DATA SCIENCE &
SCIENTIFIC COMPUTING


Istituto Officina
dei Materiali


# L03: Parallel Programming concepts


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# Agenda

- HPC Concepts (part 2)
  - Parallel programming paradigms
  - Parallel programming concepts
  - Ahmdal law / Gustafson law
  - Strong/weak scalability

# Introduction to HPC programming principles

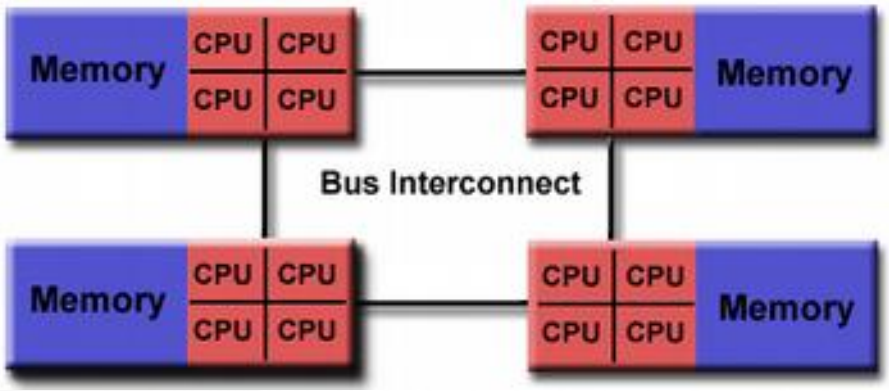
# Two main programming paradigms

- Dictated by the HW architecture:
  - shared memory
    - Single memory view, all processes (usually threads) could directly access the whole memory
  - distributed memory ( Message Passing)
    - all processes could directly access only their local memory

# Parallel programming

TAKE HOME MESSAGE:Great responsibility of the programmer

## Shared memory

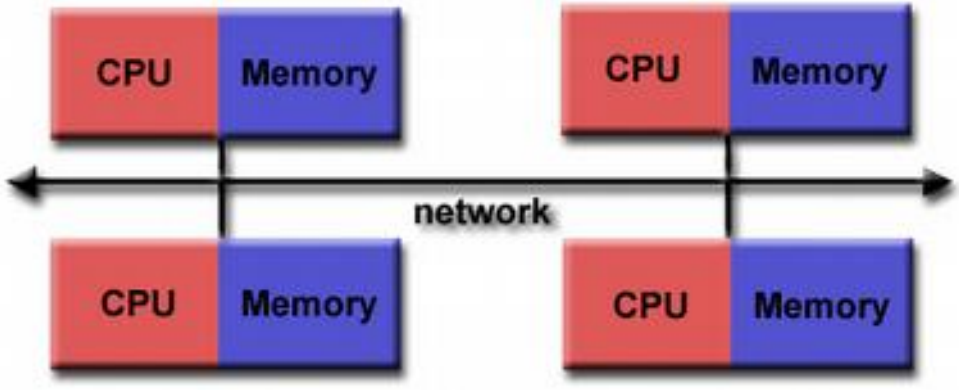



- Pros
- Global address space provides a user-friendly programming perspective to memory
- Data sharing between tasks is both fast and uniform due to the proximity of memory to CPUs

### Cons

- Cannot scale to large number of cores
- Programmer responsibility for synchronization constructsthat ensure "correct" access of global memory.

## Distributed memory




- Pros
- Memory is scalable with the number of processors. Increase the number of processors and the size of memory increases proportionately.

### Cons

- Data is scattered on separeted address spaces
- The programmer is responsible for many of the details associated with data communication between processors.
- Non-uniform memory access times - data residing on a remote node takes longer to access than node local data.

# Parallel Programming Paradigms, cont.

| Programming Environments | |
|---|---|
| **Message Passing** | **Shared memory** |
| Standard compilers | Ad hoc compilers |
| Communication Libraries | Source code Directive |
| Ad hoc commands to run the program | Standard Unix shell to run the program |
| Standards: **MPI** | Standards: **OpenMP** |

# How to program shared memory machine ?

- Automatic (implicit) parallelization:
  - compilers do (part of) the job for you not much
- Manual parallelization:
  - Insert parallel directives by yourself to help compilers
  - OpenMP THE standard simple but done manually
- Multi threading programming:
  - more complex but more efficient
  - use a threads library to create task by yourself
- Use already threaded libraries..

# Shared memory

- Central concept: execution thread
- A piece of the programm is assigned to each thread, which runs on a core of the CPU
- Approaches
  - POSIX threads Low level, performant!
  - OpenMP Good middle ground
  - Intel TBB

# Shared memory

- Simple example: loop parallelization with OpenMP

```
#pragma omp parallel for
for(int i=0; i<n; ++i)
    c[i]= a[i]+b[i];
```

- To compile with gcc add '-fopenmp' to compilation line

```
gcc -fopenmp mycode.c
```

NOTE:OpenMP = 1 process THAT SPAWN a given number of THREAD

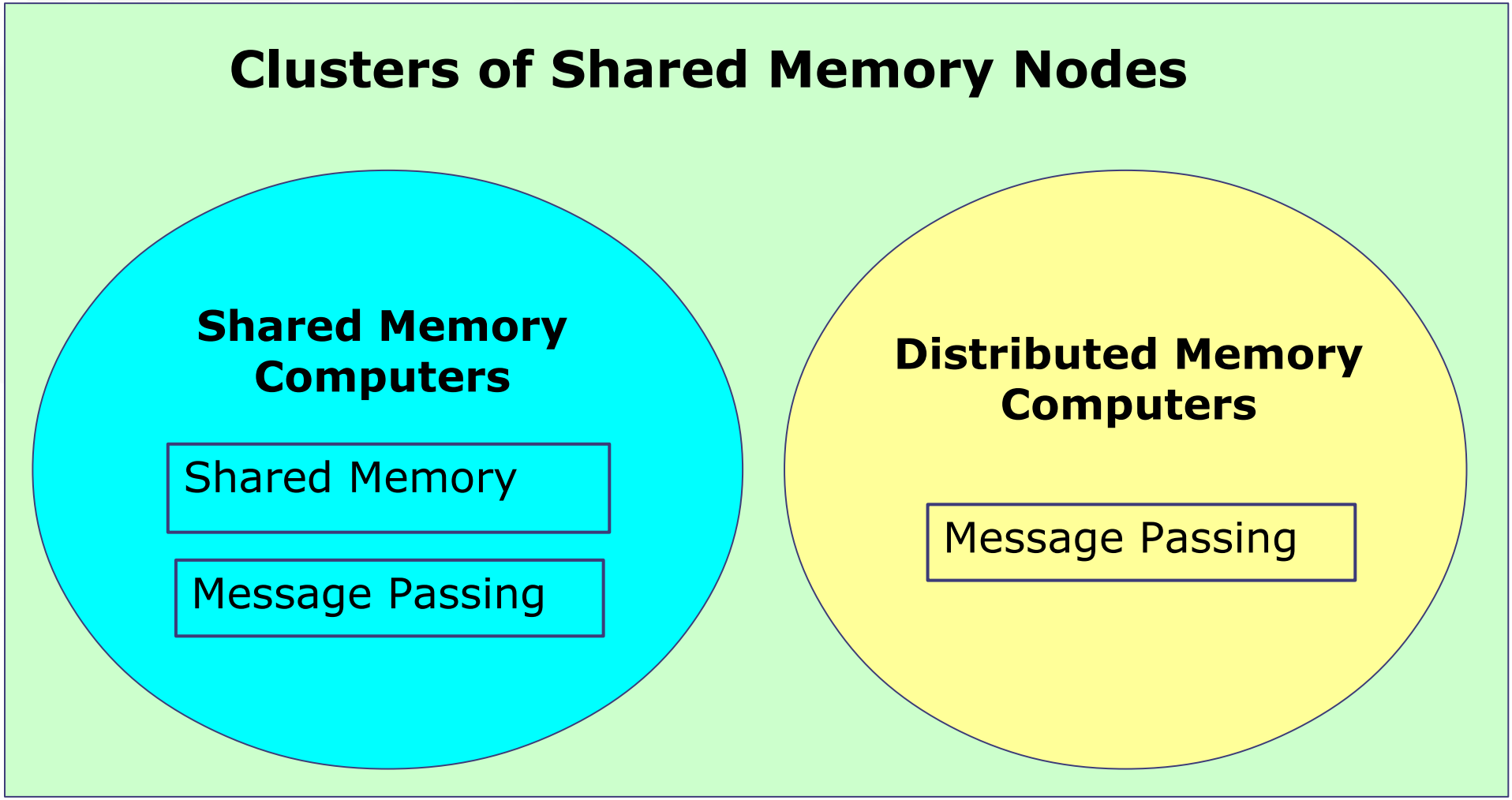
The OpenMP execution model is "simple";Good performance and scalability IF

BEWARE of PRIVATE VARIABLES that ensure execution.number of threads and so on...

# How to program using message passing ?

- Using the de-facto standard : MPI message passing interface
  - A standard which defines how to send/receive message from a different processes
- Many different implementation
  - OpenMPI
  - Intel-MPI
  - They all provide a library which provide all communication routines
- To compile your code you have to link against a library
  - Generally a wrapper is provided (mpif90/mpicc)

# Architectures vs. Paradigms



# Parallel programming:  a short summary..

Message passing is MUCH MORE COMPLEXBut NOT SLOWER! (because of more granular control!)HOWEVER in some cases, using OpenMP MAY BE

| Architectures | |
|---|---|
| Distributed Memory | Shared Memory |
| **Programming Paradigms/Environment** | |
| Message Passing  | Shared Memory  |
| **Parallel Programming Models** | |
| Domain Decomposition<br>99% of the "parallelism" | Functional Decomposition |

# Other paradigm are now available

- Mixed/hybrid approach..
  - MPI + OpenMP

Modern take!

- Specific SDK for specific devices
  - CUDA for Nvdia GPU

Accelerator SDKs in general

- Write once run everywhere:
  - OpenCL

Support for AMD/ATI Radeon (which is usually cheaper);;

  - OpenACC:

Like CUDA but NOT proprietary!

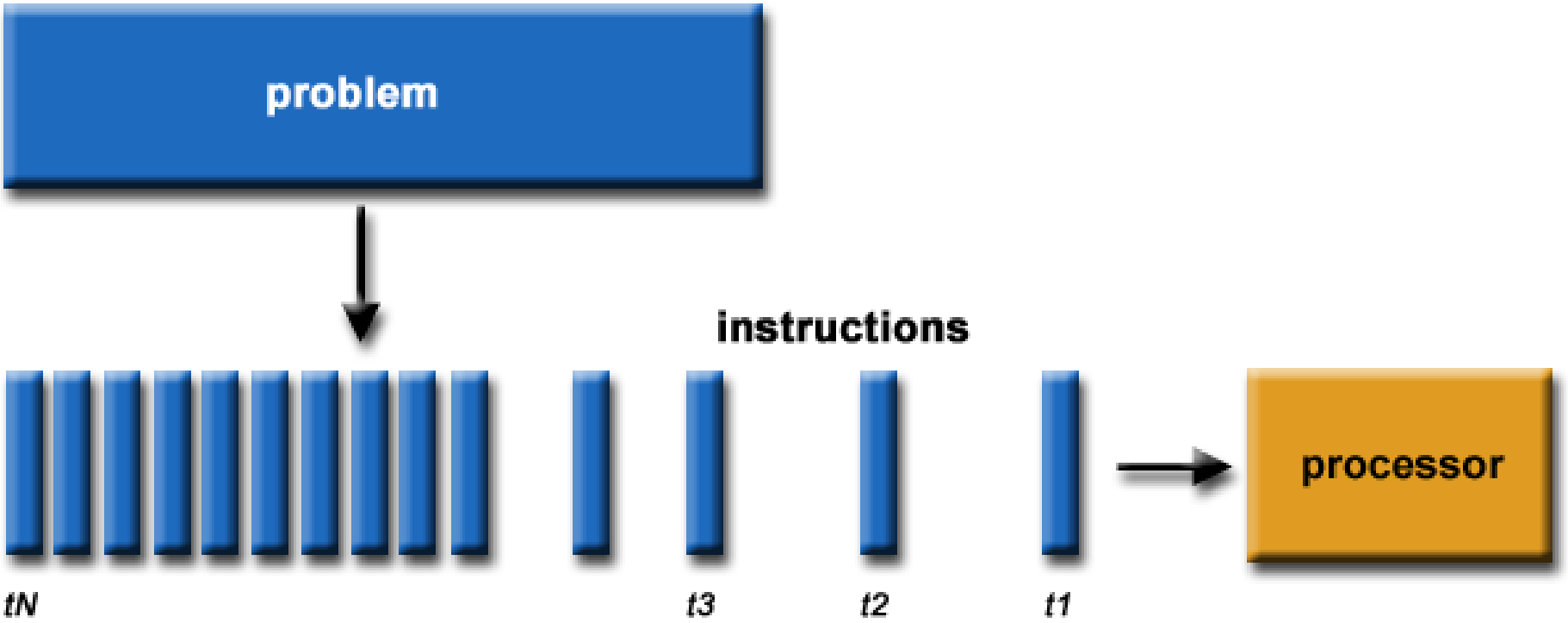
    - OpenACC is about giving programmers a set of tools to port their codes to new heterogeneous system without having to rewrite the codes in proprietary languages.

# Principle of parallel computing

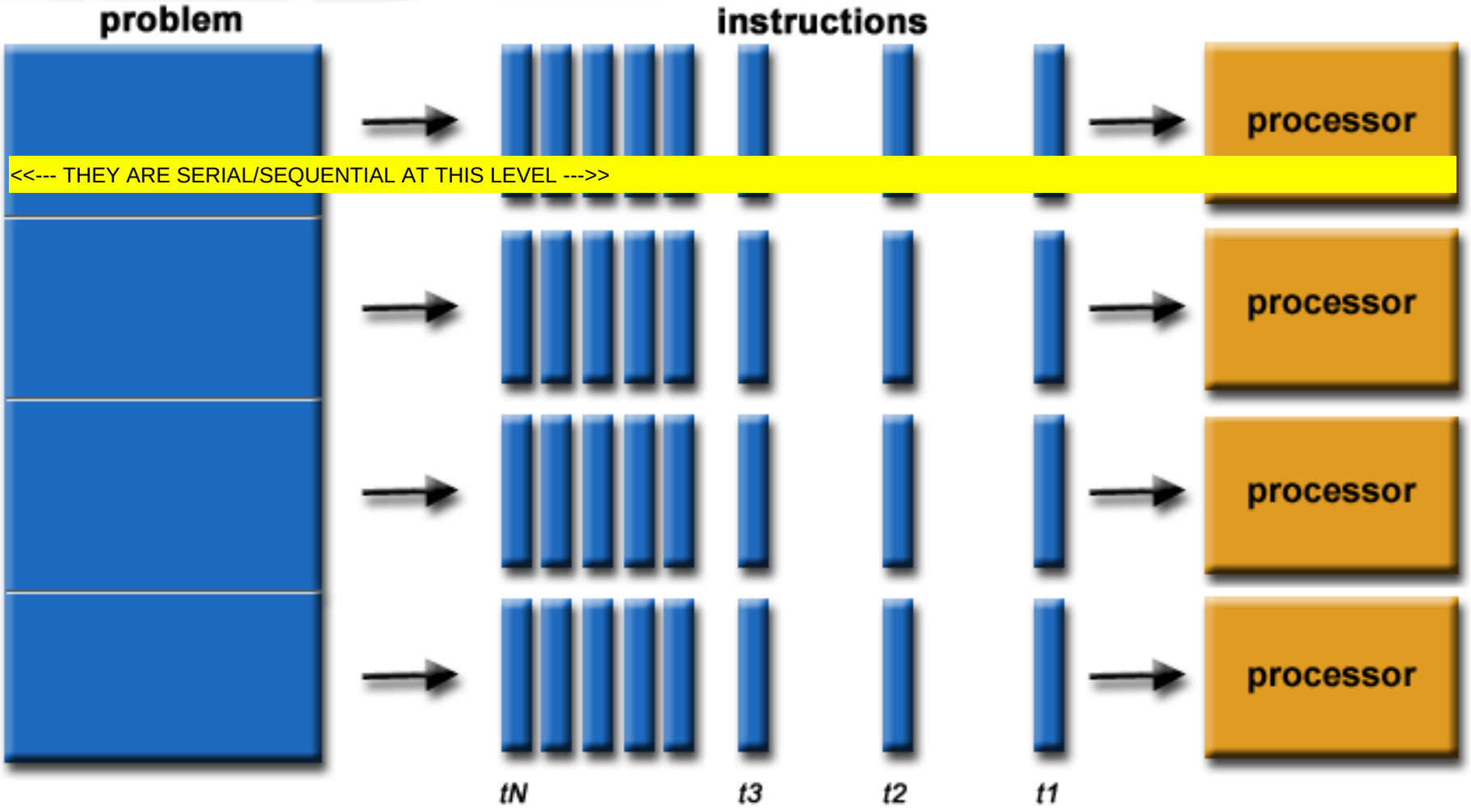
- Speedup, efficiency
  - Ahmdal Law/Gustafson Law
- Finding and exploiting parallelism — Exploiting the possibility of running code in parallel
- Finding and exploiting data locality — Exploiting the possibility of accessing data while they are local
- Load balancing — When LOAD (work to be done) is unevenly distributed: NOTE: walltime is the slowest runn
- Coordination and synchronization — i.e. Master/Slave approach
- Performance modeling

All of these things make parallel programming more difficult than sequential programming.

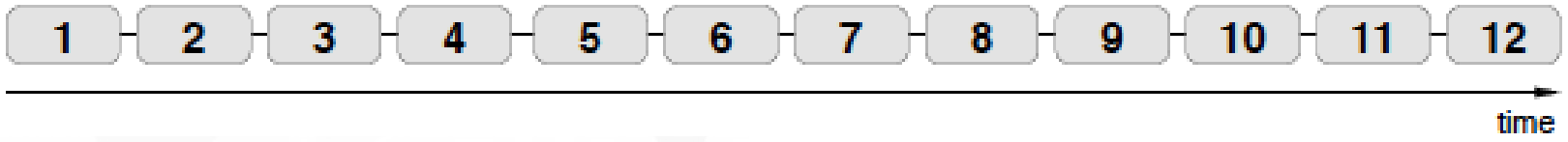
# Serial execution

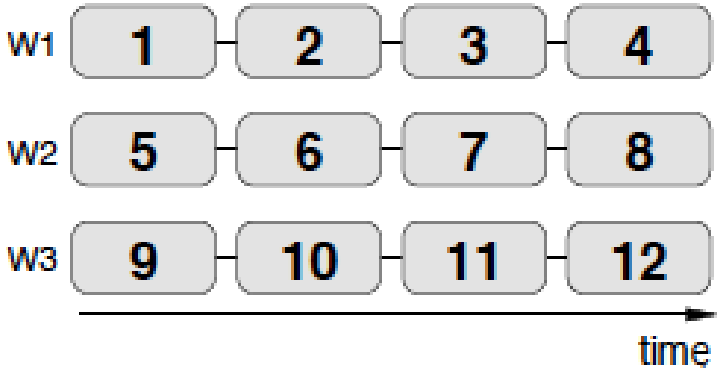


# Parallel execution



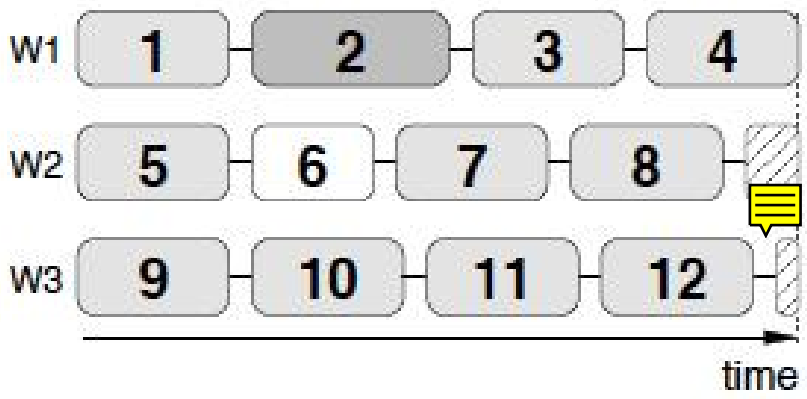
# Running in parallel



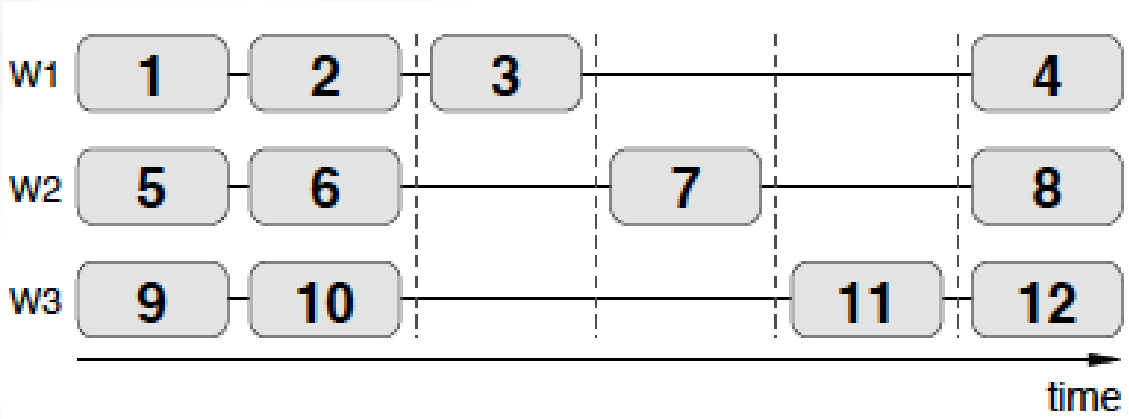

- Execution time reduces from 12 secs to 4 secs!

# Load imbalance




- What if all processors can't execute tasks with the same speed?
  - Load imbalance (ending parts for W2 and W3)

# Dependence amongst tasks




- What if tasks 3, 7 and 11 are dependent?
  - Execution time increases from 4 to 6!

Interdependency:workflow/serial-parallel interplay

# Introducing Scalability

- How much faster can a given problem be solved with N workers instead of one?
- How much more work can be done with N workers instead of one?
- What impact for the communication requirements of the parallel application have on performance?
- What fraction of the resources is actually used productively for solving the problem?

# Scalability

MODEL of SCALABILITY

- Simple model

$$s + p = 1,$$

s: serial part  p: parallel part

- Why serial part?
  - Imperfect load balancing (some processors have more work) (Starvation)
  - Cost of communication (Latency)
  - Synchronization time (Overhead )
  - Cost of contention for resources, e.g., memory bus, I/O (Waiting )

Sometimes it's not always that the LOAD is unbalanced. Just the fact that some parts

# Scaling

- Strong Scaling: Keeping the problem size fixed and pushing in more workers or processors Same problem, faster
  - Goal: Minimize time to solution for a given problem
- Weak Scaling: Keeping the work per worker fixed and adding more workers/processors (the overall problem size increases)
  - Goal: solve the larger problems Same time (ideally), bigger problem solved

# Speed up

The speedup of a parallel application is

$$Speedup(p) = Time(1)/Time(p)$$

where

Time(1) = execution time for a single processor

Time(p) = execution time using p parallel processor

If Speedup(p) = p we have perfect speedup (also called linear scaling)

Holy grail of parallel programmer! ;-)

speedup compares an application with itself on one and on p processors

more useful to compare

The execution time of the best serial application on 1 processor

versus More accurate!

The execution time of best parallel algorithm on p processors

# Scaling…

- Scaling  or scalability:  some sort of ration between the performance and the “size” of the HPC infrastructure
  - Usual way to measure size: # of processors
- The ability for some application to increases  speed when the size of the HPC is increased strong
- The ability to for some application to solve larger problems when the size of the HPC increases.. weak

# Efficiency

- The parallel efficiency of an application is defined as
  - Efficiency(p) = Speedup(p)/p
- Efficiency(p) <= 1
- For perfect speedup Efficiency (p) = 1 Linear scaling
- We will rarely have perfect speedup: Lack of perfect parallelism in the application or algorithm
- Understanding why an application is not scaling linearly will help will help finding ways improving the applications performance on parallel computers.

# Superlinear speedup

Question: can we find "*superlinear*" speedup, that is

Speedup(p) > p ?

Usually not; however...

Choosing a bad "baseline" for T(1)

WRONG !!!

Old serial code has not been updated with optimizations

"fake" speedup

Shrinking the problem size per processor

GOOD

The code actually exploits parallelism!

- May allow it to fit in small fast memory (cache)

i.e. SWAPPING AVOIDANCE!Even with SSDs: VERY LOW speed bottleneck between DISK ar

NEVER EVER TRY/ATTEMPT TO SWAP MEMORY ON DISK in HPC.>> Solution: allocate m

# Amdahl's law

What is the maximum speedup for P processors?

assumes perfect speedup for parallel part

Speedup(p) = T(1)/T(p)
p=1-s
T(p) = (1-s)*T(1)/P +s*T(1)
T(p) = T(1)*((1-s) + P*s)/P

Speedup(p) = P/(1 + (P-1)*s)
= 1/ (1-s)/P +s)

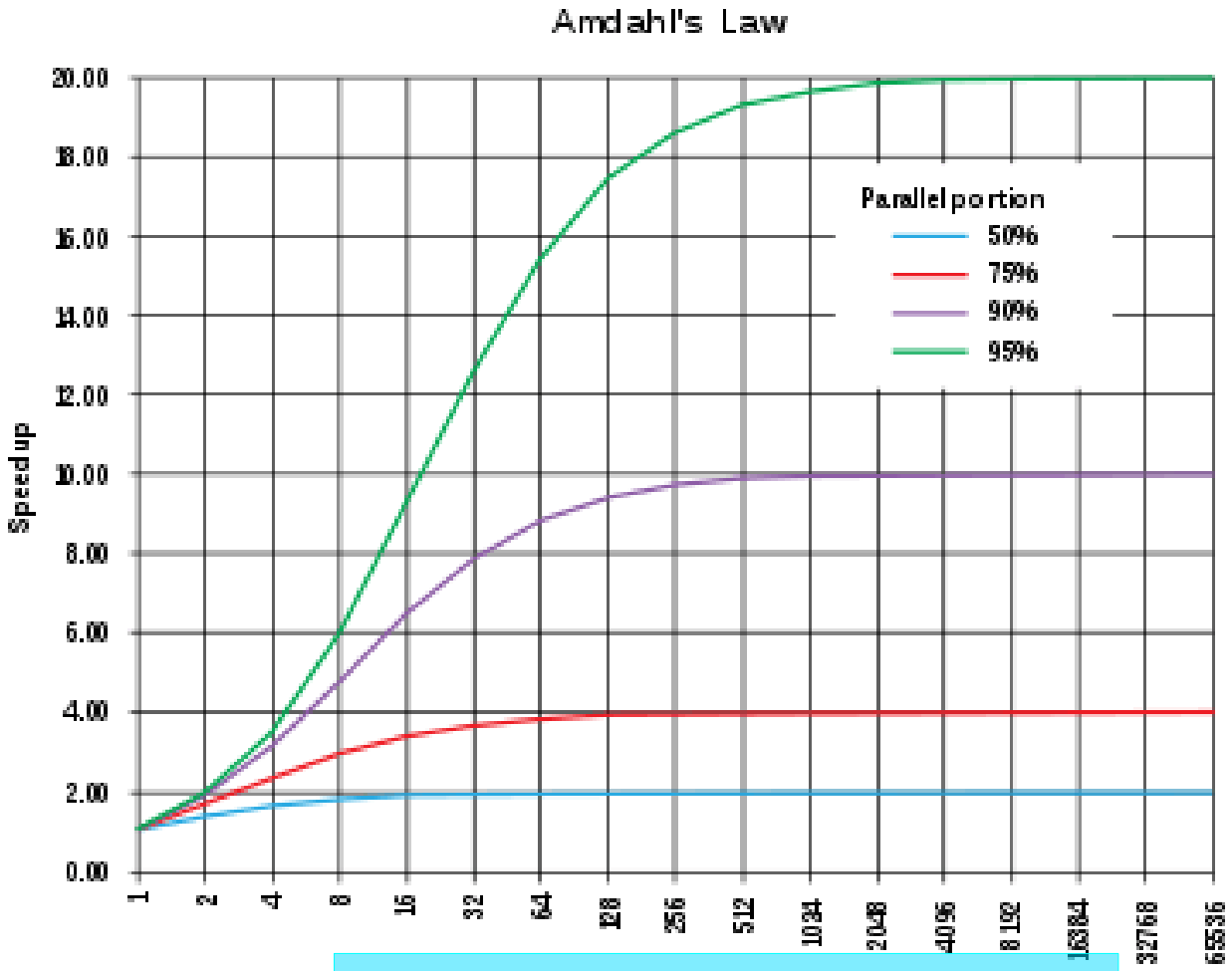
P->inifnity S=1/s

Speedup given by PERFECT SCALABILITY!Limited by the serial part only.

Even if the parallel part speeds up perfectly,
we may be limited by the sequential portion of code.

# Amdahl's law

- Which fraction of serial code is it allowed ?




Great waste of resources DUE TO SERIAL

What about Scalability ???

# Ahmdal law: communication overhead

- Tp = T1*s + T1*p/P +Tc
- S= T1/(T1/P +Tc)

  == > S = P/ (1 +P*(Tc/T1))

- P should not exceed the ratio between computing time and communication time !!! very important to scale well:i.e. the part (1+ P*(...)) ~ 1.

# Example: sum of N numbers

- Serial Algorithm : n-1 operations
  - $T_s = n * T_{comp}$
  - $T_{comp}$=time to compute a floating point operation
- Parallel Algorithm : master-slave

  1) read n and distribute n to P slaves ===> $T_{read} + (P-1) * T_{comm}$

  $T_{comm}$ = time each processor takes to communicate one message, i.e. latency..

  $T_{read}$ =time master takes to read

  2) n/p sum over each processors (including master) ===> $T_{comp}/P$

  3) Slaves send partial sum ===> $(P-1)T_{comm}$

  4) Master performs final sum ===> $T_{comp}$

  $$T_p = T_{comp}(1 + n/P) + T_{read} + 2(P-1) * T_{comm}$$

# Example: sum of N numbers

- Compute Scalability:
- Estimate for your computer $T_{read}$ $T_{comp}$ $T_{comm}$ f
- Formulate some scalability curve as function of N
- Implement a program to solve the exercise
- Check if our performance model is adequate

(DECENT) SCALABILITY:Usually afte

IN THE CASE OF:Very high (i.e.) read time=> I NEED TO INCREASE THE (1+p

# Problem scaling

- Amdahl's Law is relevant only if serial fraction is independent of problem size, which is rarely true
- Fortunately "The proportion of the computations that are sequential (non parallel) normally decreases as the problem size increases " (a.k.a. Gustafon's Law)
- Check this on the previous example

# Gustafson law

- $T_p = T(s + p)$ whit $s+p=1$
- $T_1 = sT + p*P*T$
- $S(P) = T_1/T_p = (s+Pp)/(s+p) = s+Pp = p-1 +Pp = s+ P(1-s) =$

$$S(P) = P - (P-1)*s$$

Gustafson's LAW:>> Not possible to PERFECTLY S

USUALLY:>> The time/amount of... required to communicate

# So What Is Scalability?

- to get N times more work done on N processors
- compute a fixed-size problem N times faster
  - Strong scaling
    - Speedup S = $T_1$ / $T_N$ ; linear speedup occurs when S = N
    - Can't achieve it due to Amdahl's Law (no speedup for serial parts)
- compute a problem N times bigger in the same amount of time:
  - Weak scaling
    - Speedup depends on the amount of serial work remaining constant or increasing slowly as the size of the problem grows
    - Assumes amount of communication among processors also remains constant or grows slowly

# Why weak scaling tends to work better..

- Strong scaling: fixed data/problem set; measure speedup with more processors
  - Ahmdal law
- Weak scaling: data/problem set increases with more processors; measure if speed(efficiency) is the same
  - Gustafson law

# References

- 
- https://computing.llnl.gov/tutorials/parallel_comp/
- Reference 2 : chapter 2 section 2.1 2.2