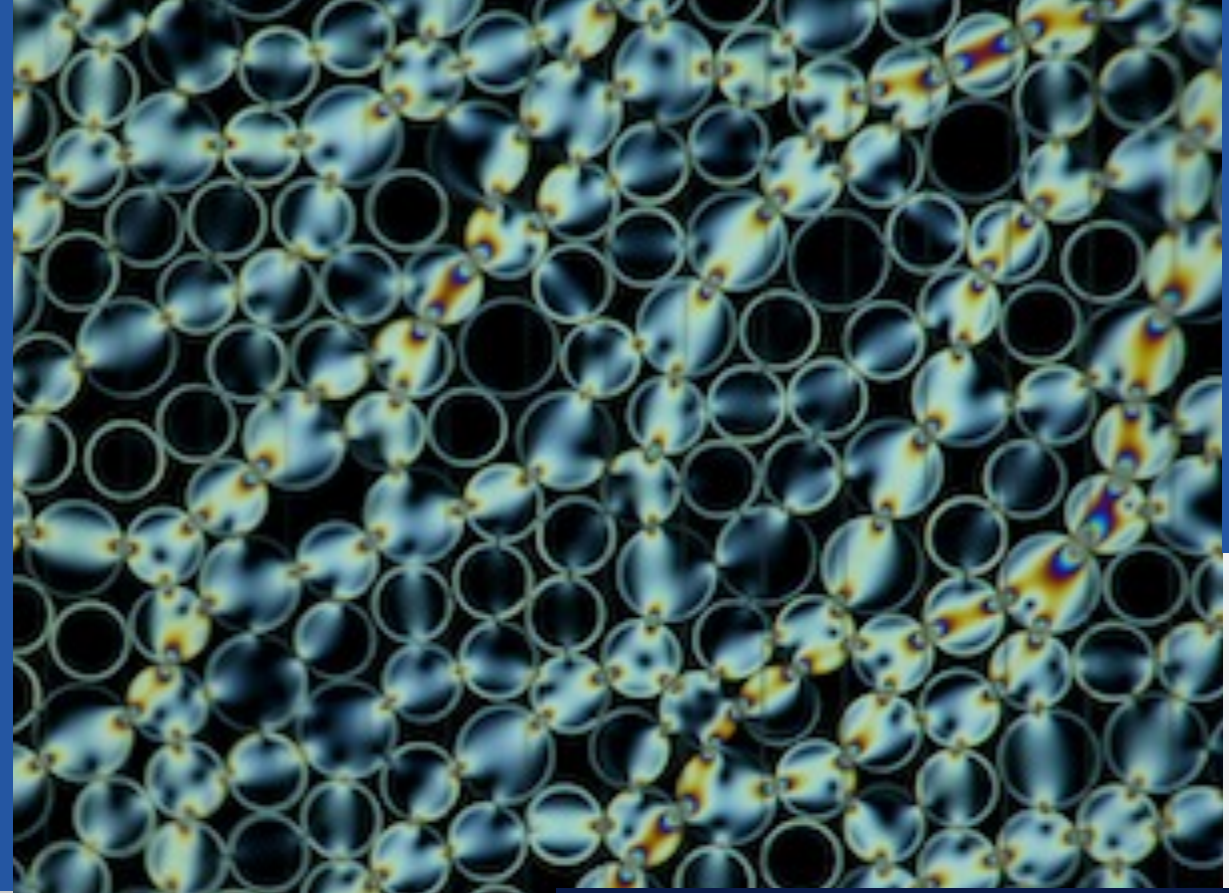
Thinking Parallel 101



Ivan Girotto
(igirotto@ictp.it)

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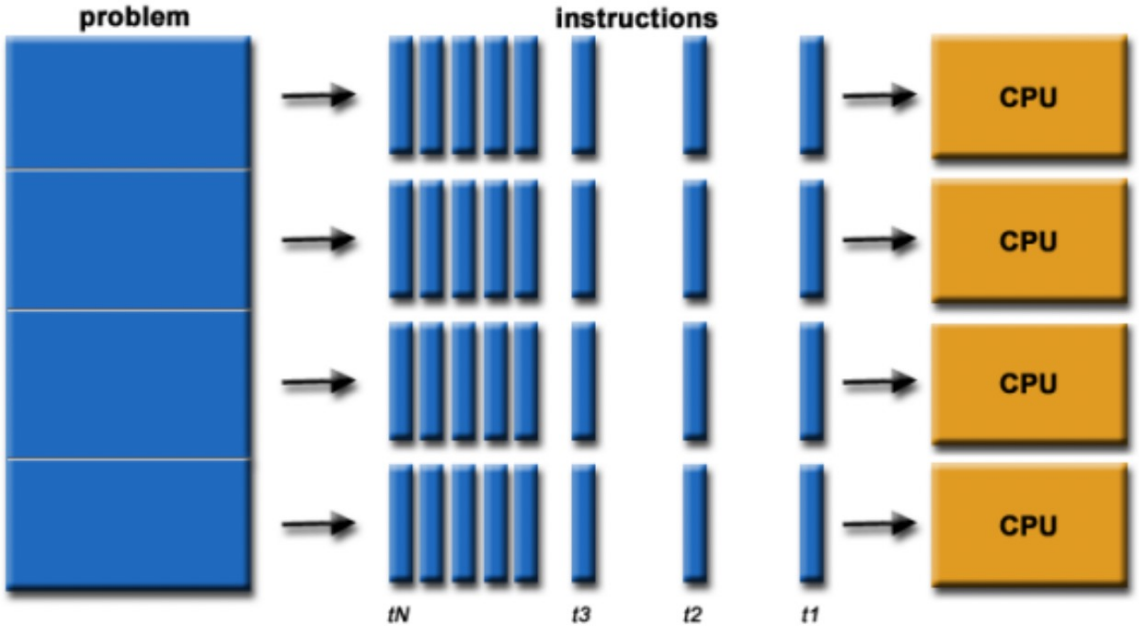
The Abdus Salam International Centre for Theoretical Physics

IAEA International Atomic Energy Agency

unesco United Nations Educational, Scientific and Cultural Organization

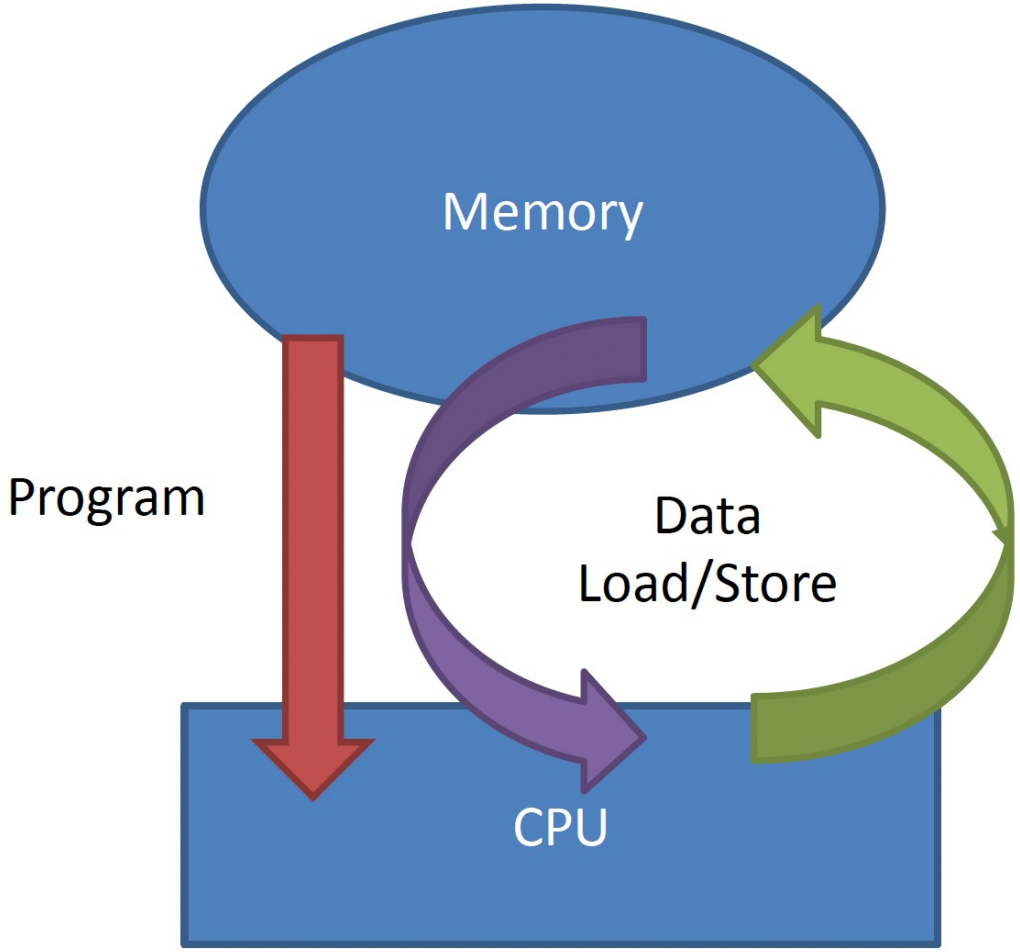
Concurrency

The first step in developing a parallel algorithm is to decompose the problem into tasks that can be executed concurrently

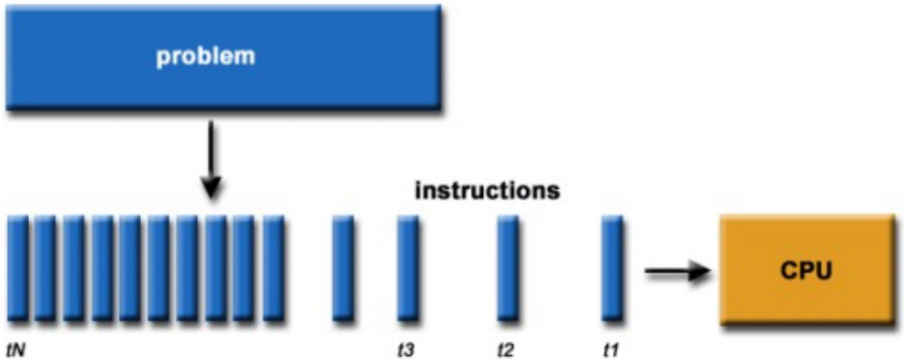


- A problem is broken into discrete parts that can be solved concurrently
- Each part is further broken down to a series of instructions
- Instructions from each part execute simultaneously on different processors
- An overall control / coordination mechanism is employed

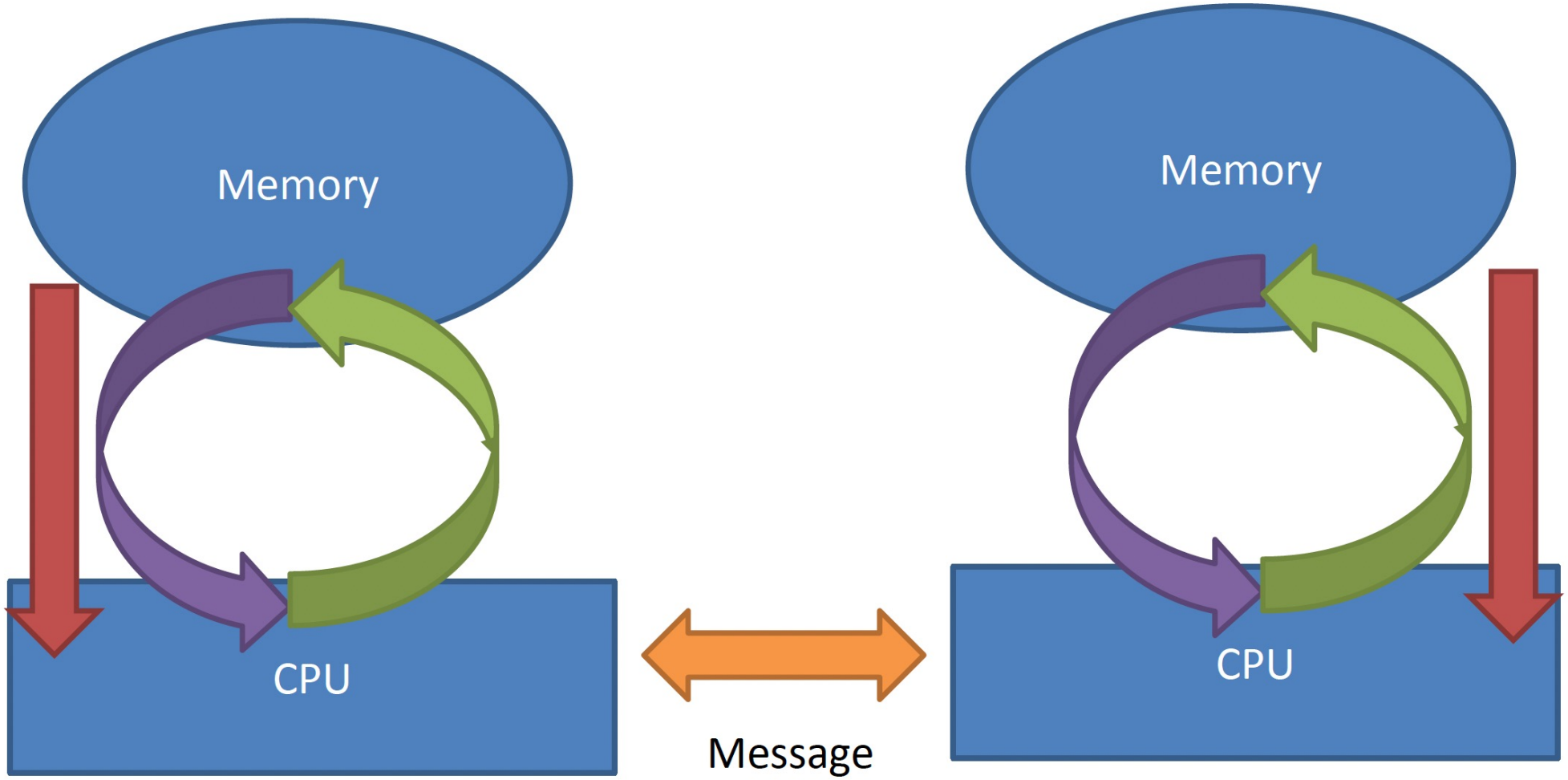
Serial Programming



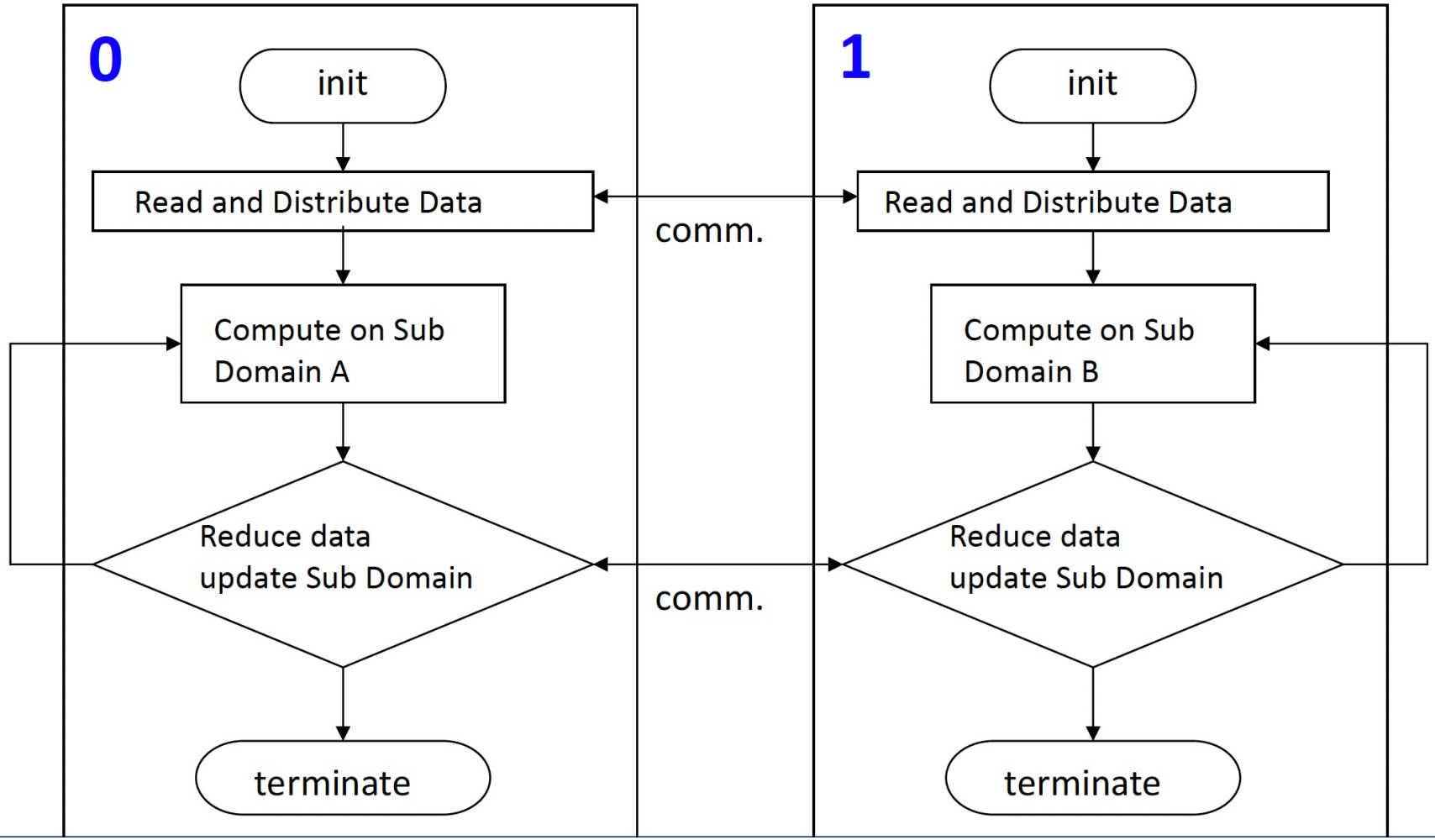
A problem is broken into a discrete series of instructions.
Instructions are executed one after another.
Only one instruction may execute at any moment in time.



Parallel Programming



What is a Parallel Program



Fundamental Steps of Parallel Design

- Identify portions of the work that can be performed concurrently
- Mapping the concurrent pieces of work onto multiple processes running in parallel
- Distributing the input, output and intermediate data associated within the program
- Managing accesses to data shared by multiple processors
- Synchronizing the processors at various stages of the parallel program execution

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

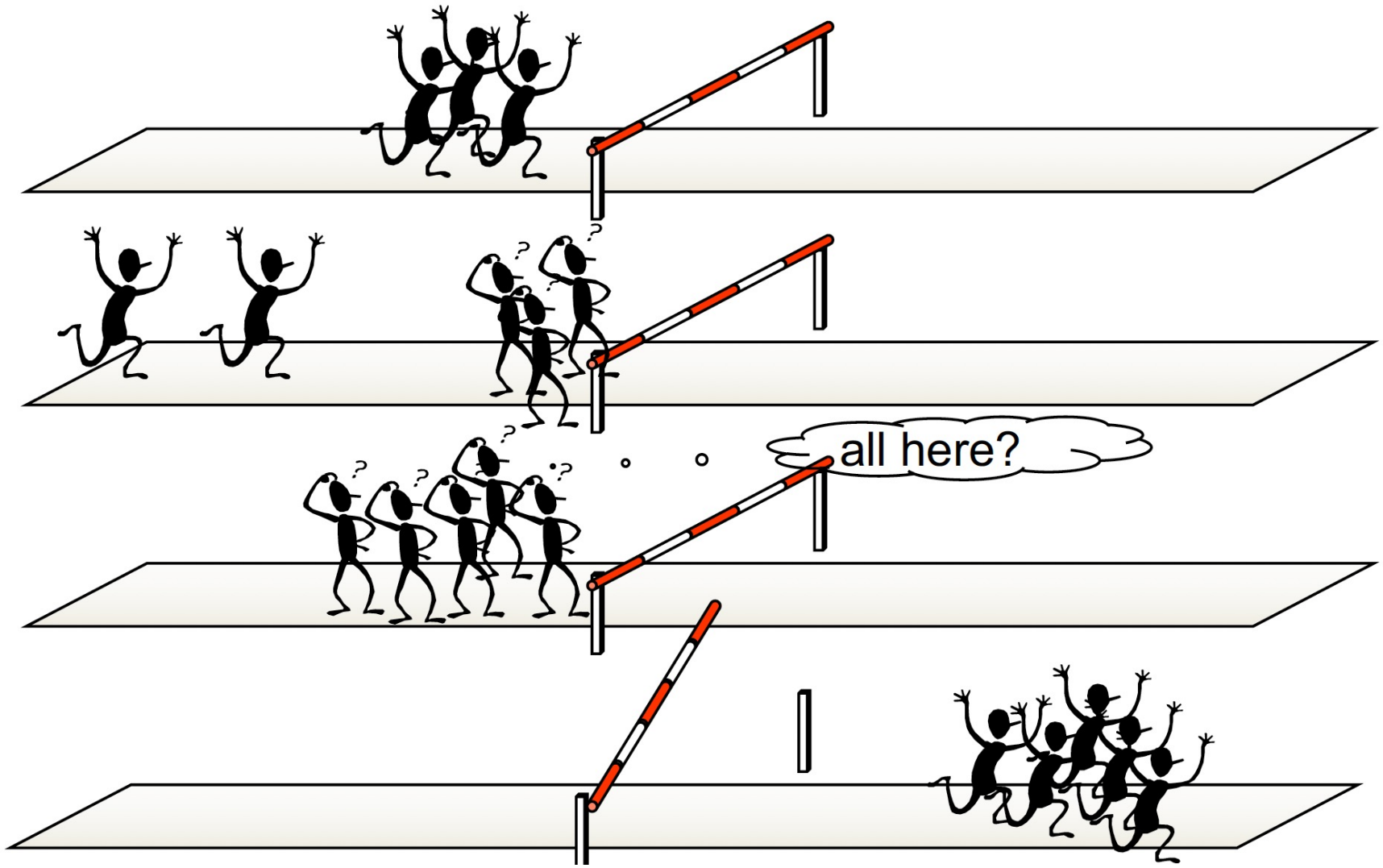
Process Interactions

- 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**)

Load Balancing

- Equally divide the work among the available resource: processors, memory, network bandwidth, I/O, ...
- This is usually a simple task for the problem decomposition model
- It is a difficult task for the functional decomposition model

Effect of Load Unbalancing



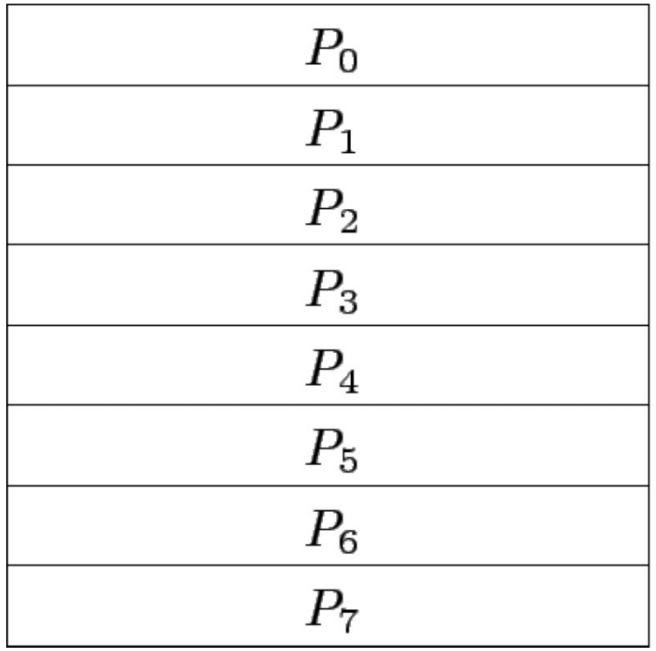
Minimizing Communication

- When possible reduce the communication events:
  - group lots of small communications into large one
  - eliminate synchronizations as much as possible. Each synchronization level off the performance to that of the slowest process

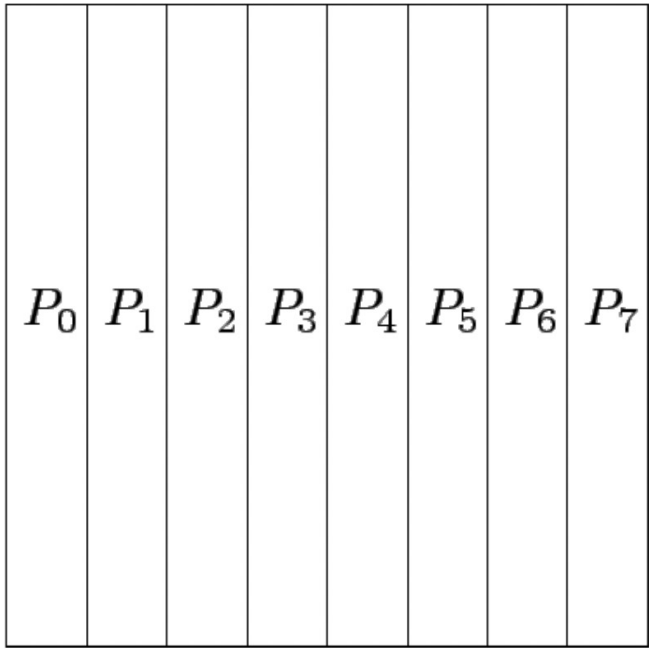
Static Data Partitioning

The simplest data decomposition schemes for dense matrices are 1-D block distribution schemes.

row-wise distribution



column-wise distribution

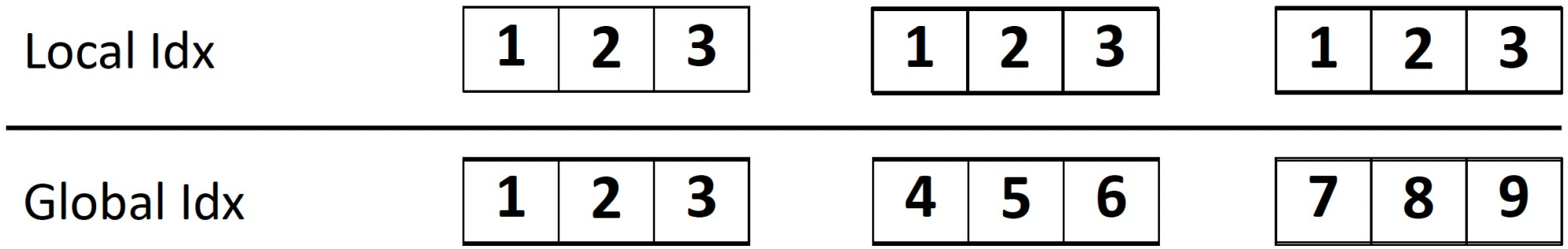


Distributed Data Vs Replicated Data

- Replicated data distribution is useful if it helps to reduce the communication among process at the cost of bounding scalability
- Distributed data is the ideal data distribution but not always applicable for all data-sets
- Usually complex application are a mix of those techniques => distribute large data sets; replicate small data

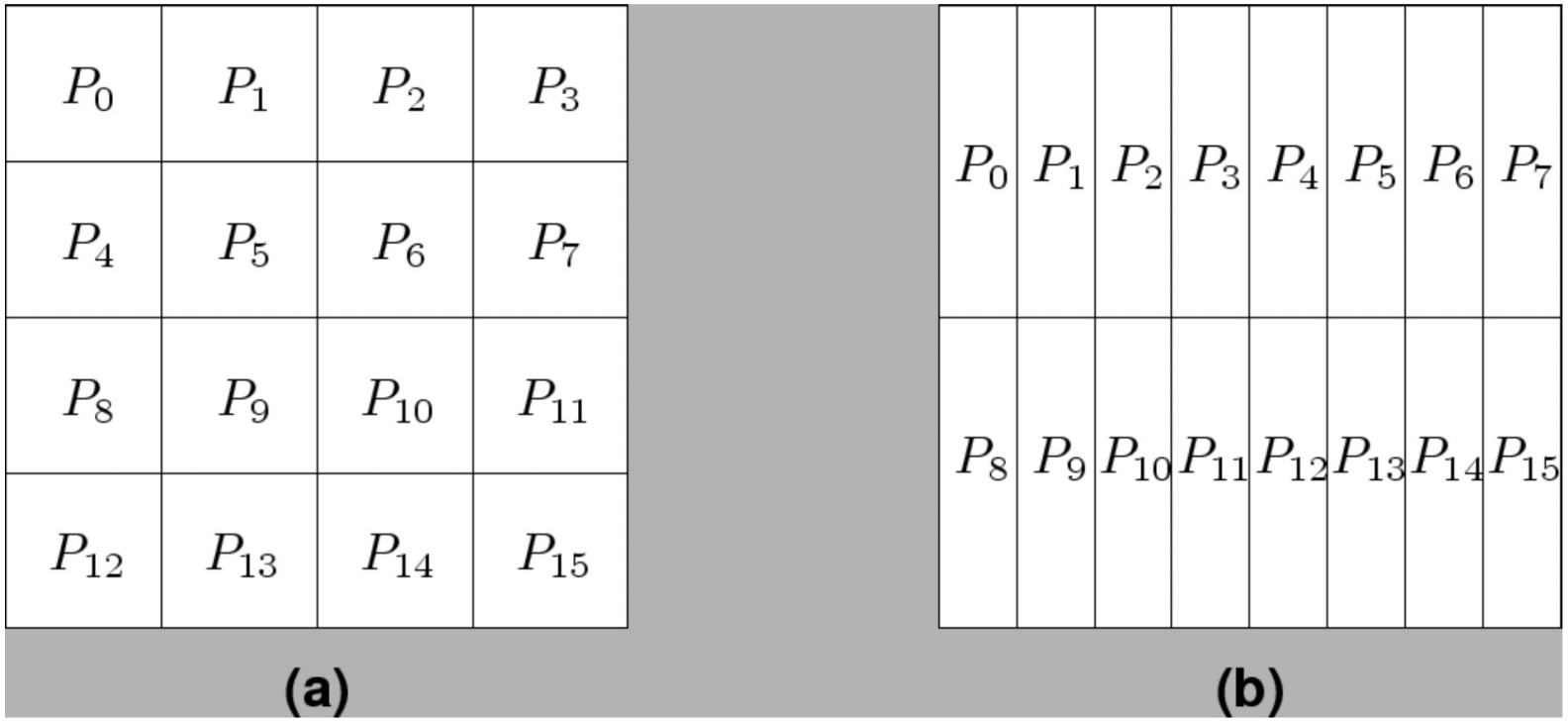
Global Vs Local Indexes

- In sequential code you always refer to global indexes
- With distributed data you must handle the distinction between global and local indexes (and possibly implementing utilities for transparent conversion)



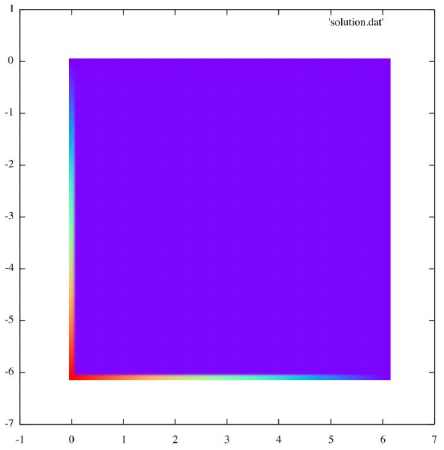
Block Array Distribution Schemes

Block distribution schemes can be generalized to higher dimensions as well.

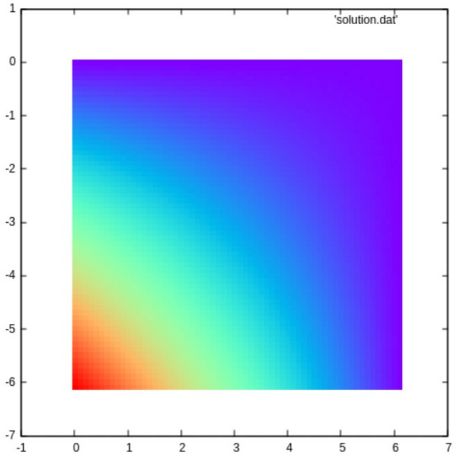


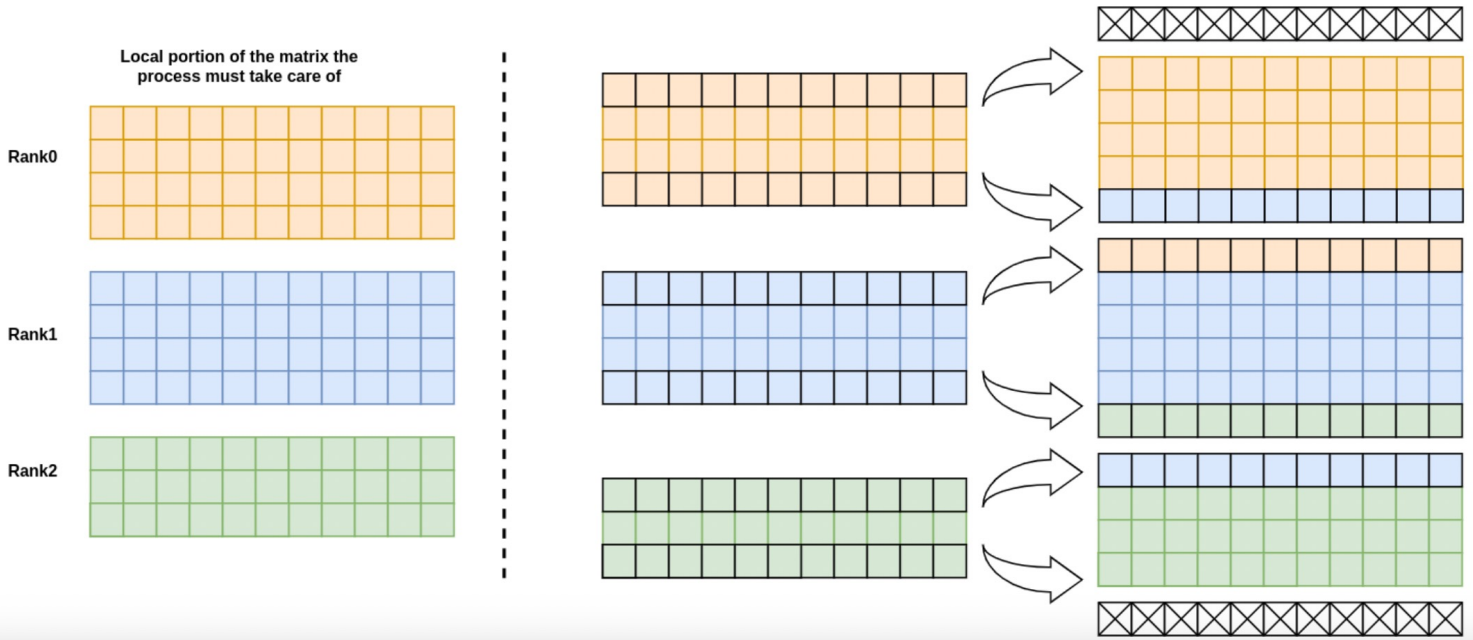
Degree to which tasks/data can be subdivided is limit to concurrency and parallel execution!!

Parallel Efficiency: Jacoby example



$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = 0$$



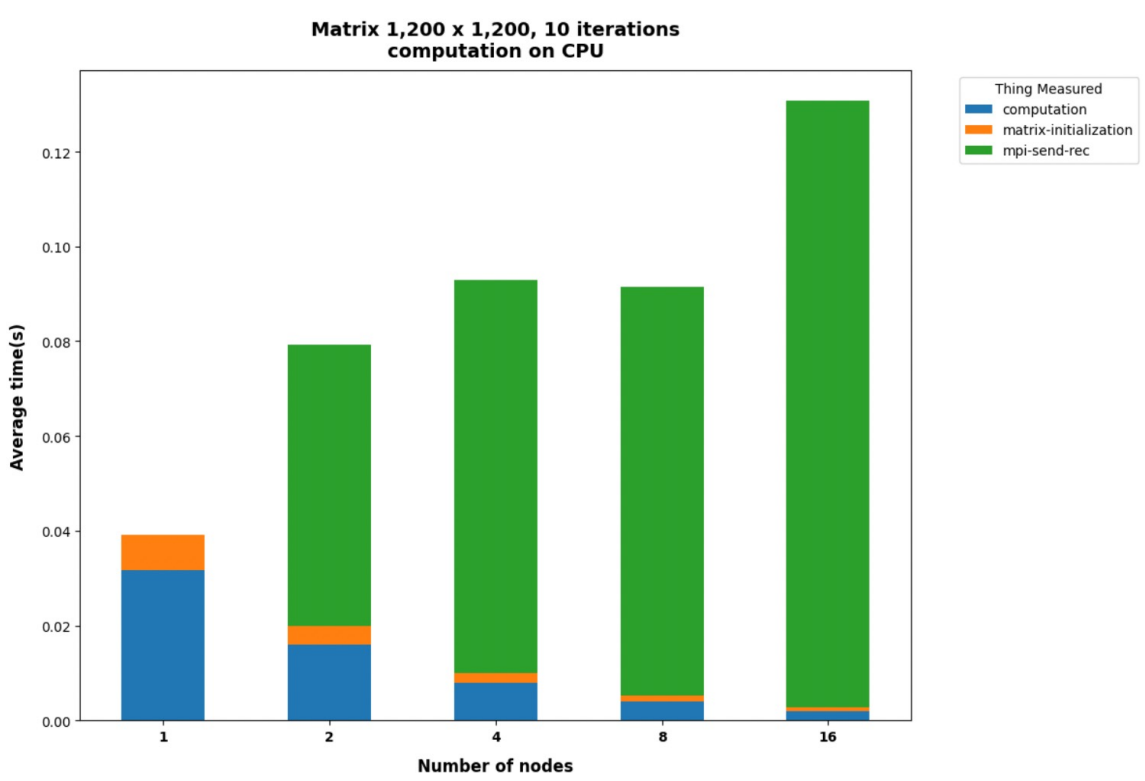


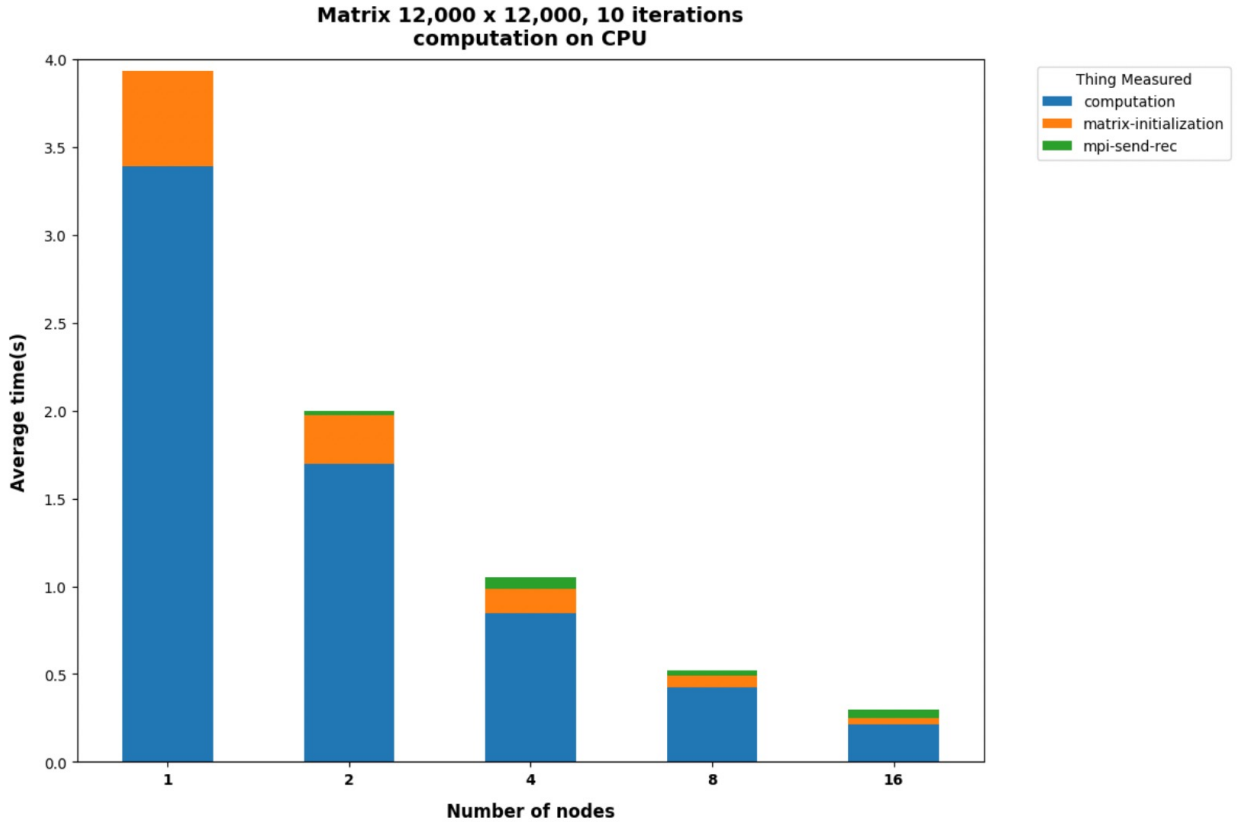
$$V_{i,j}^{new} = 0.25(V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1})$$

0	0	0	0	0	0	0	0	0	0	0
10										0
20										0
30			$V_{i+1,j}$							0
40		$V_{i,j-1}$	$V_{i,j}$	$V_{i,j+1}$						0
50			$V_{i-1,j}$							0
60										0
70										0
80										0
90										0
100	90	80	70	60	50	40	30	20	10	0

Figure 1: A diagram of the Jacobi Relaxation for Solving the Laplace's Equation on an evenly spaced 9x9 grid with the boundary conditions outlined in the text above.

Parallel Efficiency: Jacoby example





Overlap Communication and Computation

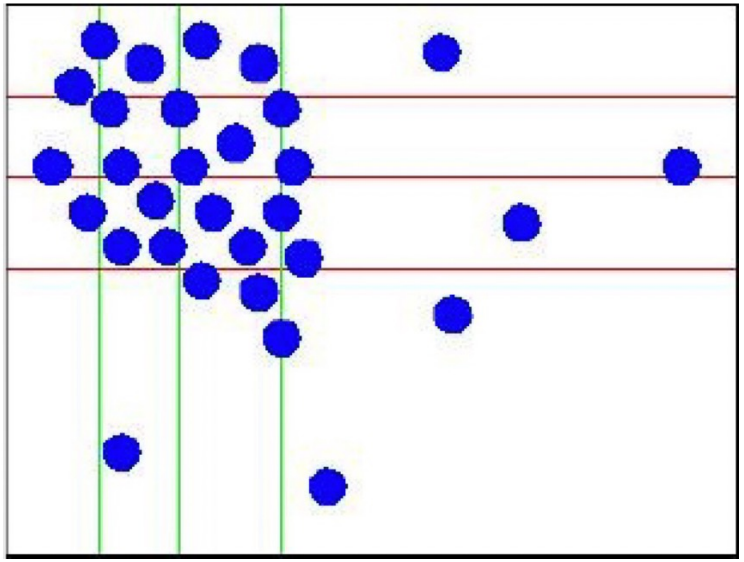
- When possible code your program in such a way that processes continue to do useful work while communicating
- This is usually a non trivial task and is afforded in the very last phase of parallelization
- If you succeed, you have done. Benefits are enormous

Granularity

- Granularity is determined by the decomposition level (number of task) on which we want divide the problem
- The degree to which task/data can be subdivided is limit to concurrency and parallel execution
- Parallelization has to become “topology aware”
  - coarse grain and fine grained parallelization has to be mapped to the topology to reduce memory and I/O contention
  - make your code modularized to enhance different levels of granularity and consequently to become more “platform adaptable”

Limitations of Parallel Computing

- Fraction of serial code limits parallel speedup
- Degree to which tasks/data can be subdivided is limit to concurrency and parallel execution
- Load imbalance:
  - parallel tasks have a different amount of work
  - CPUs are partially idle
  - redistributing work helps but has limitations
  - communication and synchronization overhead



Shared Resources

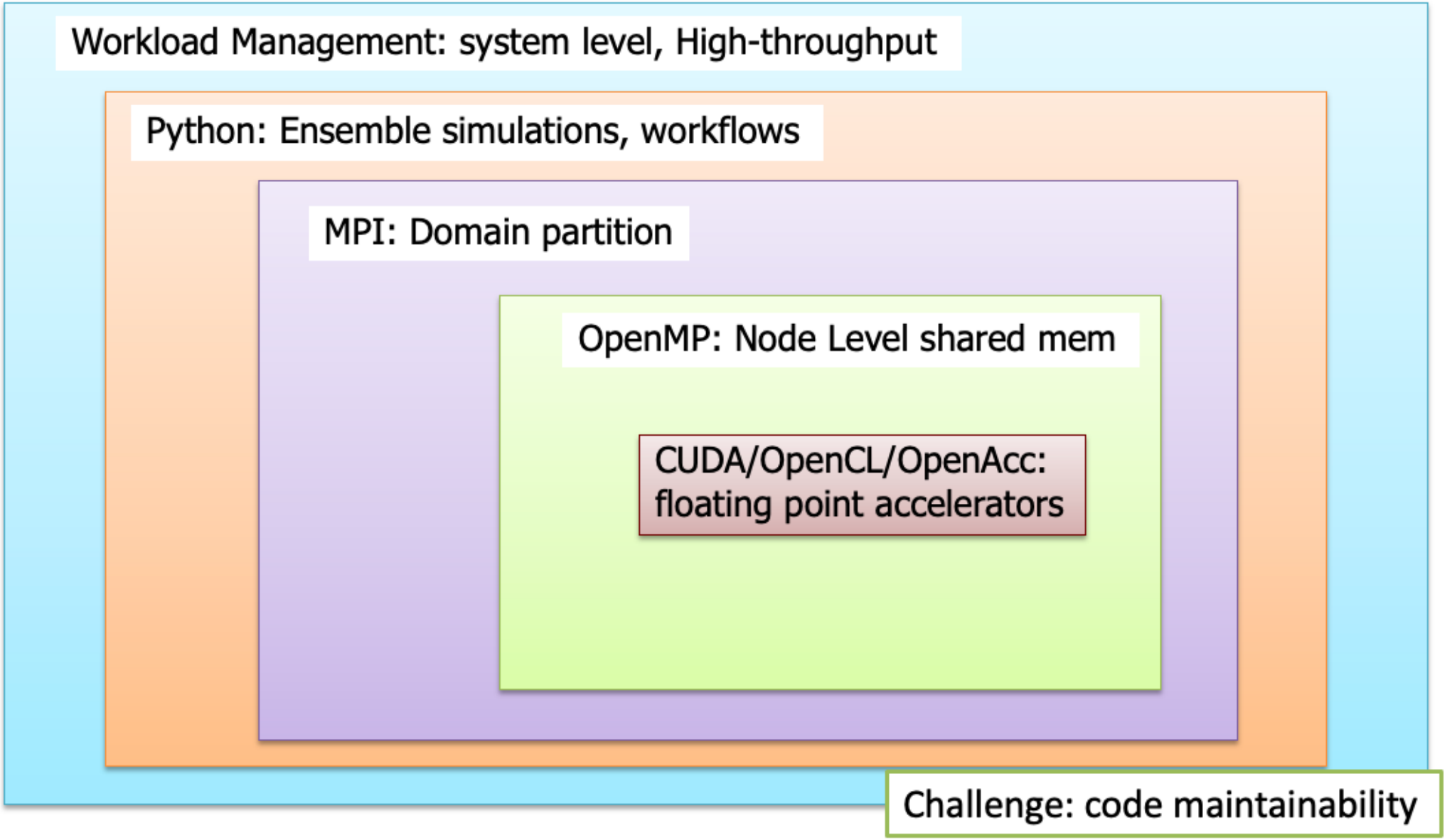
- In parallel programming, developers must manage exclusive access to shared resources
- Resources are in different forms:
  - concurrent read/write (including parallel write) to shared memory locations
  - concurrent read/write (including parallel write) to shared devices
  - a message that must be send and received

Fundamental Tools of Parallel Programming

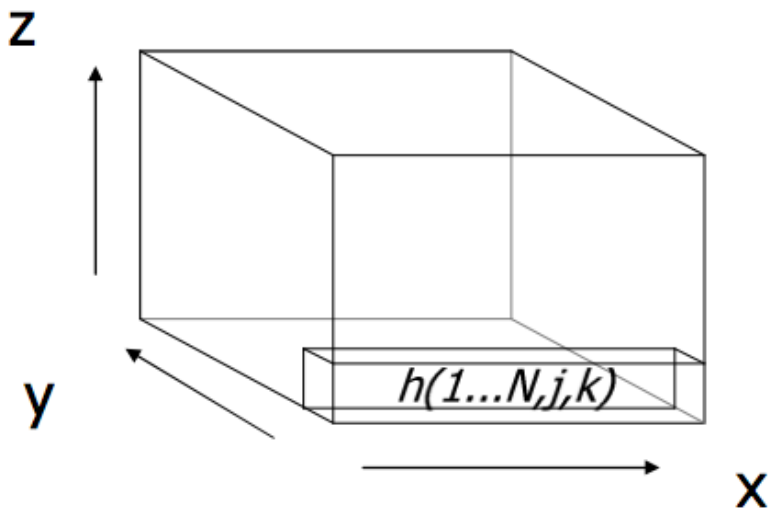
Programming Parallel Paradigms

- 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

OpenMP™


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

Multidimensional FFT



1) For any value of ***j*** and ***k***
transform the column (1…N, j, k)

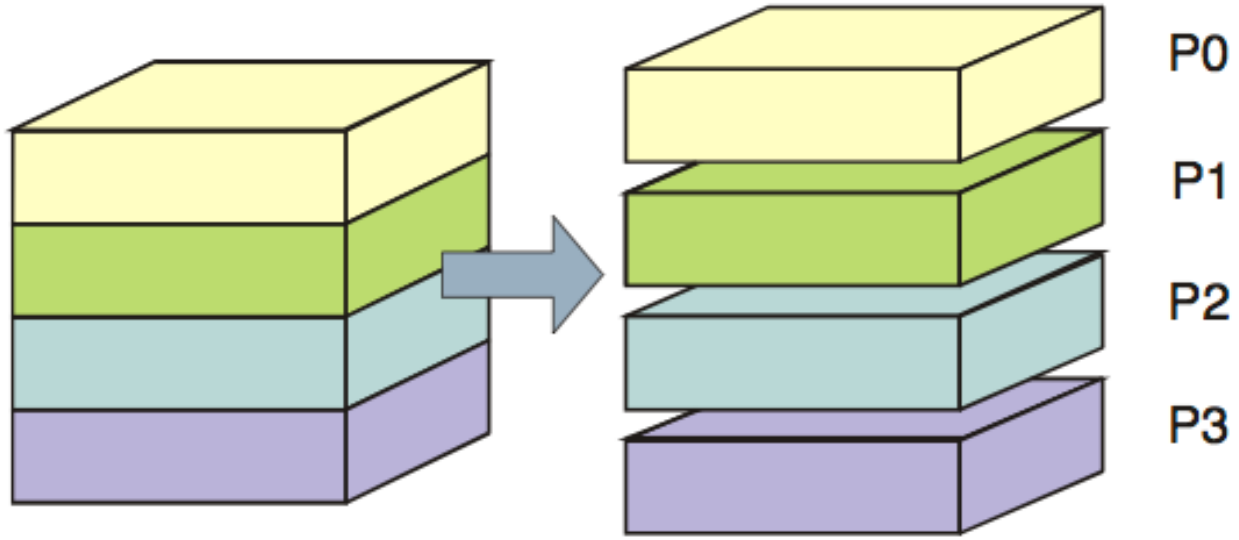
2) For any value of ***i*** and ***k***
transform the column (i, 1…N, k)

3) For any value of ***i*** and ***j***
transform the column (i, j, 1…N)

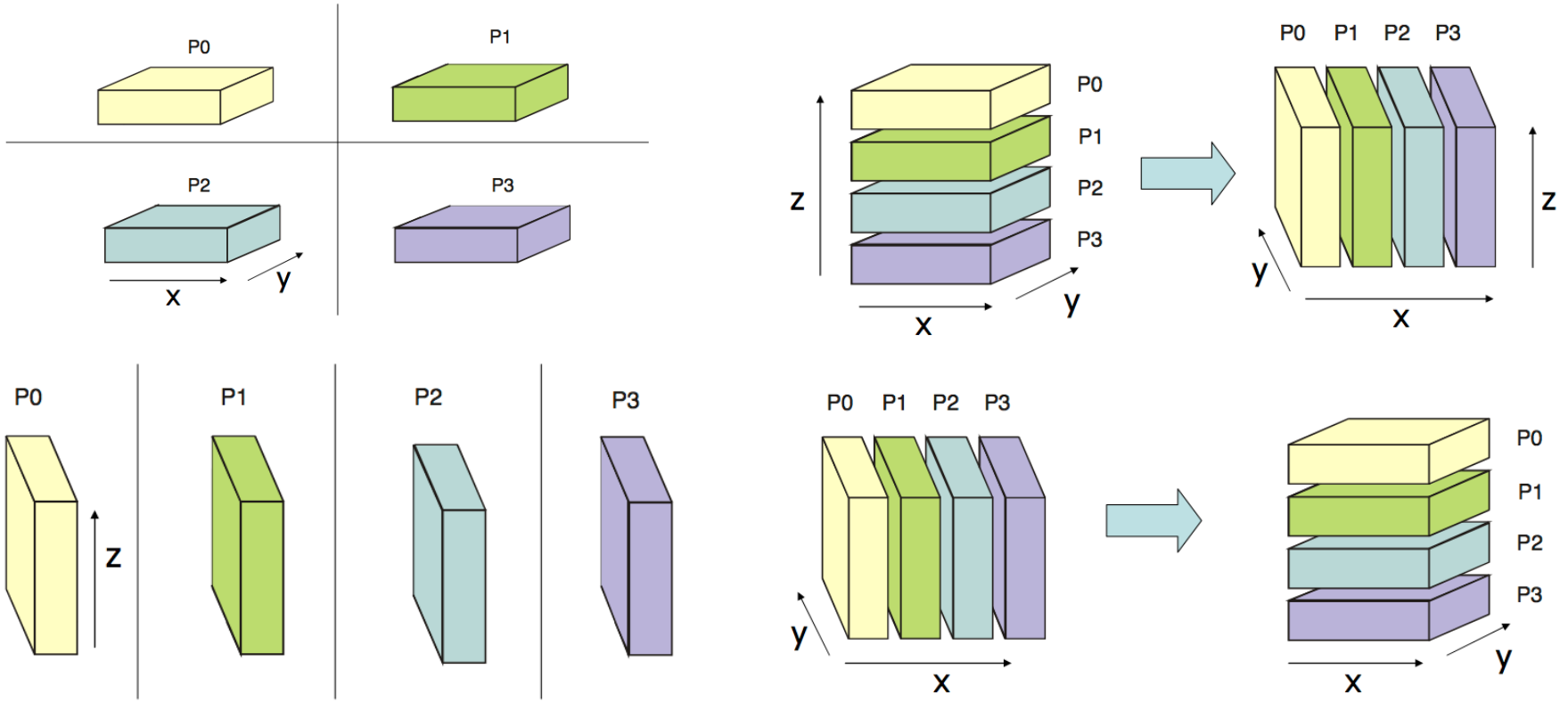
$$f(x,y,z) = \frac{1}{N_z N_y N_x} \sum_{z=0}^{N_z-1} \Big(\sum_{y=0}^{N_y-1} \underbrace{\Big(\sum_{x=0}^{N_x-1} F(u,v,w)\, e^{-2\pi i \frac{xu}{N_x}} \Big)}_{\text{DFT long x-dimension}} e^{-2\pi i \frac{yv}{N_y}} \Big)}_{\text{DFT long y-dimension}} e^{-2\pi i \frac{zw}{N_z}}$$

DFT long z-dimension

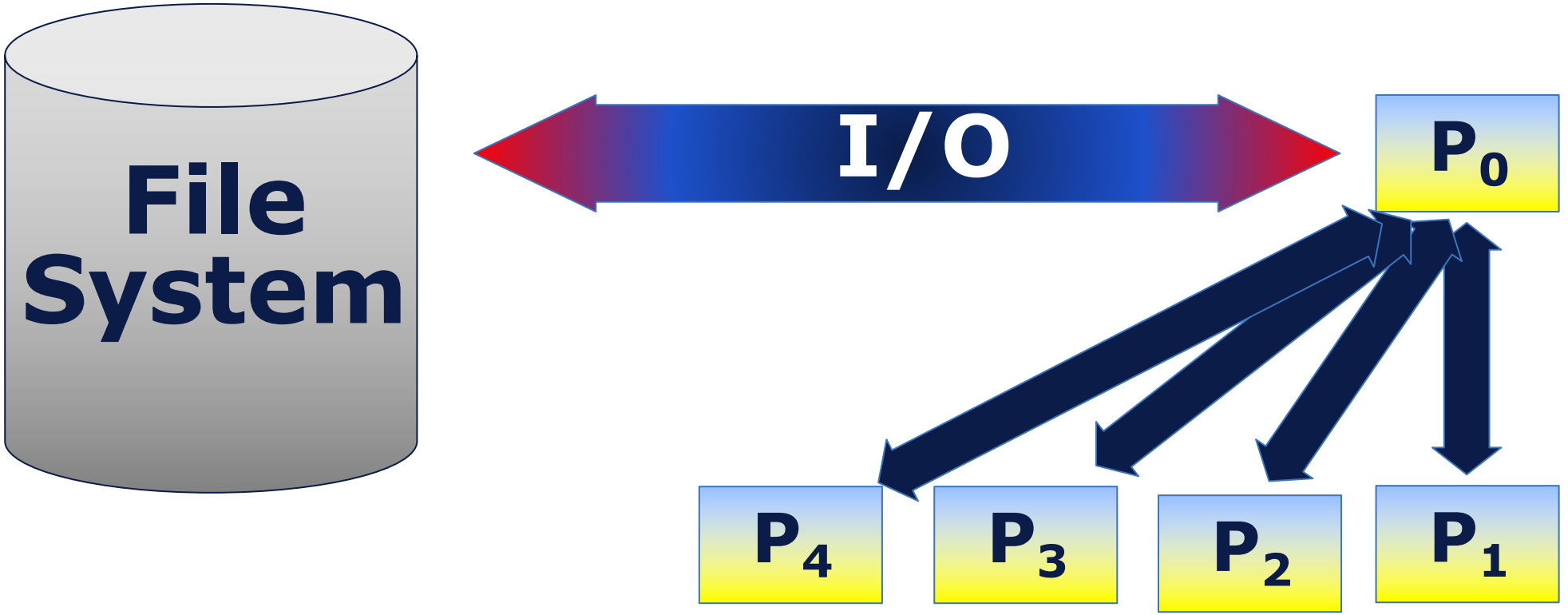
Parallel 3DFFT / 1



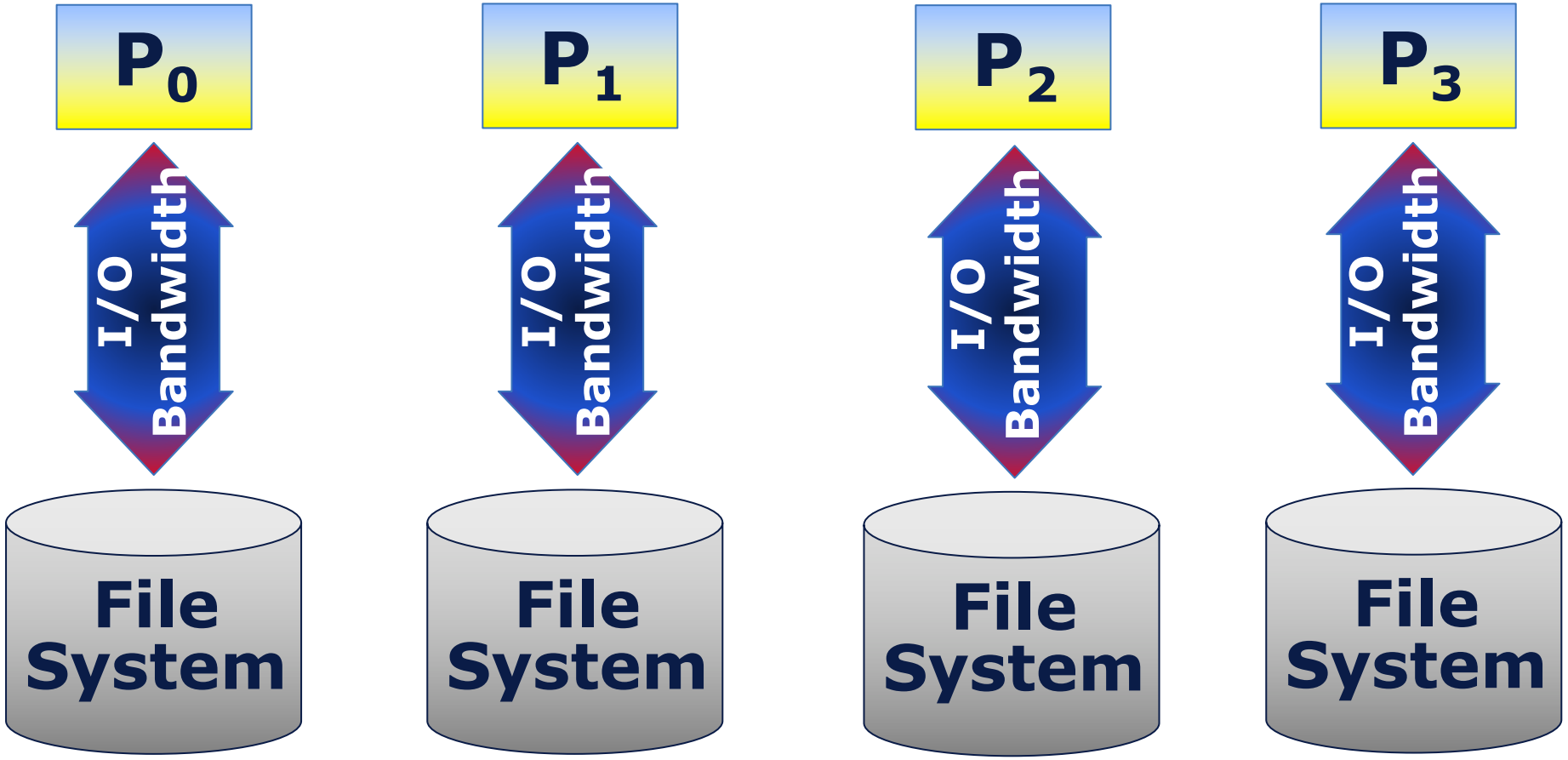
Parallel 3DFFT / 2



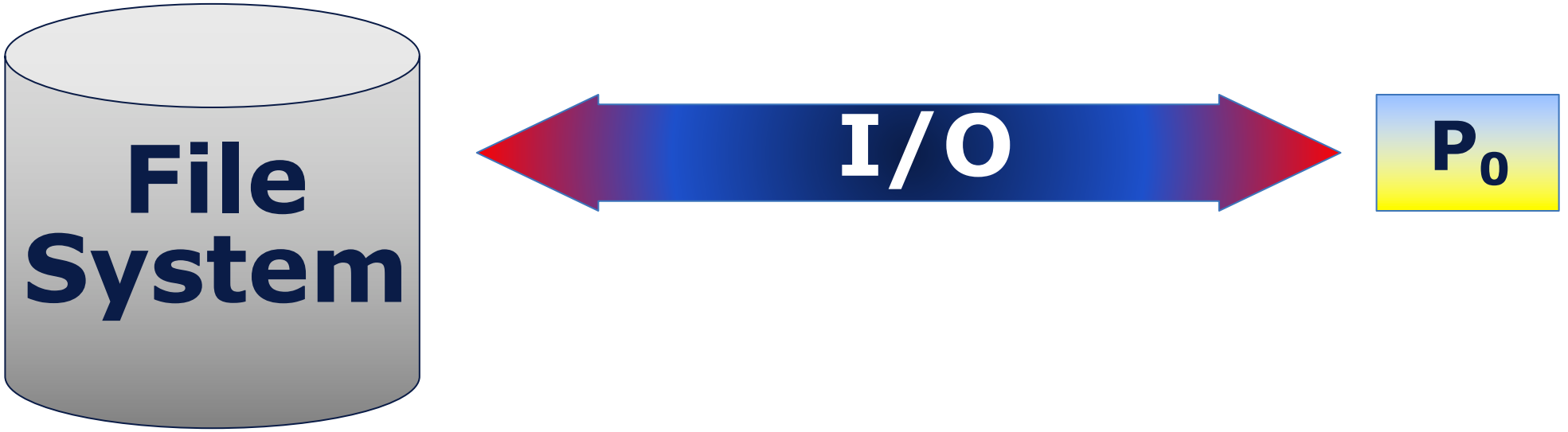
Parallel I/O



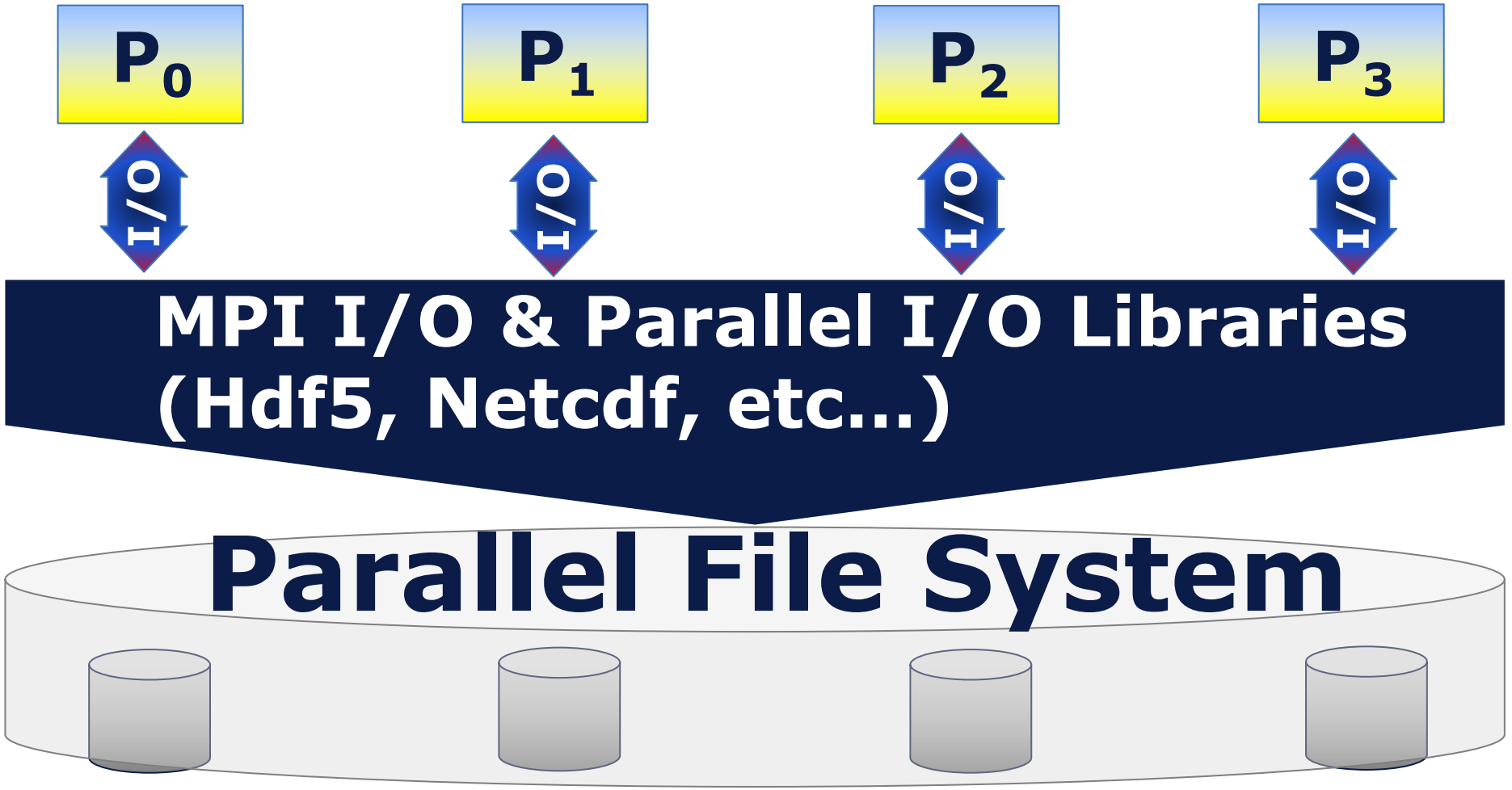
Parallel I/O

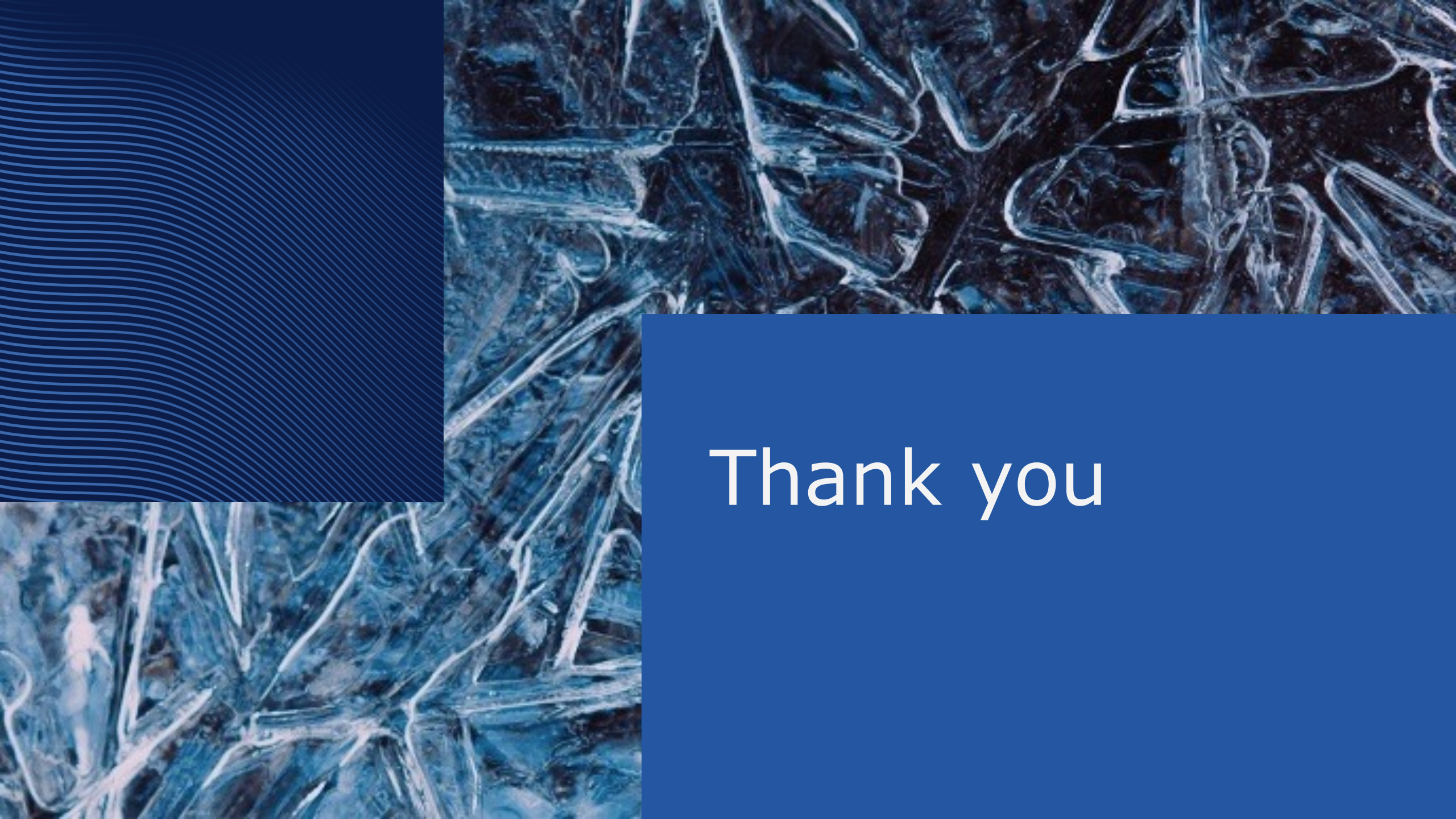

P0
P1
P2
P3
I/O Bandwidth
I/O Bandwidth
I/O Bandwidth
I/O Bandwidth
File System
File System
File System
File System

Serial I/O



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



Thank you