MPI: Message-Passing Interface

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MPI Overview

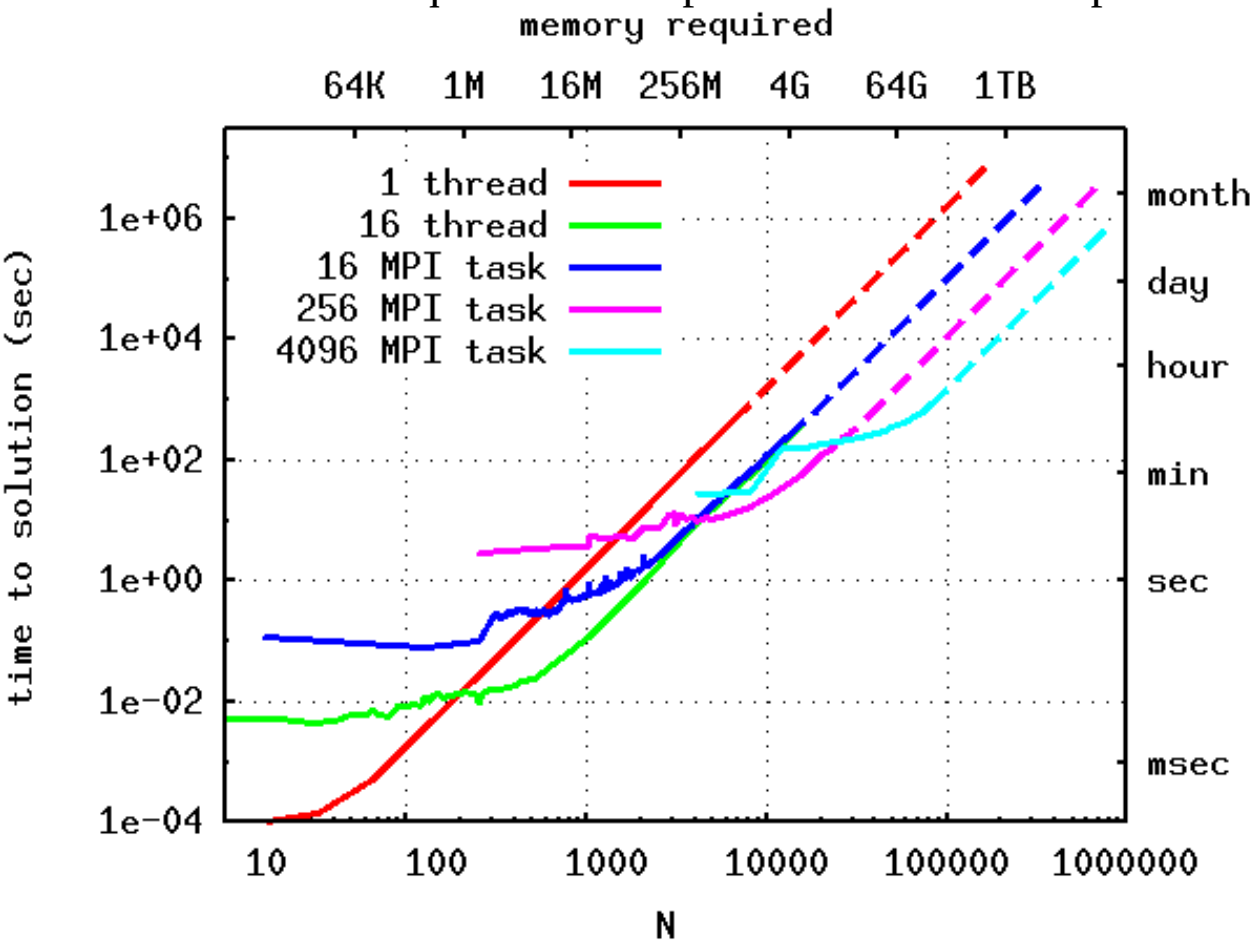
- Most widely used for programming parallel computers (clusters of workstations)
- Key attributes:
  - Partitioned address space
  - Explicit parallelization
- Process interactions
  - Send and receive data

MPI Overview

- Communications
  - Sending and receiving messages
  - Primitives
    - send(buff, size, destination)
    - receive(buff, size, source)
    - Blocking vs non-blocking
    - Buffered vs non-buffered
  - Message Passing Interface (MPI)
    - Popular message passing library
    - ~125 functions

Scale: Practical Importance

Time required to compute the NxN matrix product C=A*B



Assuming you can address 64GB from one task, can you wait a month?

How to balance computational goal vs. compute resources?

Choose the right scale!

Let's jump to an example

- Sharks and Fish II : N^2 parallel force evalulation
- e.g. 4 CPUs evaluate force for 125 fish

31	31	31	32

- Domain decomposition: Each CPU is "in charge" of ~31 fish, but keeps a fairly recent copy of all the fishes positions (replicated data)
- Is it not possible to uniformly decompose problems in general, especially in many dimensions
- This toy problem is simple, has fine granularity and is 2D
- Let's see how it scales

Sharks and Fish II : Program

Data:

n_fish → global

my_fish → local

$fish_i$ = {x, y, …}

Dynamics:

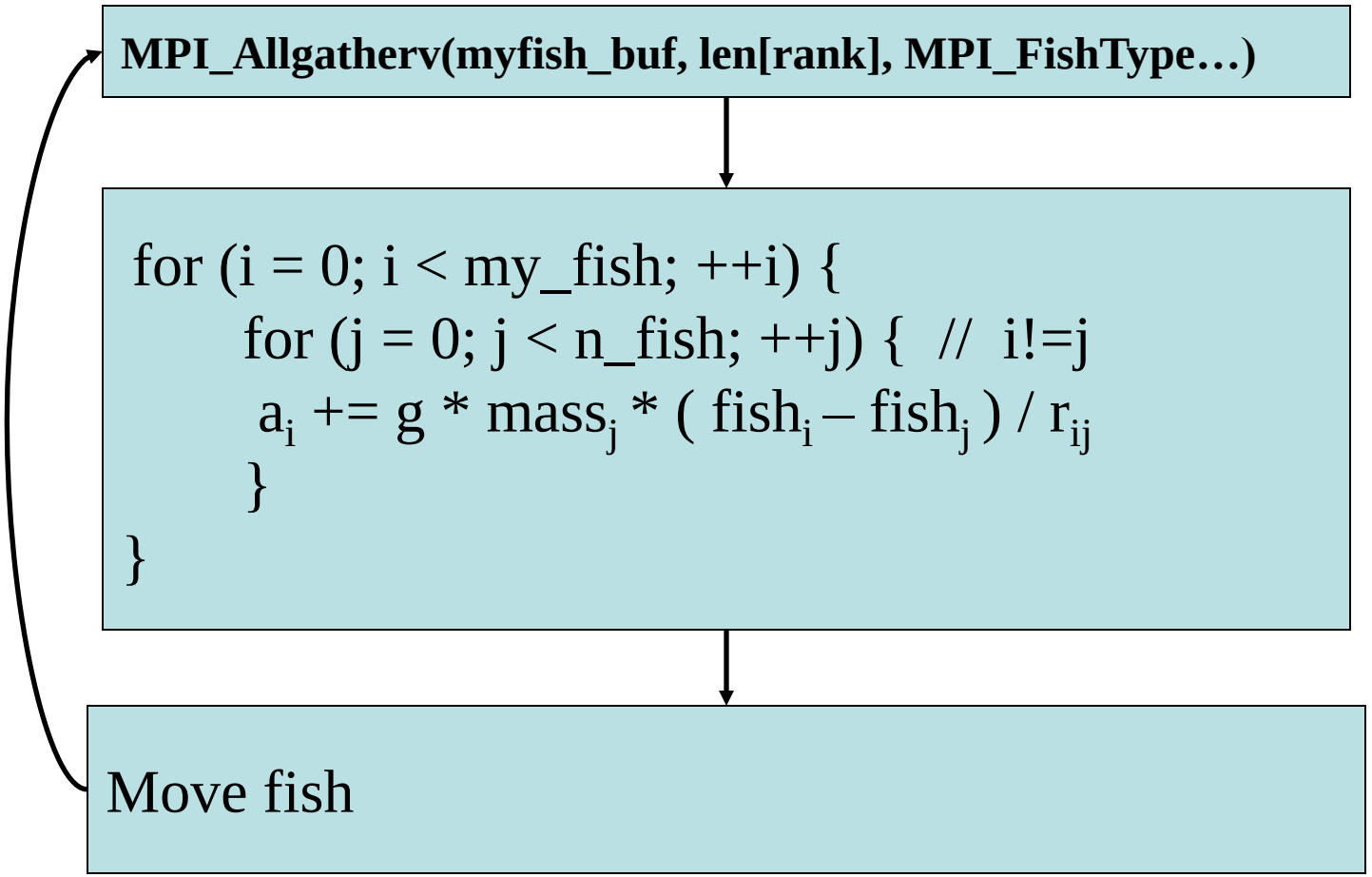
F = ma

…

$V = \Sigma\ 1/r_{ij}$

dq/dt = m * p

dp/dt = -dV/dq



Sharks and Fish II: How fast?

- 100 fish can move 1000 steps in
  - 1 task → 5.459s
  - 32 tasks → 2.756s

  x 1.98 speedup

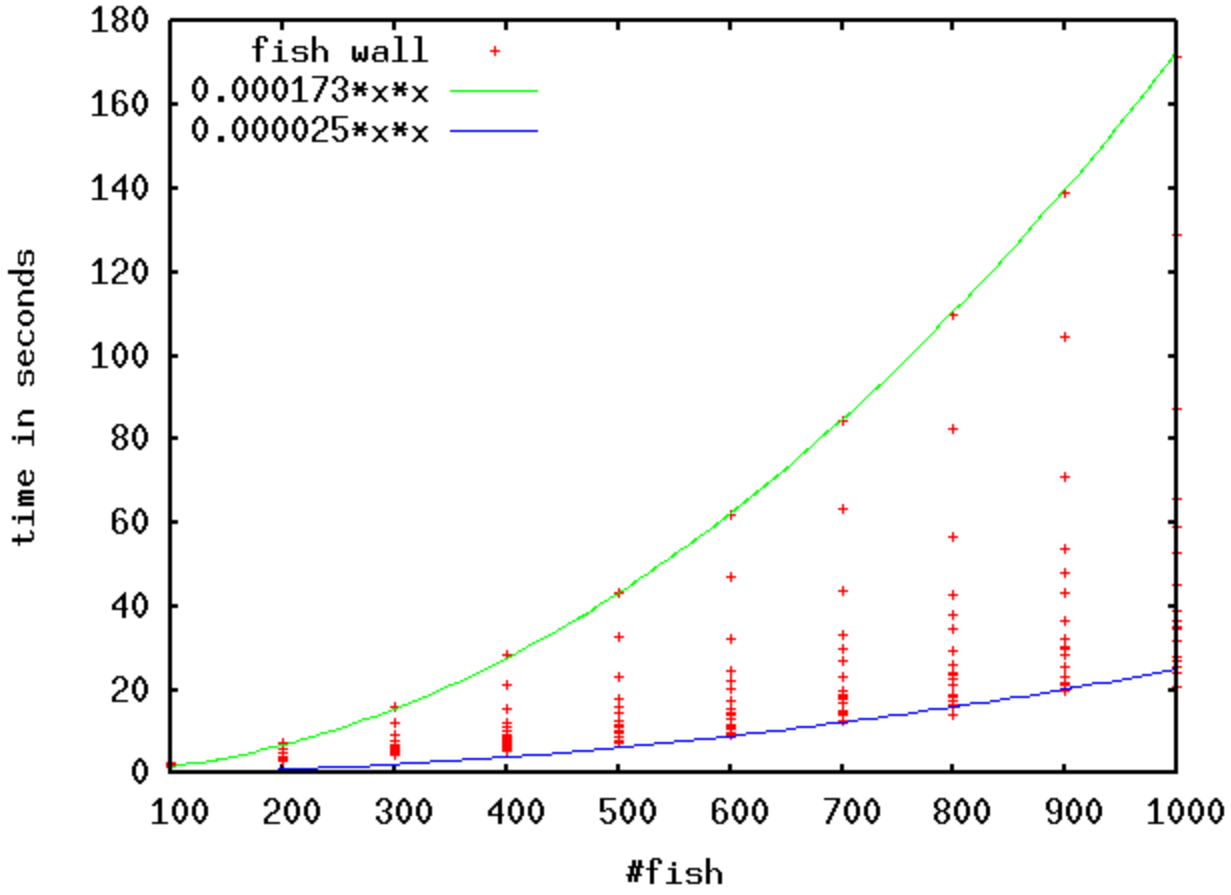
- 1000 fish can move 1000 steps in
  - 1 task → 511.14s
  - 32 tasks → 20.815s

  x 24.6 speedup

- So what's the "best" way to run?
  - How many fish do we really have?
  - How large a computer (time) do we have?
  - How quickly do we need the answer?

Scaling: Good 1st Step: Do runtimes make sense?

Running fish_sim for 100-1000 fish on 1-32 CPUs we see



1 Task

…

32 Tasks

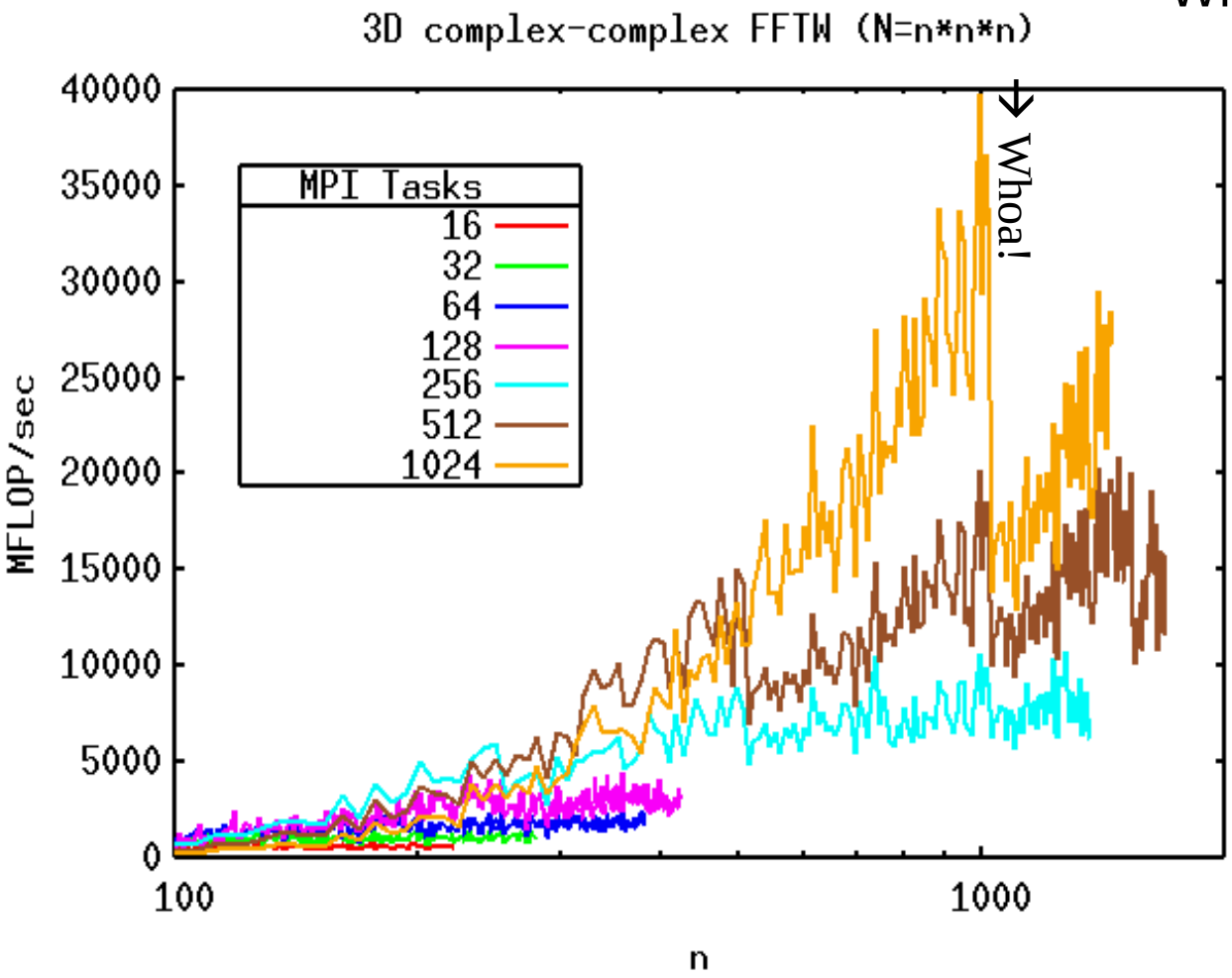
time ~ fish^2 ✓

Scaling: terminology

- Scaling studies involve changing the degree of parallelism. Will we be changing the problem also?
  - Strong scaling →Fixed problem size
  - Weak scaling→ Problem size grows with additional compute resources
- How do we measure success in parallel scaling?
  - Speed up = $T_s/T_p(n)$
  - Efficiency = $T_s/(n*T_p(n))$

Multiple definitions exist!

Scaling: Analysis



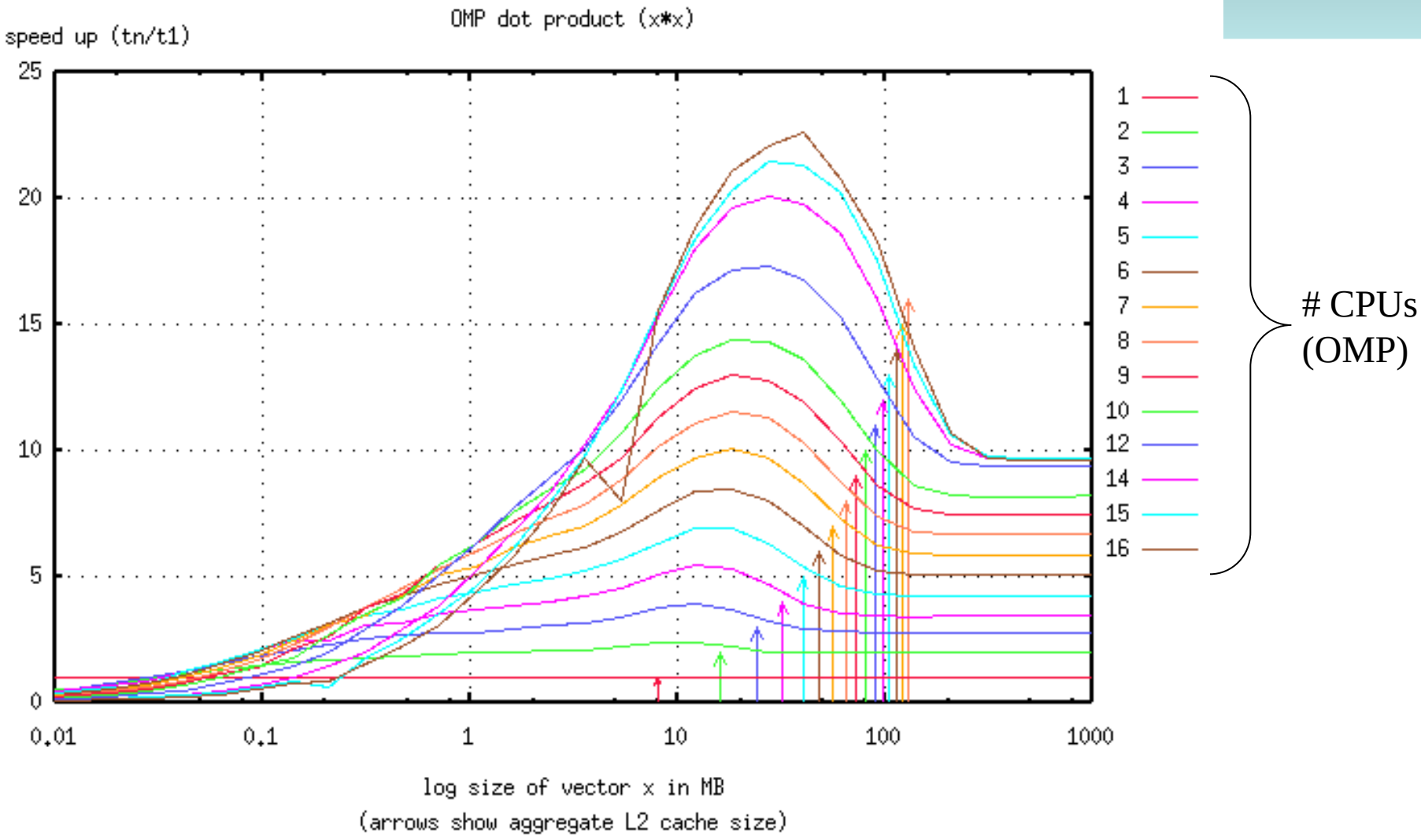
Why does efficiency drop?

- Serial code sections → Amdahl's law
- Surface to Volume → Communication bound
- Algorithm complexity or switching
- Communication protocol switching
- Scalability of computer and interconnect

Scaling: Analysis

- In general, changing problem size and concurrency expose or remove compute resources. Bottlenecks shift.
- In general, first bottleneck wins.
- Scaling brings additional resources too.
  - More CPUs (of course)
  - More cache(s)
  - More memory BW in some cases

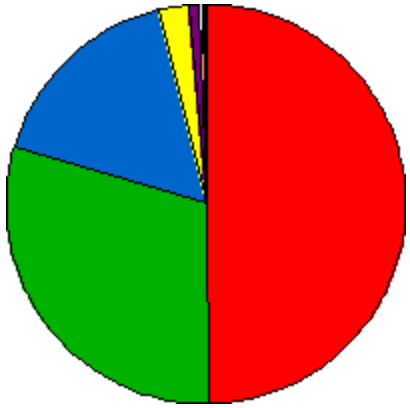
Scaling: Superlinear Speedup



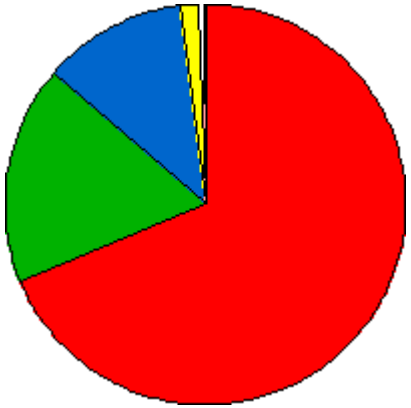
Strong Scaling: Communication Bound

64 tasks , 52% comm

192 tasks , 66% comm



768 tasks , 79% comm



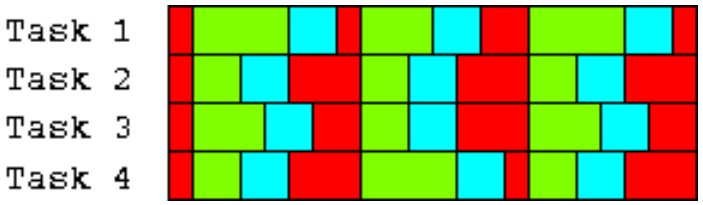
MPI_Allreduce buffer size is 32 bytes.

Q: What resource is being depleted here?
A: Small message latency

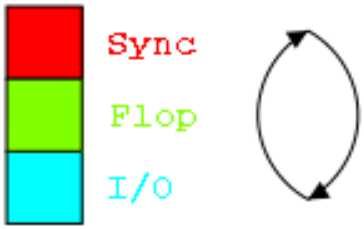
1) Compute per task is decreasing
2) Synchronization rate is increasing
3) Surface:Volume ratio is increasing

Load Balance : Application Cartoon

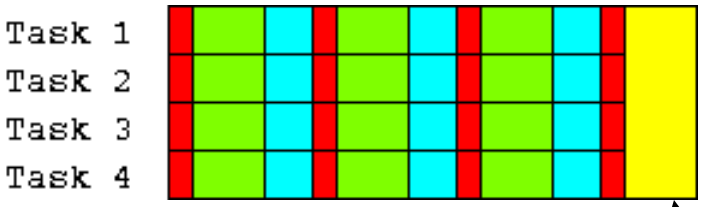
Unbalanced:



Universal App



Balanced:

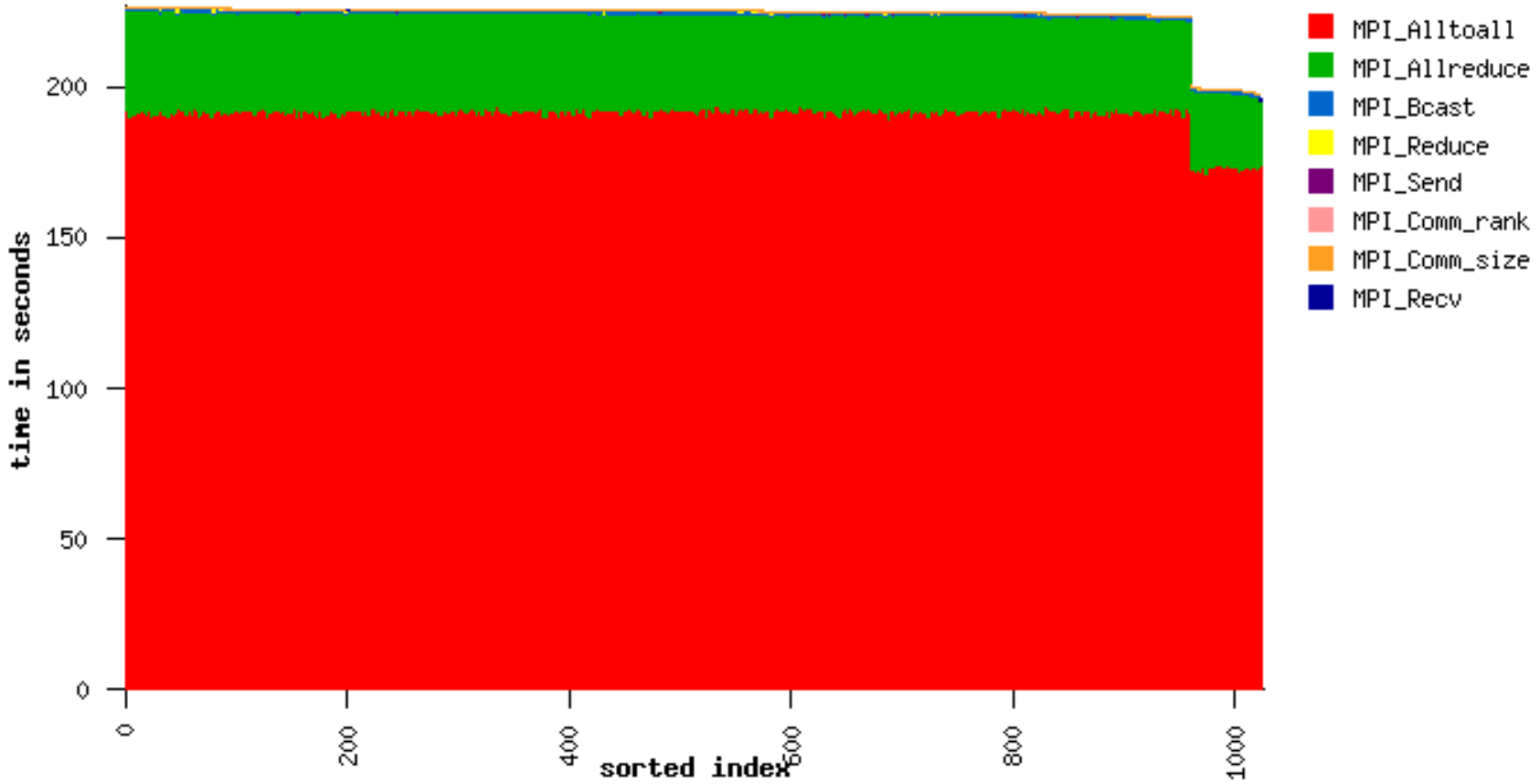


Time saved by load balance

Will define synchronization later

Load Balance : performance data

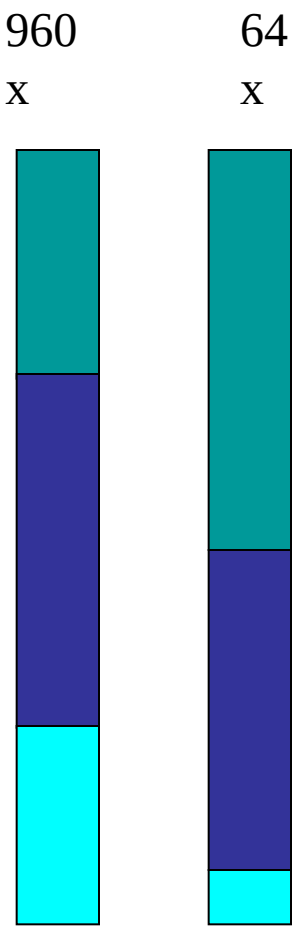
Communication Time: 64 tasks show 200s, 960 tasks show 230s



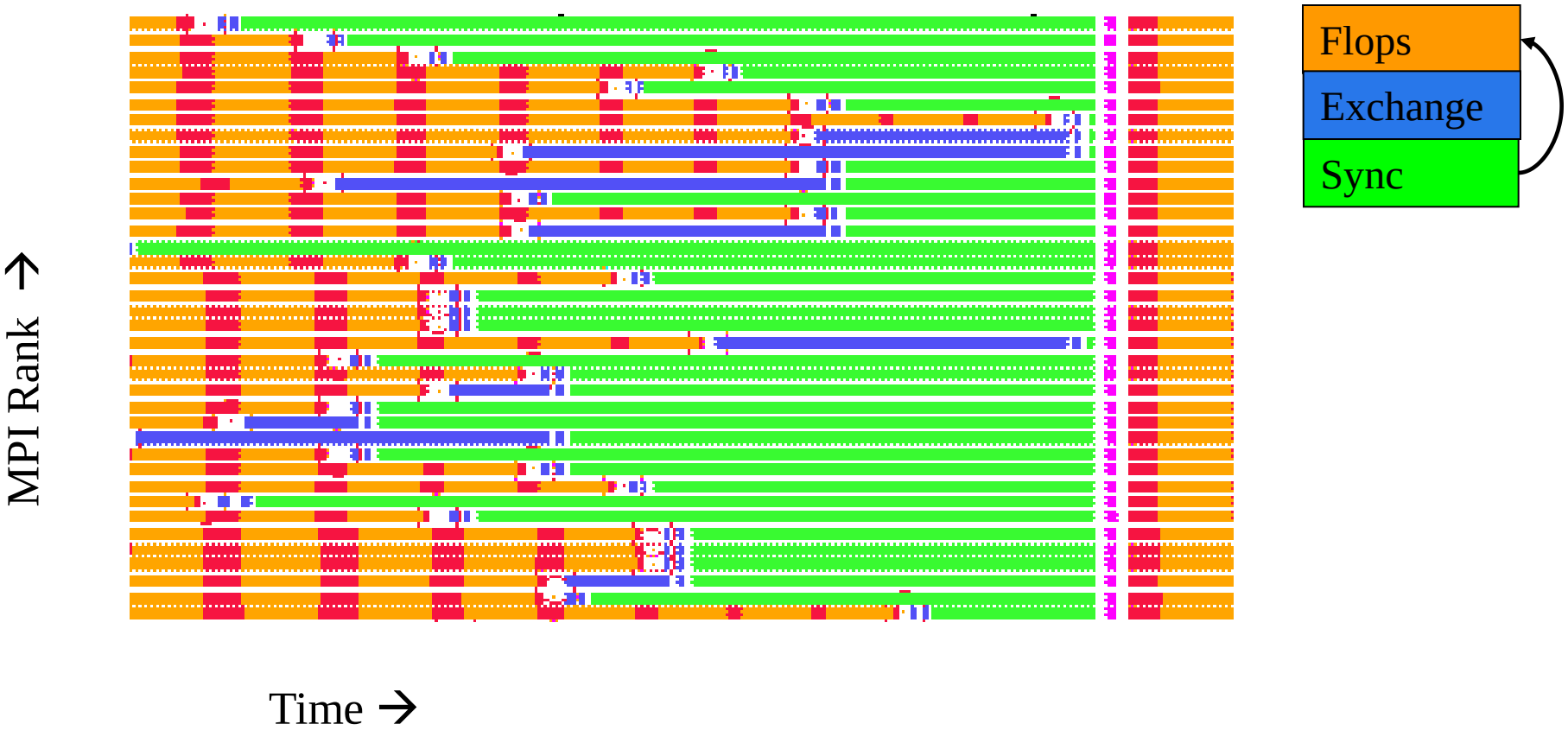
MPI ranks sorted by total communication time

Load Balance: ~code

```
while(1) {
  do_flops(N_i);
  MPI_Alltoall();
  MPI_Allreduce();
}
```



Load Balancing



Load Balancing

Flops

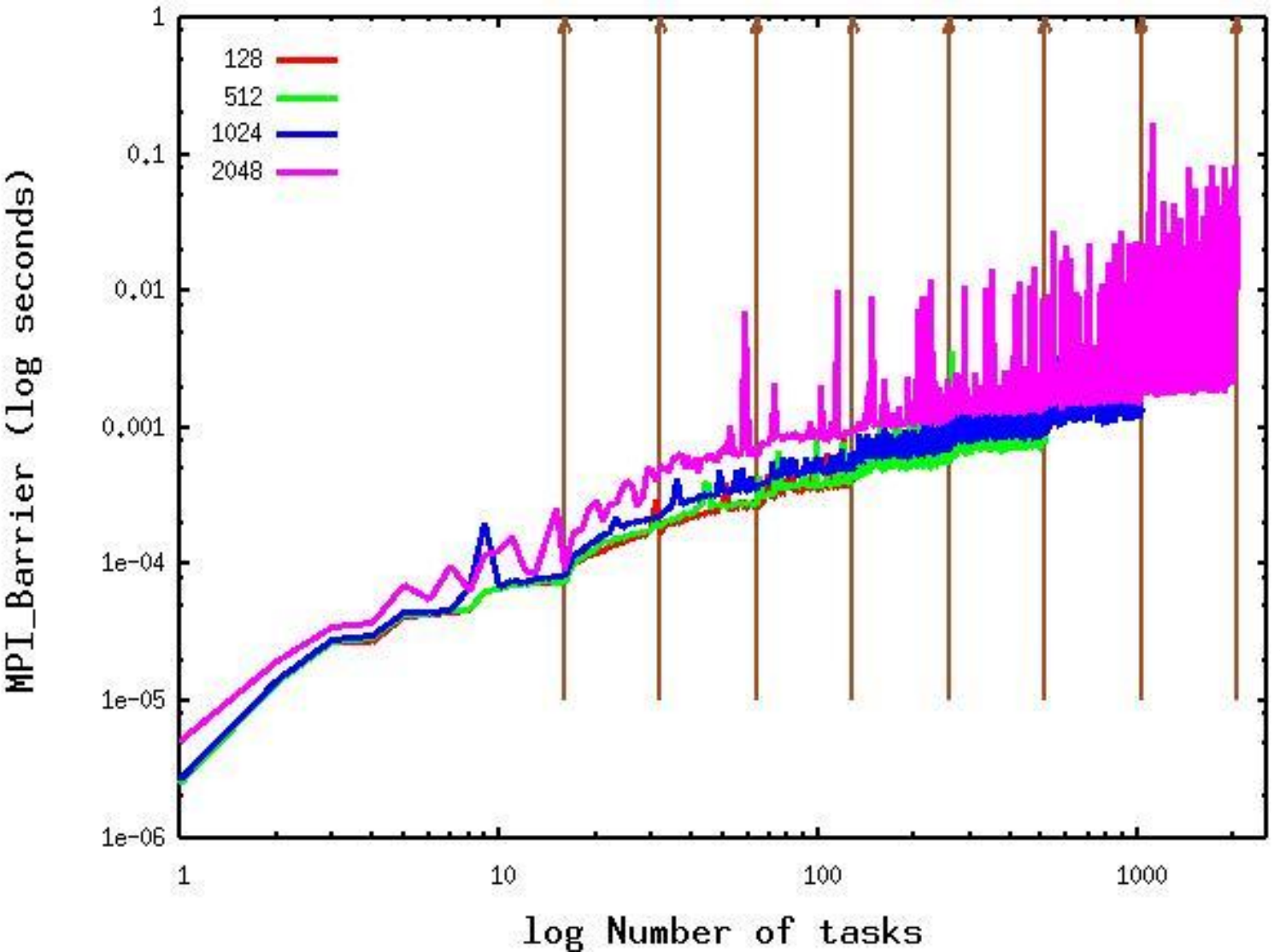
Exchange

Sync

Load Balance : analysis

- The 64 slow tasks (with more compute work) cause 30 seconds more “communication” in 960 tasks
- This leads to 28800 CPU*seconds (8 CPU*hours) of unproductive computing
- All load imbalance requires is one slow task and a synchronizing collective!
- Pair well problem size and concurrency.
- Parallel computers allow you to waste time faster!

Scaling of MPI_Barrier()



four orders of magnitude

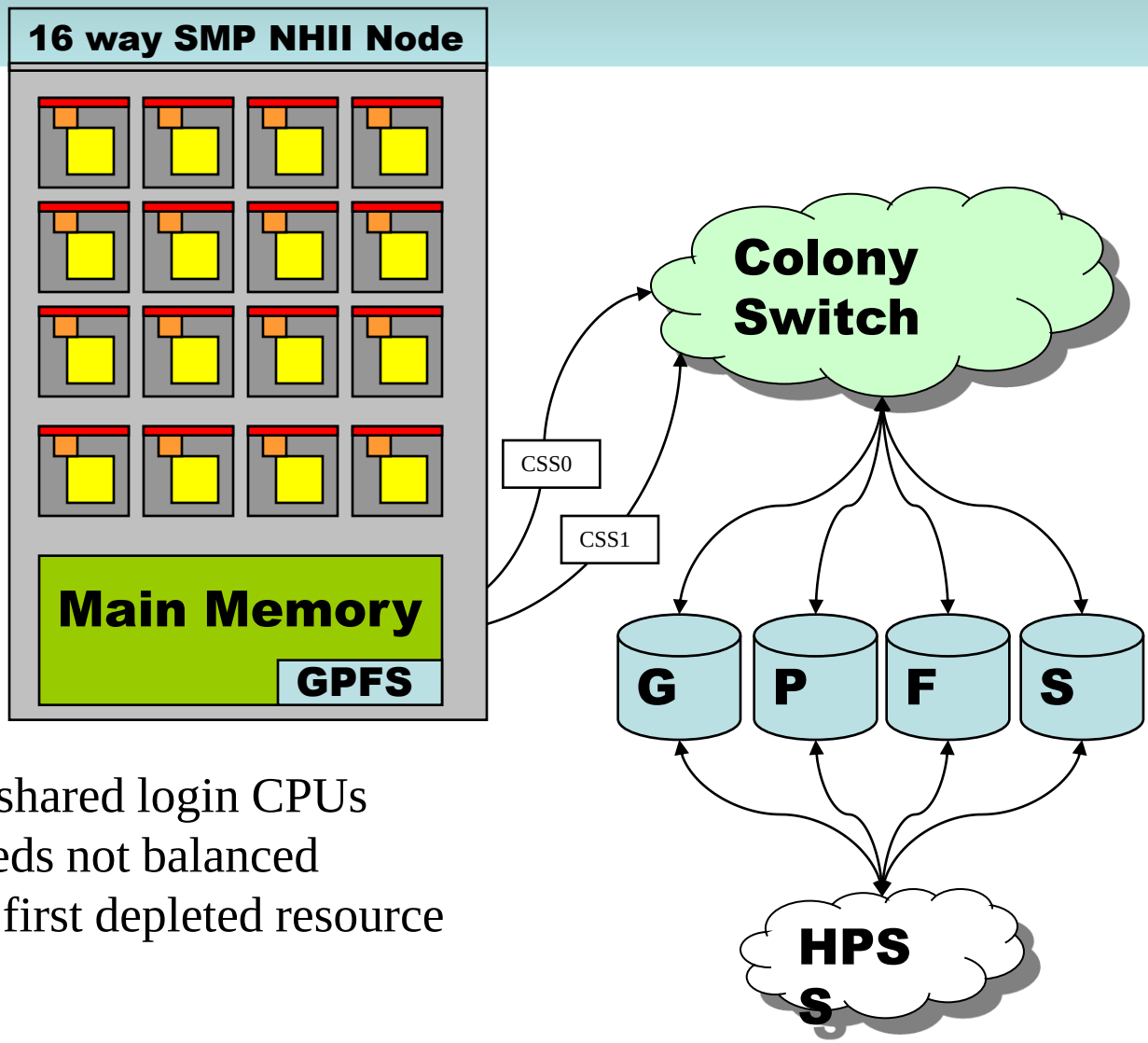
Synchronization

- It's hard to discuss synchronization outside of the context a particular parallel computer
- MPI timings depend on HW, SW, and environment
  - How much of MPI is handled by the switch adapter?
  - How big are messaging buffers?
  - How many thread locks per function?
  - How noisy is the machine (today)?
- This is hard to model, so take an empirical approach based on an IBM SP which is largely applicable to other clusters…

Memory Hierarchy

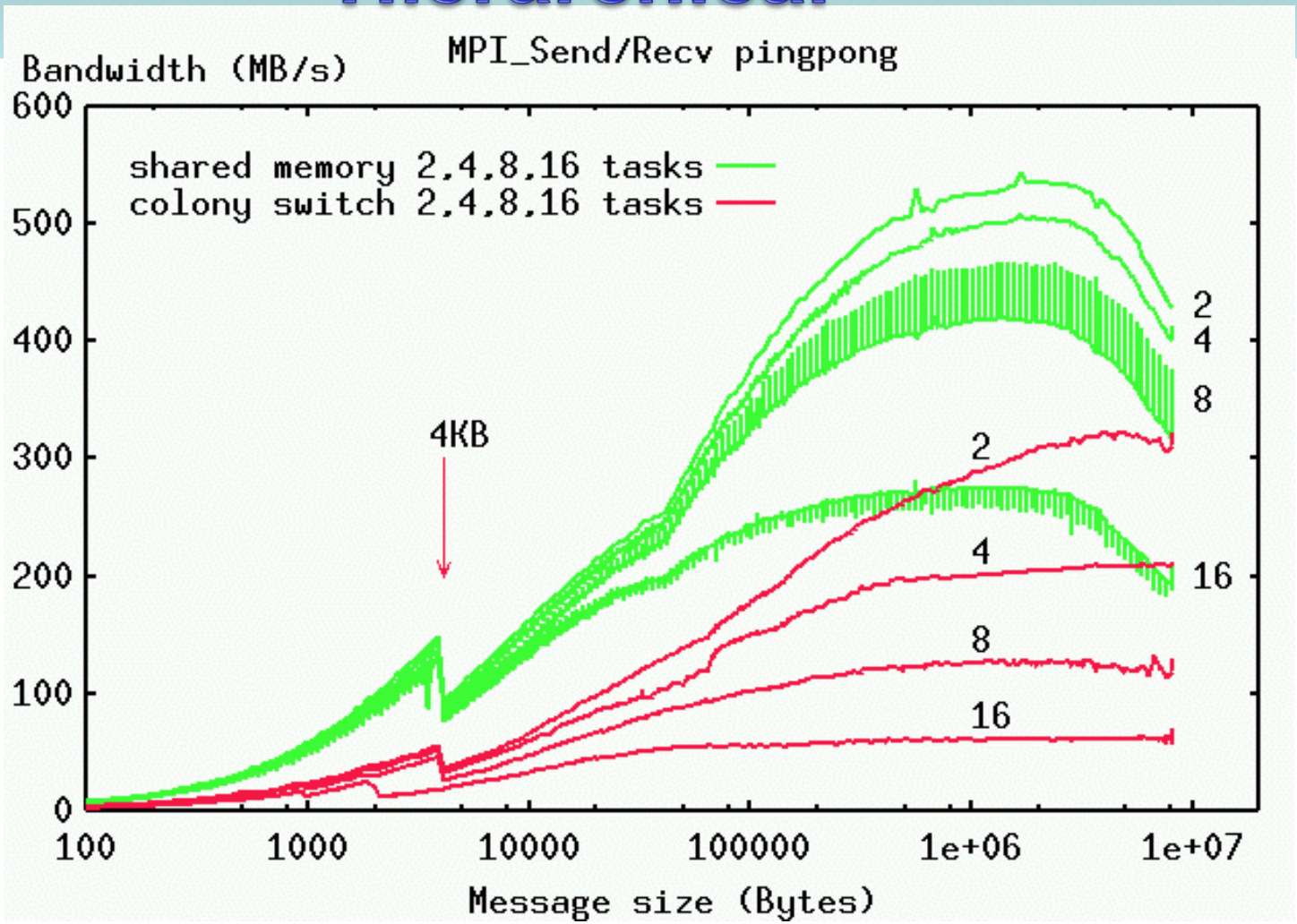
IBM SP **380 x**

Resource	Speed	Bytes
Registers	3 ns	2560 B
L1 Cache	5 ns	32 KB
L2 Cache	45 ns	8 MB
Main Memory	300 ns	16 GB
Remote Memory	19 us	7 TB
GPFS	10 ms	50 TB
HPSS	5 s	9 PB



- 6080 dedicated CPUs, 96 shared login CPUs
- Hierarchy of caching, speeds not balanced
- Bottleneck determined by first depleted resource

MPI Performance is often Hierarchical



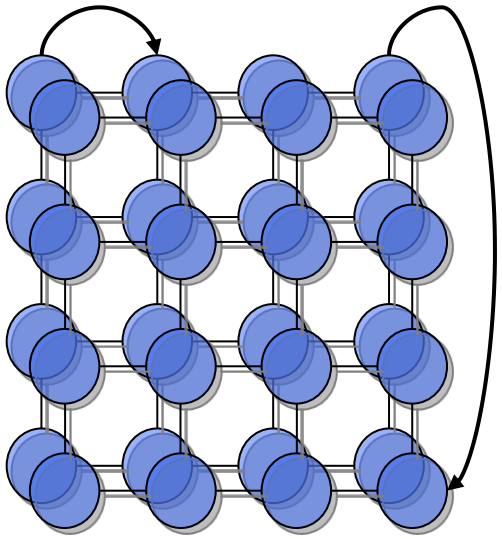
Intra

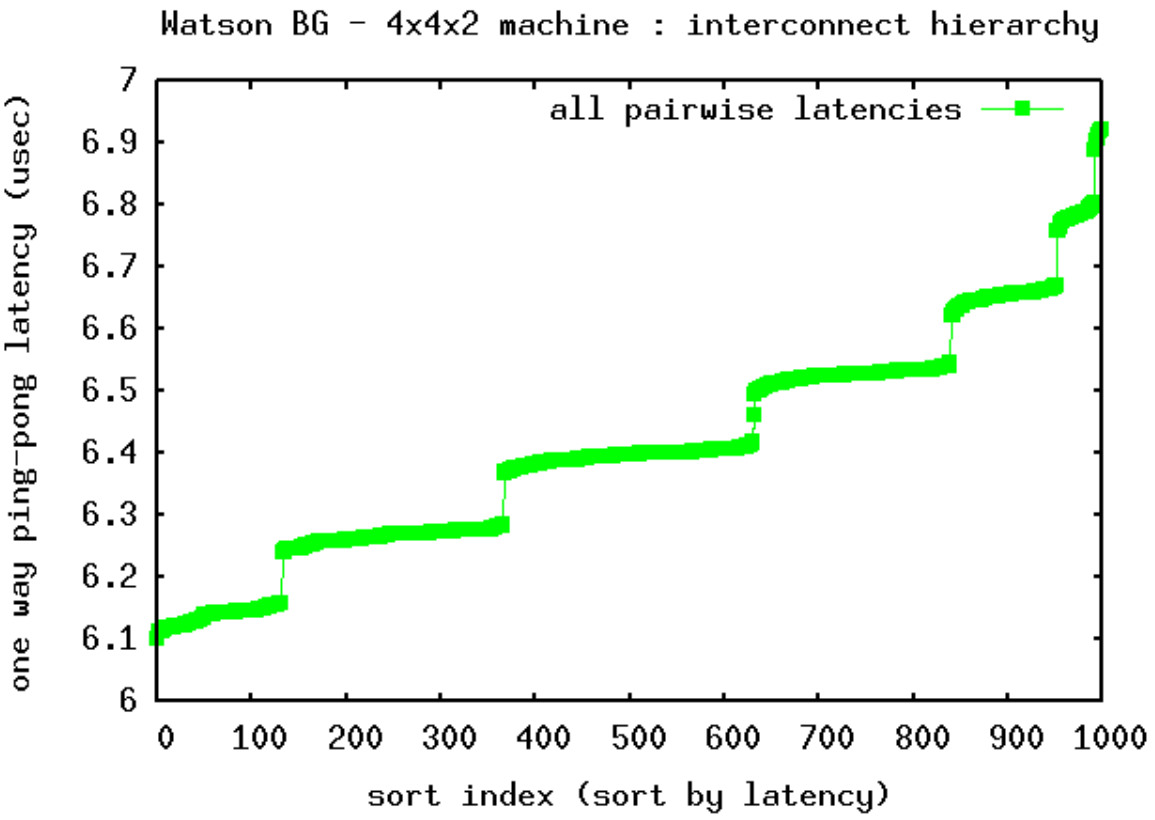
Inter

message size and task placement are key to performance

MPI: Latency not always 1 or 2 numbers

The set of all possibly latencies describes the interconnect geometry from the application perspective

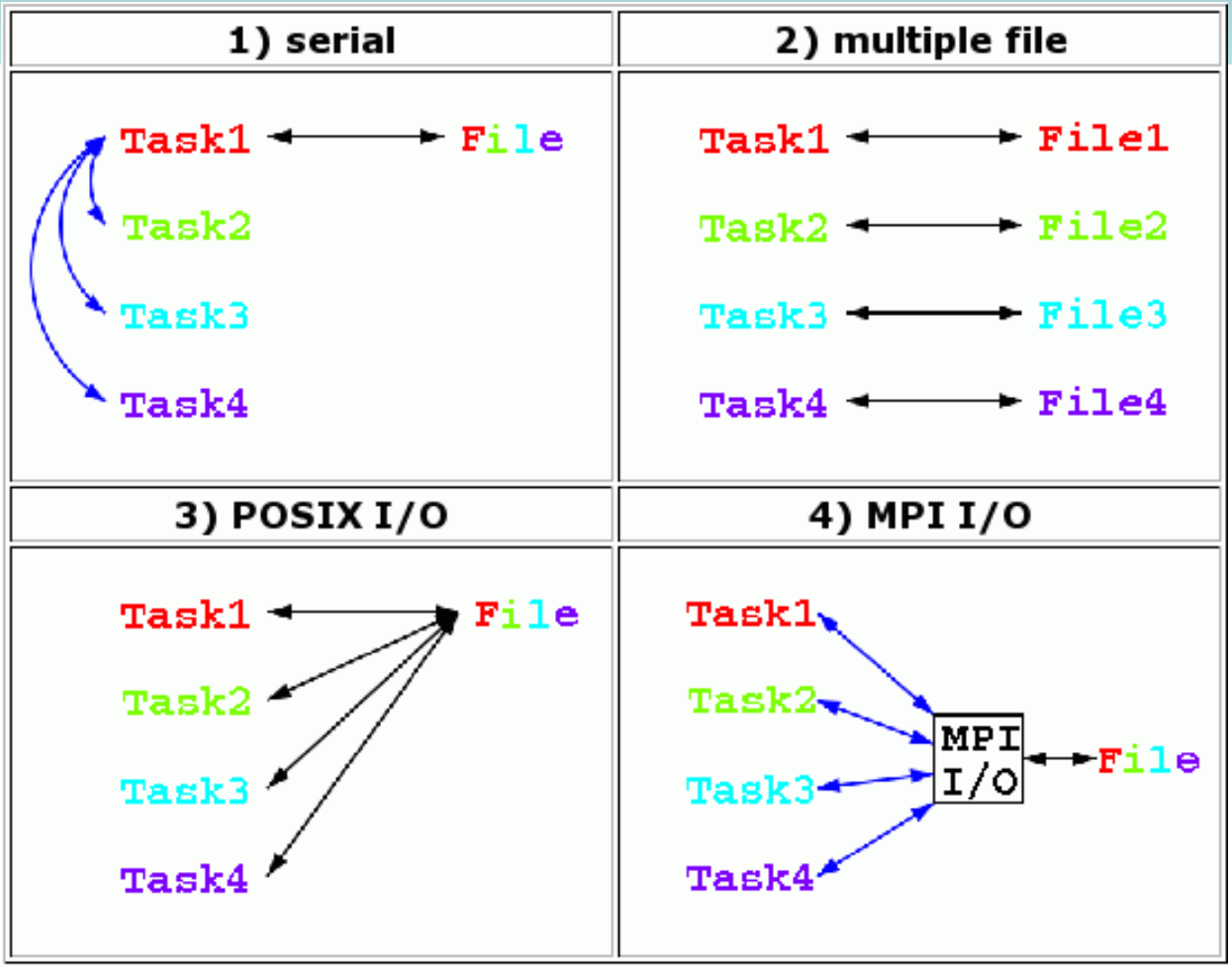


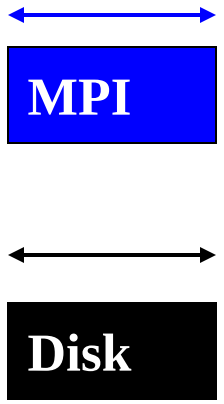


Synchronization : Summary

- As a programmer you can control
  - Which MPI calls you use (it's not required to use them all).
  - Message sizes, Problem size (maybe)
  - The temporal granularity of synchronization, i.e., where do synchronization occur.
- Language writers and system architects control
  - How hard is it to do the above
  - The intrinsic amount of noise in the machine

Parallel File I/O : Strategies

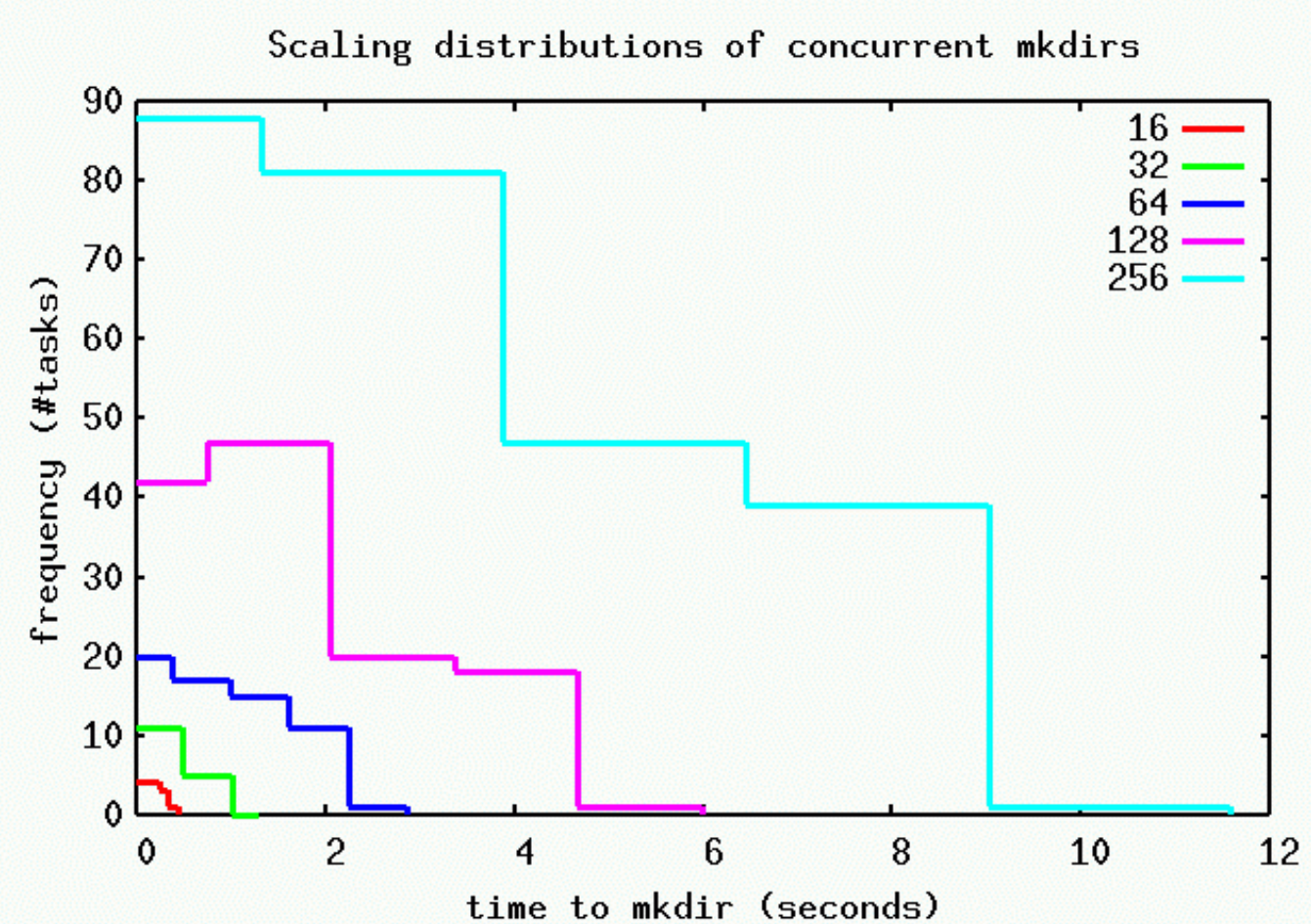




Some strategies fall down at scale

Parallel File I/O: Metadata

- A parallel file system is great, but it is also another place to create contention.
- Avoid uneeded disk I/O, know your file system
- Often avoid file per task I/O strategies when running at scale



Questions