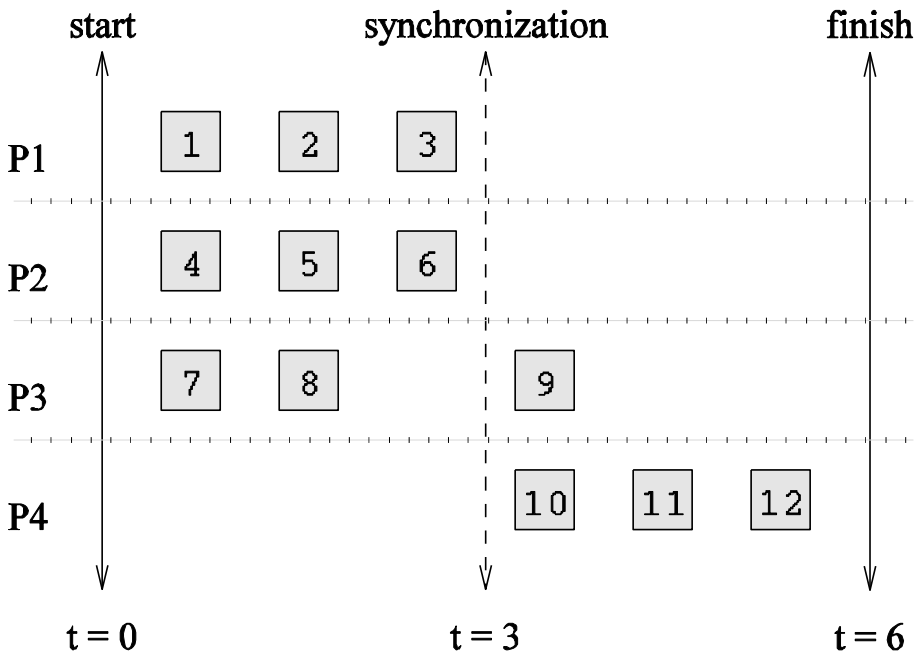
Effect of load-unbalancing



Mapping and Synchronization



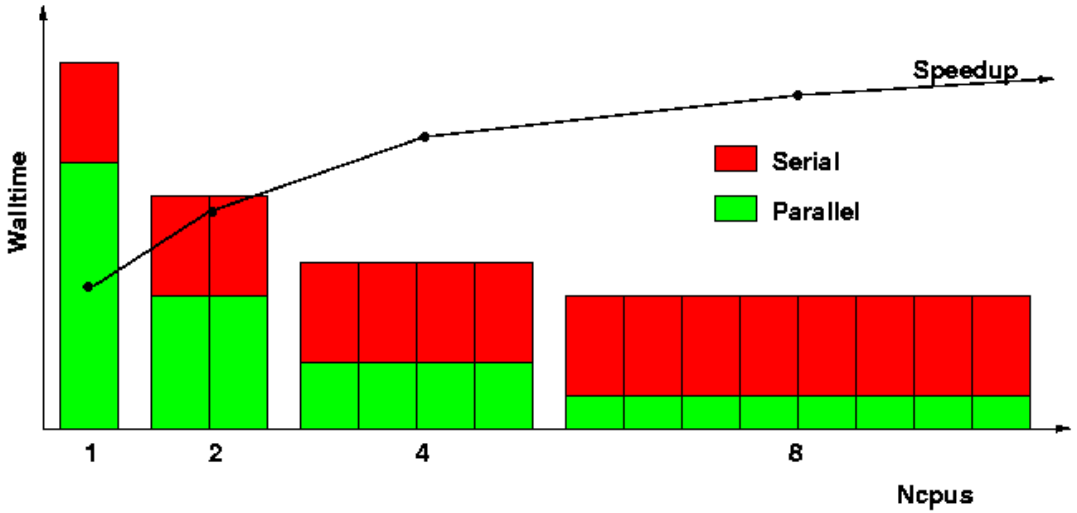
(a)



(b)

Amdahl's law

In a massively parallel context, an upper limit for the scalability of parallel applications is determined by the fraction of the overall execution time spent in non-scalable operations (Amdahl's law).



maximum speedup tends to
$1 / (1 - P)$
P= parallel fraction

1000000 core

P = 0.999999

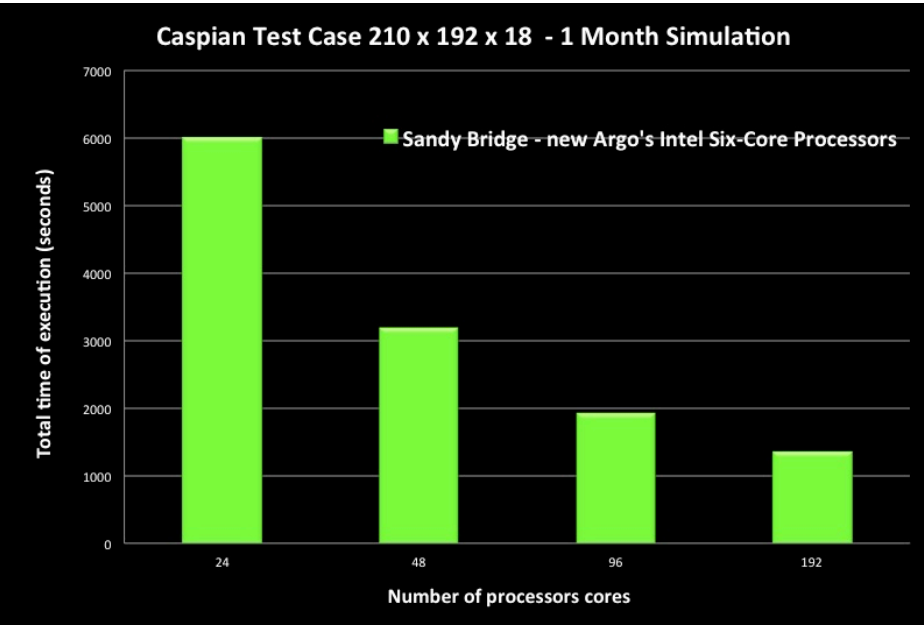
serial fraction= 0.000001

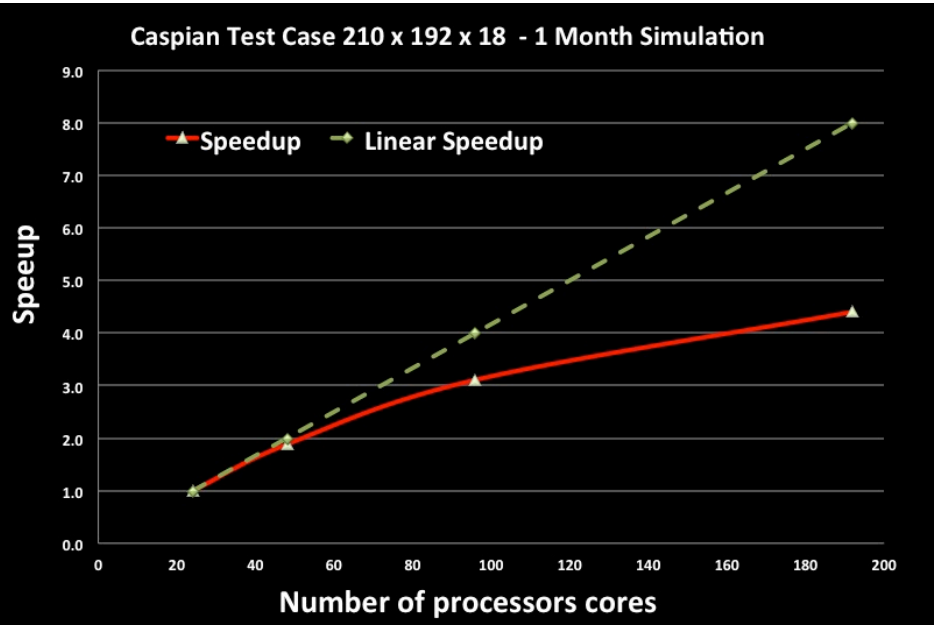
How do we evaluate the improvement?

- We want estimate the amount of the introduced overhead => $T_o = n_{pes} T_P - T_S$
- But to quantify the improvement we use the term **Speedup**:

$$S_P = \frac{T_S}{T_P}$$

Speedup


Caspian Test Case 210 x 192 x 18 - 1 Month Simulation
Sandy Bridge - new Argo's Intel Six-Core Processors
Total time of execution (seconds)
7000
6000
5000
4000
3000
2000
1000
0
24
48
96
192
Number of processors cores

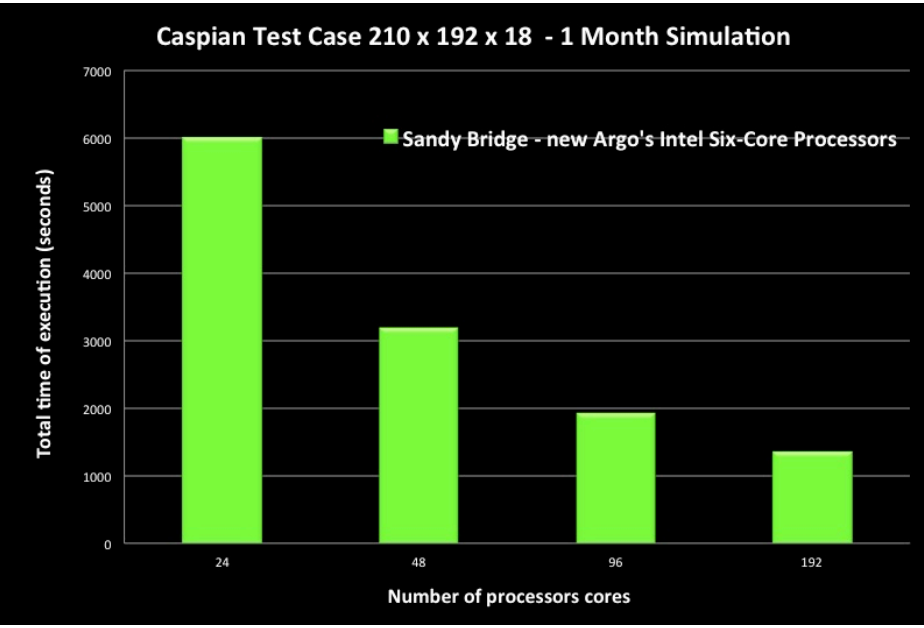

Caspian Test Case 210 x 192 x 18 - 1 Month Simulation
Speedup
Linear Speedup
Speeup
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
0
20
40
60
80
100
120
140
160
180
200
Number of processors cores

Efficiency

- Only embarrassing parallel algorithm can obtain an ideal Speedup
- The **Efficiency** is a measure of the fraction of time for which a processing element is usefully employed:

$$E_P = \frac{S_P}{p}$$

Efficiency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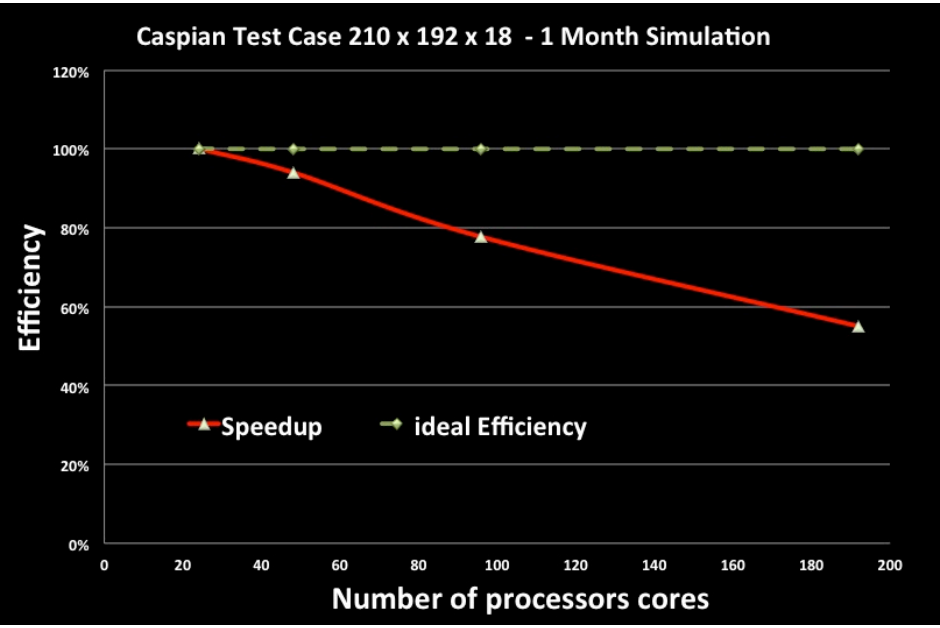
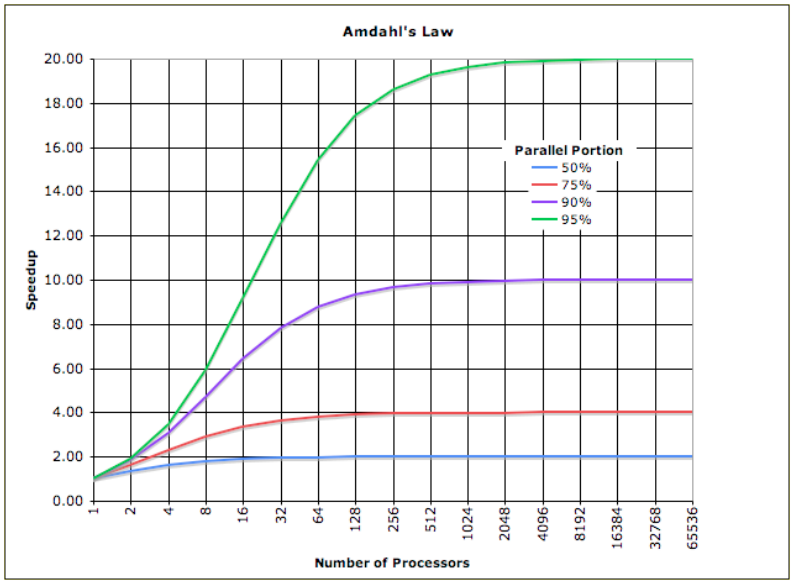
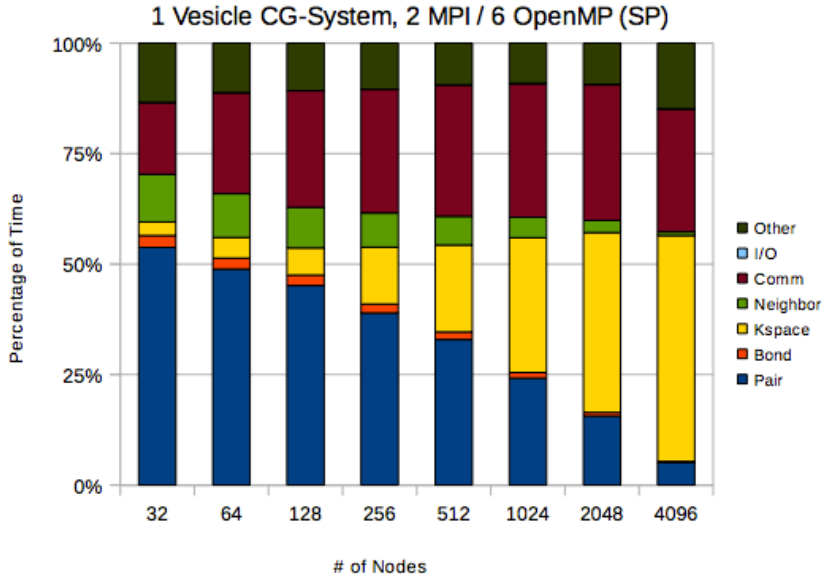

Caspian Test Case 210 x 192 x 18 - 1 Month Simulation
Efficiency
120%
100%
80%
60%
40%
20%
0%
Speedup
ideal Efficiency
0
20
40
60
80
100
120
140
160
180
200
Number of processors cores

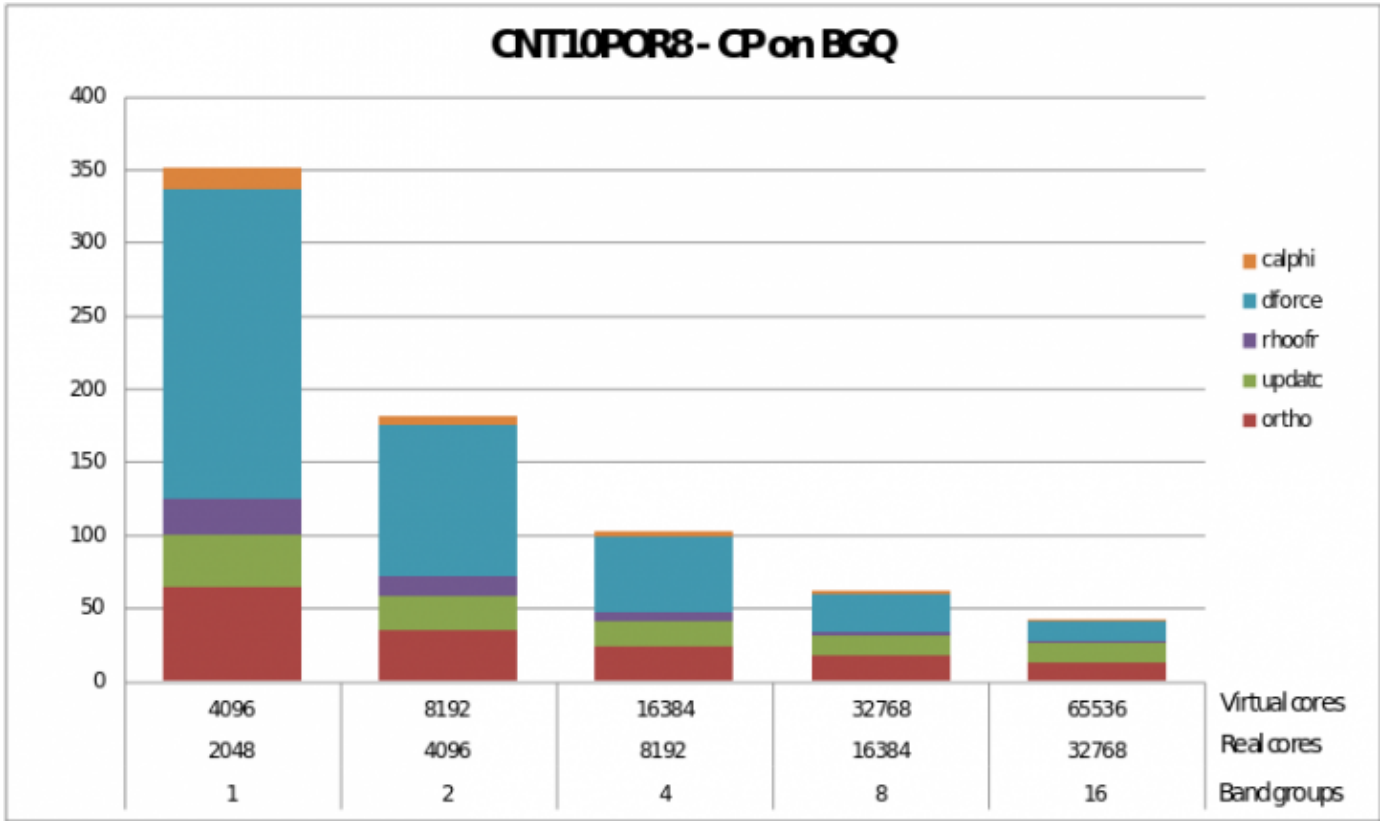
Amdal's Law And Real Life

- The speedup of a parallel program is limited by the sequential fraction of the program
- This assumes perfect scaling and no overhead





Scaling - QE-CP on Fermi BGQ @ CINECA



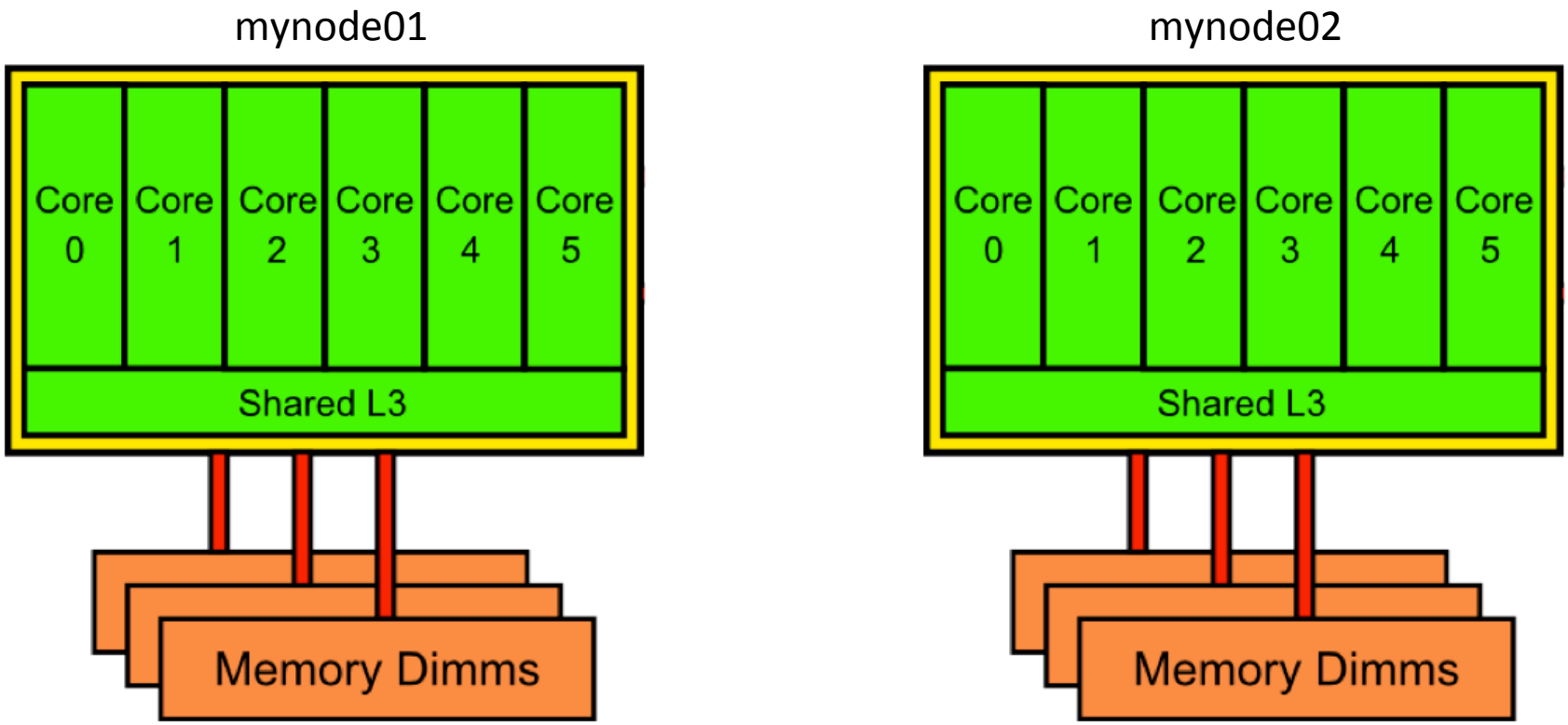
Easy Parallel Computing

- Farming, embarrassingly parallel
  - Executing multiple instances on the same program with different inputs/initial cond.
  - Reading large binary files by splitting the workload among processes
  - Searching elements on large data-sets
  - Other parallel execution of embarrassingly parallel problem (no communication among tasks)
- Ensemble simulations (weather forecast)
- Parameter space (find the best wing shape)

Single Program on Multiple Data

- performing the same program (set of instructions) among different data
- Same model adopted by the MPI library
- A parallel tool is needed to handle the different processes working in parallel
- The MPI library provides the *mpirun* application to execute parallel instances of the same program

```
$ mpirun -np 12 my_program.x
```



Ivan Girotto

```
[igirotto@mynode01 ~]$ mpirun -np 12 /bin/hostname
mynode01
mynode02
mynode01
mynode02
mynode01
mynode02
mynode01
mynode02
mynode01
mynode02
mynode01
mynode02
```

PATH name common to all processes !!

Parallel Operations in Practice

- Parallel reading and computing in parallel is always allowed
- Parallel writing is extremely dangerous!
- To control the parallel flow each process should be unique and identifiable (ID)
- The OpenMPI implementation of the MPI library provides a series of environment variables defined for each MPI process

OMPI_COMM_WORLD_SIZE - the number of processes in this process' MPI Comm_World

OMPI_COMM_WORLD_RANK - the MPI rank of this process

OMPI_COMM_WORLD_LOCAL_RANK - the relative rank of this process on this node within its job. For example, if four processes in a job share a node, they will each be given a local rank ranging from 0 to 3.

OMPI_UNIVERSE_SIZE - the number of process slots allocated to this job. Note that this may be different than the number of processes in the job.

OMPI_COMM_WORLD_LOCAL_SIZE - the number of ranks from this job that are running on this node.

OMPI_COMM_WORLD_NODE_RANK - the relative rank of this process on this node looking across ALL jobs.

http://www.open-mpi.org

In Python

```
import os
myid = os.environ['OMPI_COMM_WORLD_RANK']
[...]
```

In BASH

```
#!/bin/bash
myid=${OMPI_COMM_WORLD_RANK}
[...]
```

```
[igirotto@mynode01 ~]$ mpirun ./myprogram.[py/sh...]
```

Possible Applications

- Executing multiple instances on the same program with different inputs/initial cond.
- Reading large binary files by splitting the workload among processes
- Searching elements on large data-sets
- Other parallel execution of embarrassingly parallel problem (no communication among tasks)

Conclusions

- Task Farming is a simple model to parallelize simple problems that can be divided in independent task
- The *mpirun* application aids to easily perform multiple processes, includes environment setting
- Load balancing remains a main problem, but moving from serial to parallel processing can substantially speed-up time of simulation

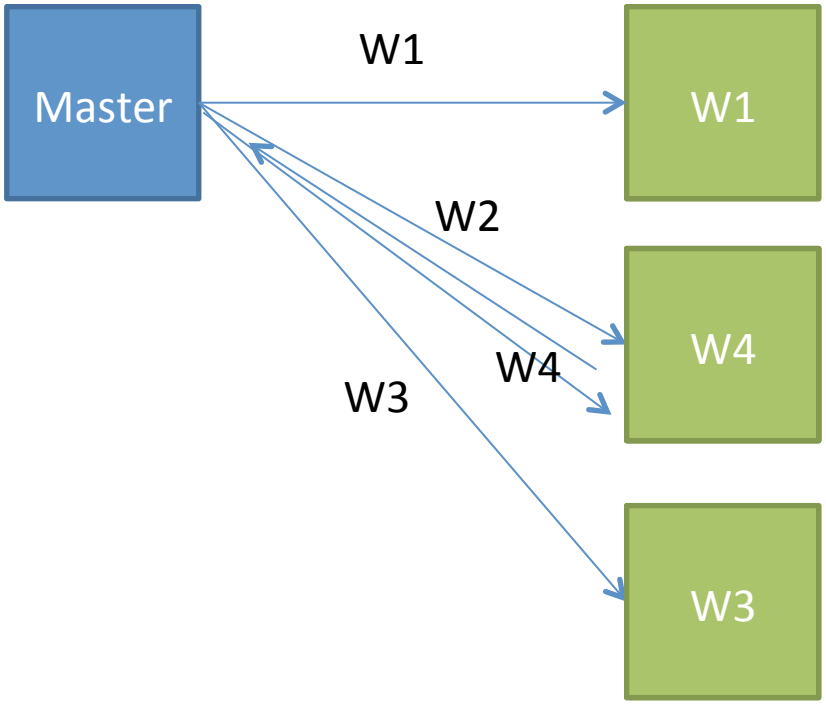
Task Farming

- Many independent programs (tasks) running at once
  - each task can be serial or parallel
  - "independent" means they don't communicate directly
  - Processes possibly driven by the mpirun framework

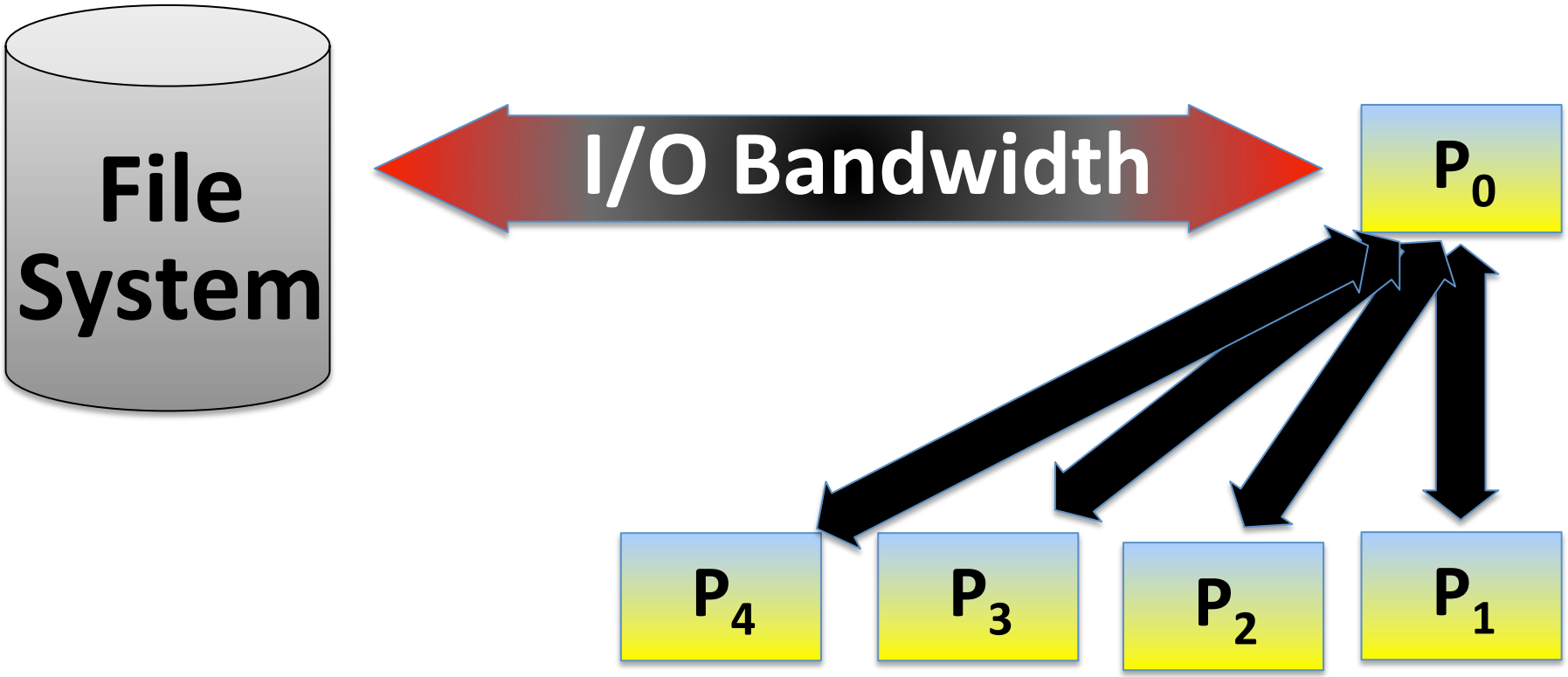
```
[igirotto@localhost]$ more my_shell_wrapper.sh
#!/bin/bash
#example for the OpenMPI implementation
./prog.x --input input_${OMPI_COMM_WORLD_RANK}.dat

[igirotto@localhost]$ mpirun -np 400 ./my_shell_wrapper.sh
```

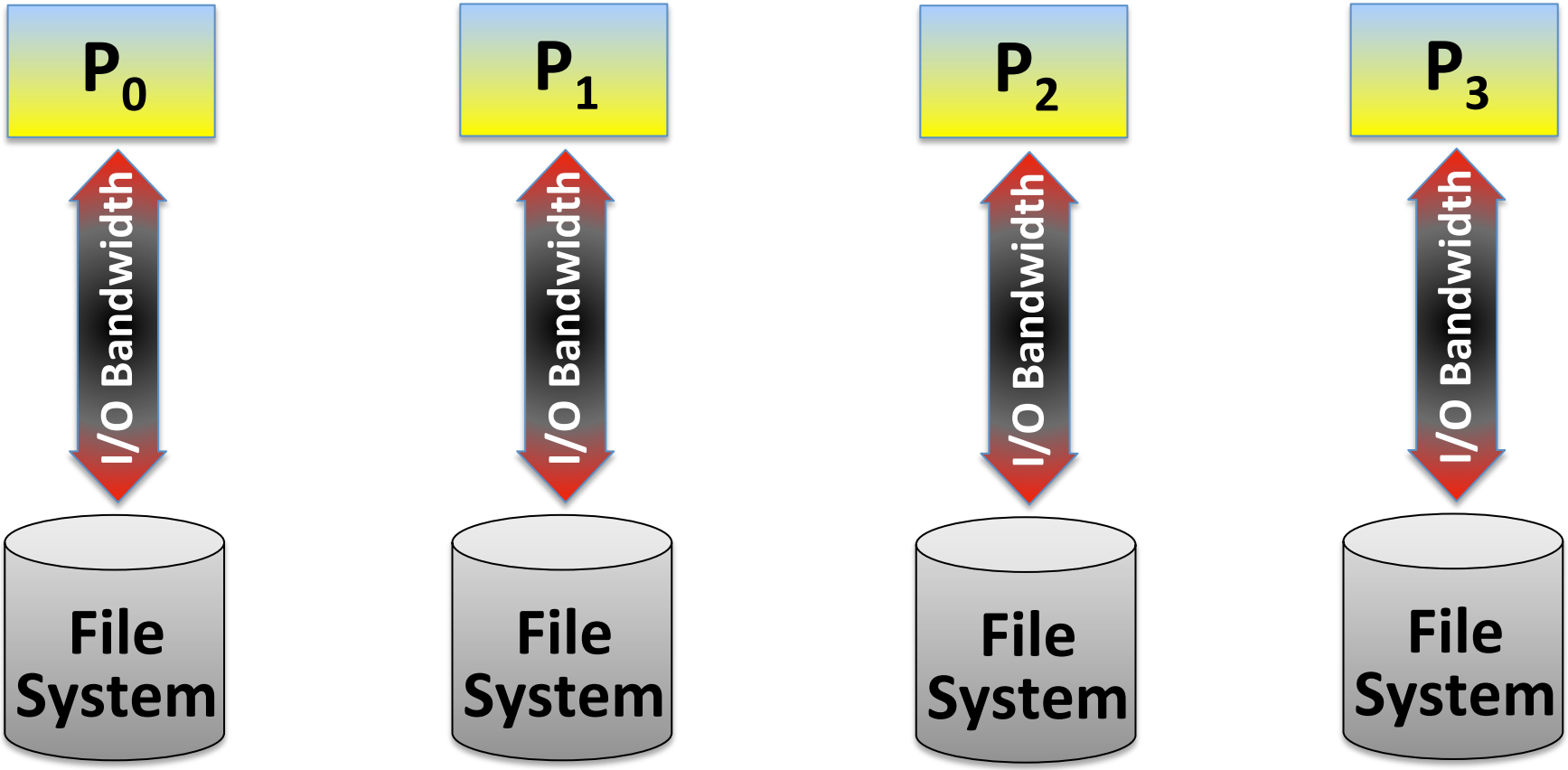
Master/Slave



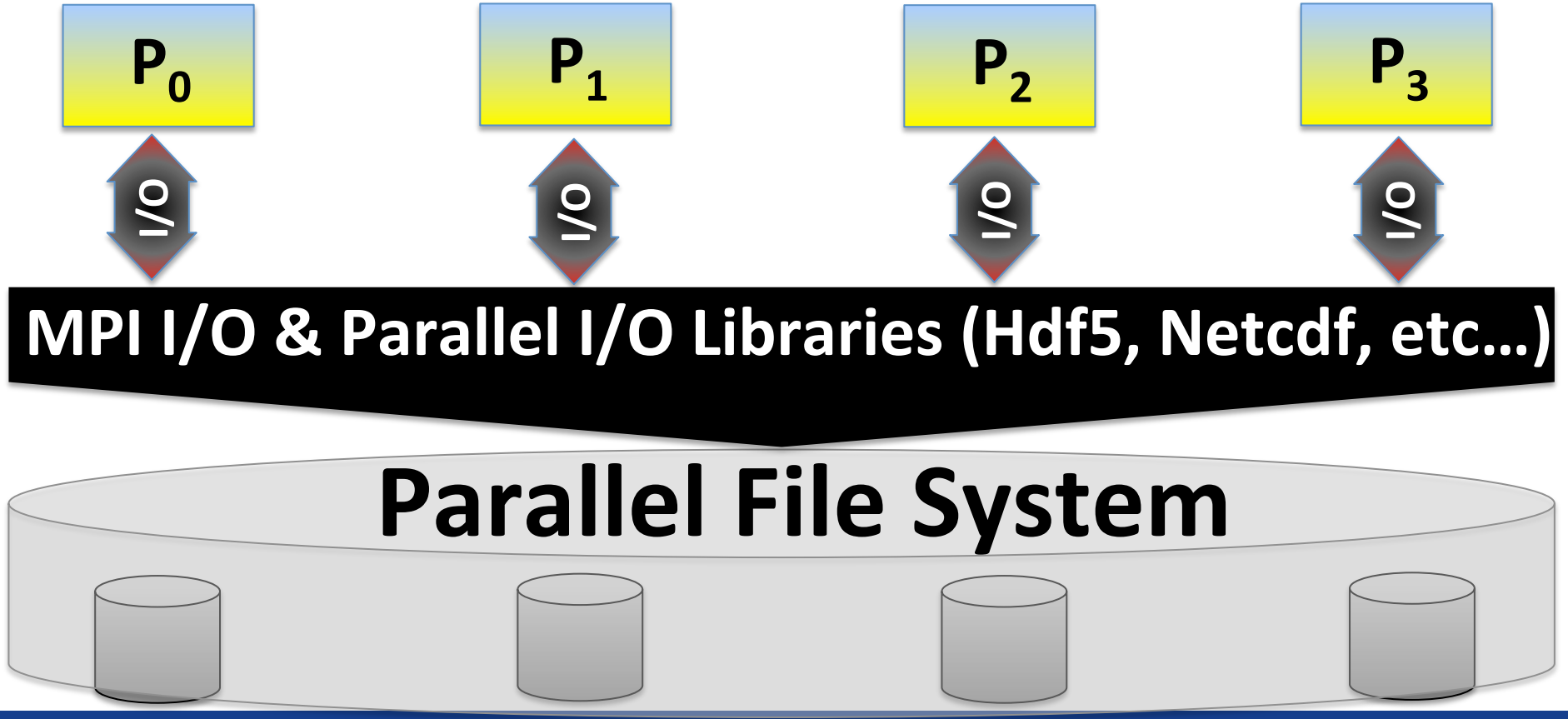
Parallel I/O



Parallel I/O


P0
P1
P2
P3
I/O Bandwidth
I/O Bandwidth
I/O Bandwidth
I/O Bandwidth
File System
File System
File System
File System

Parallel I/O


P0
P1
P2
P3
I/O
I/O
I/O
I/O
MPI I/O & Parallel I/O Libraries (Hdf5, Netcdf, etc…)
Parallel File System

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- 3 October 2016 - 14 October 2016

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READ ALL

Thanks for your attention!!