Foundations of High Performance Computing

Lecture 04: Parallel concepts and performance evaluations

"Foundation of HPC" course

DATA SCIENCE & SCIENTIFIC COMPUTING

2020-2021 Stefano Cozzini

Agenda

- Parallel programming paradigm
- Parallel programming concepts
- Parallel performance
- Ahmdal /Gustafson law

2 main parallel paradigms

DIDACTED BY MEMORY ORGANIZATION

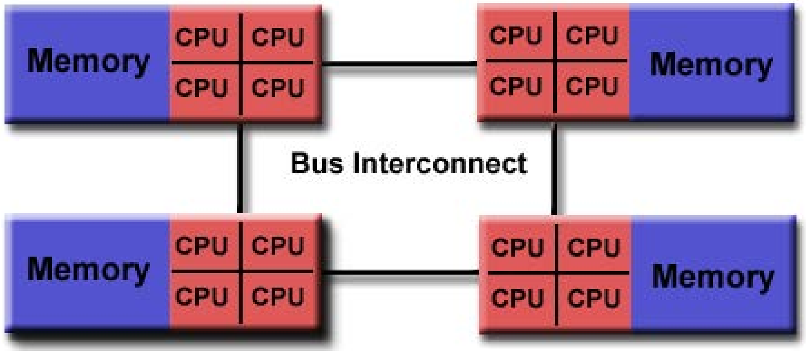
shared memory

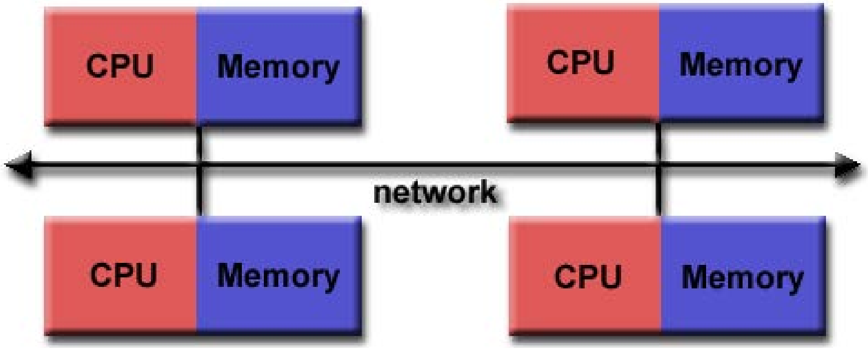
Single memory view, all processes (usually threads) could directly access the whole memory

distributed memory

Message Passing

all processes could directly access only their local memory.





Pro&Cons

- Pros
  - Unique 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 constructs that ensure "correct" access of global memory.
  - Non uniform memory access time on modern CPU architecture

- 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 separated 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.

Programming enviroment

- Shared
  - Ad hoc compilers
  - Source code directives (trivial portability)
  - Standard unix shell to run the program
  - Standard: OpenMP

- Distributed
  - Standard Compilers
  - Communication libraries (not so trivial portability_
  - Ad hoc command to run the program
  - Standard MPI

Shared memory approach: a first basic example

loop parallelization with OpenMP

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

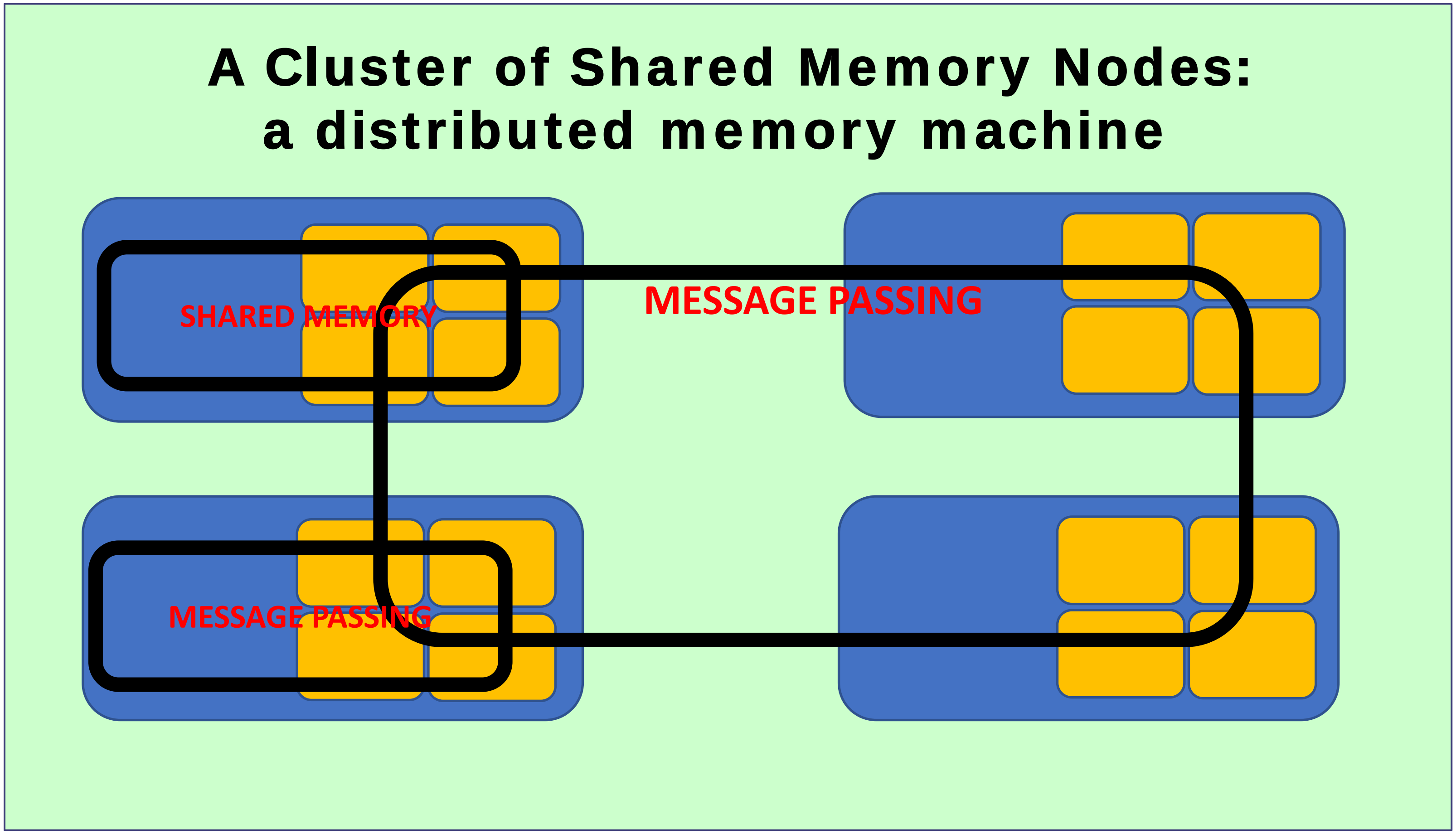
Compile with correct flag: -f openmp

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

Message Passing approach

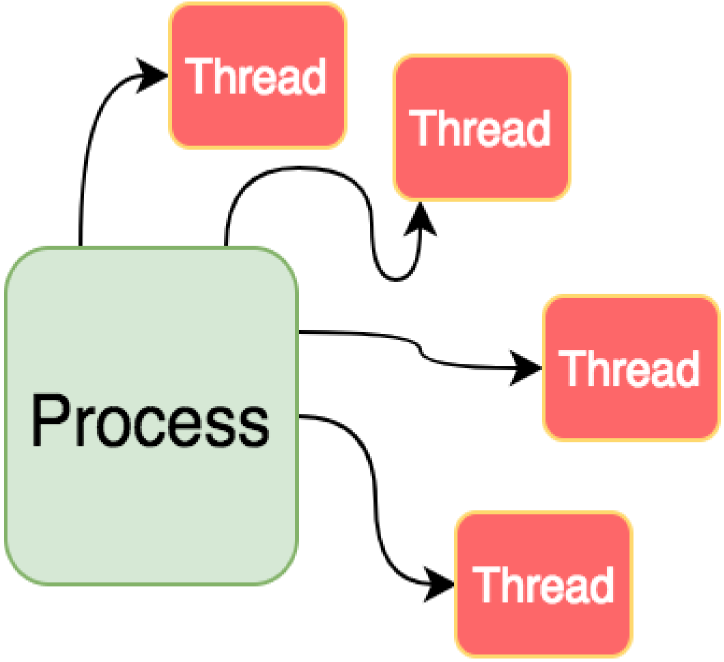
- Using the de-facto standard : MPI message passing interface
  - A standard which defines how to send/receive message from a different processes
- Many different implementation
  - OpenMPI
  - Intel-MPI
- They all provide a library which provide all communication routines
- To compile your code you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

HPC Architecture vs Paradigms



Important note

- It is trivial to implement MP approach on Shared Memory machine..
    - Each Linux process has its own private memory
- It is impossible to implement shared memory approach on distribute memory machine.
    - Threads are spawned by a single linux process and so they share the same memory



Picture from https://www.slashroot.in/difference-between-process-and-thread-linux

Architectures&Paradigms&Parallel programming model..

Architectures	
Distributed Memory	Shared Memory
Programming Paradigms/Environment	
Message Passing	Shared Memory
Parallel Programming Models	
Domain Decomposition	Functional Decomposition

Other paradigm available

- Mixed/hybrid approach..
  - MPI + OpenMP
- Specific SDK for specific devices
  - CUDA for Nvdia GPU
- Write once run everywhere:
  - OpenCL
  - OpenACC:
    - 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.

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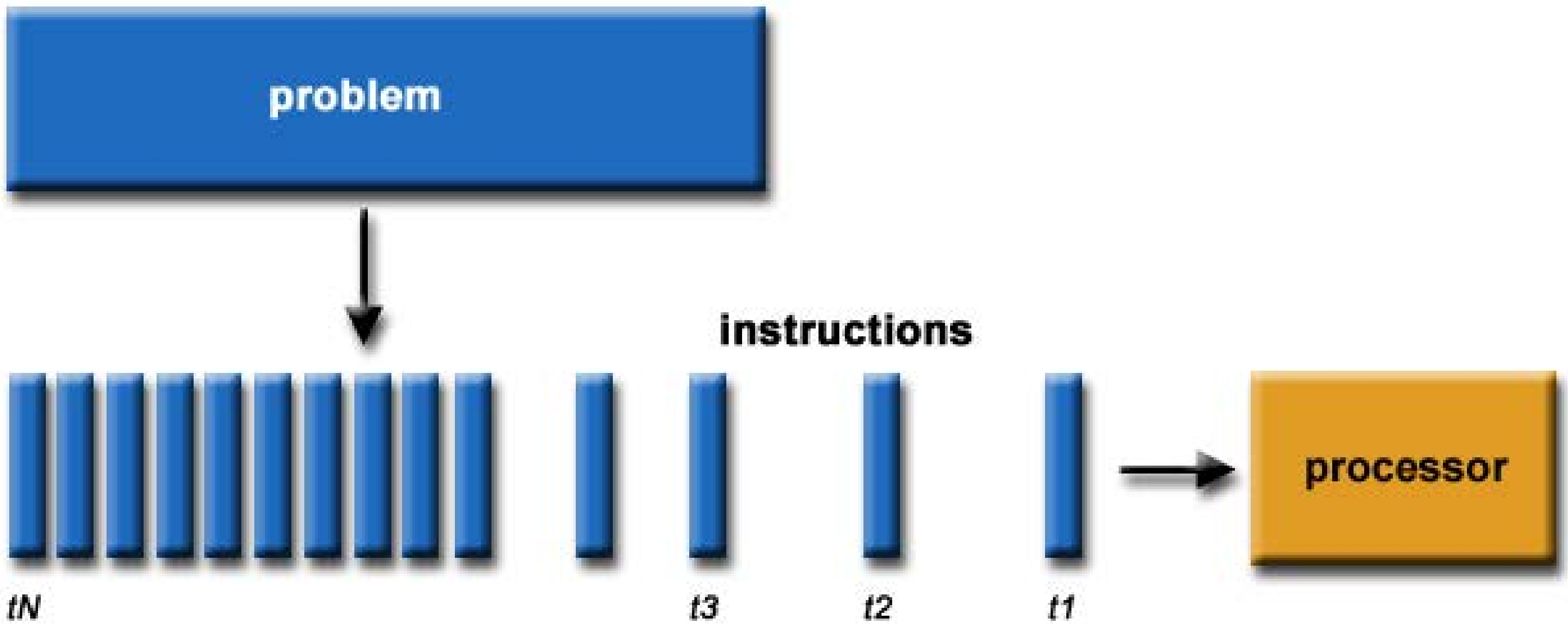
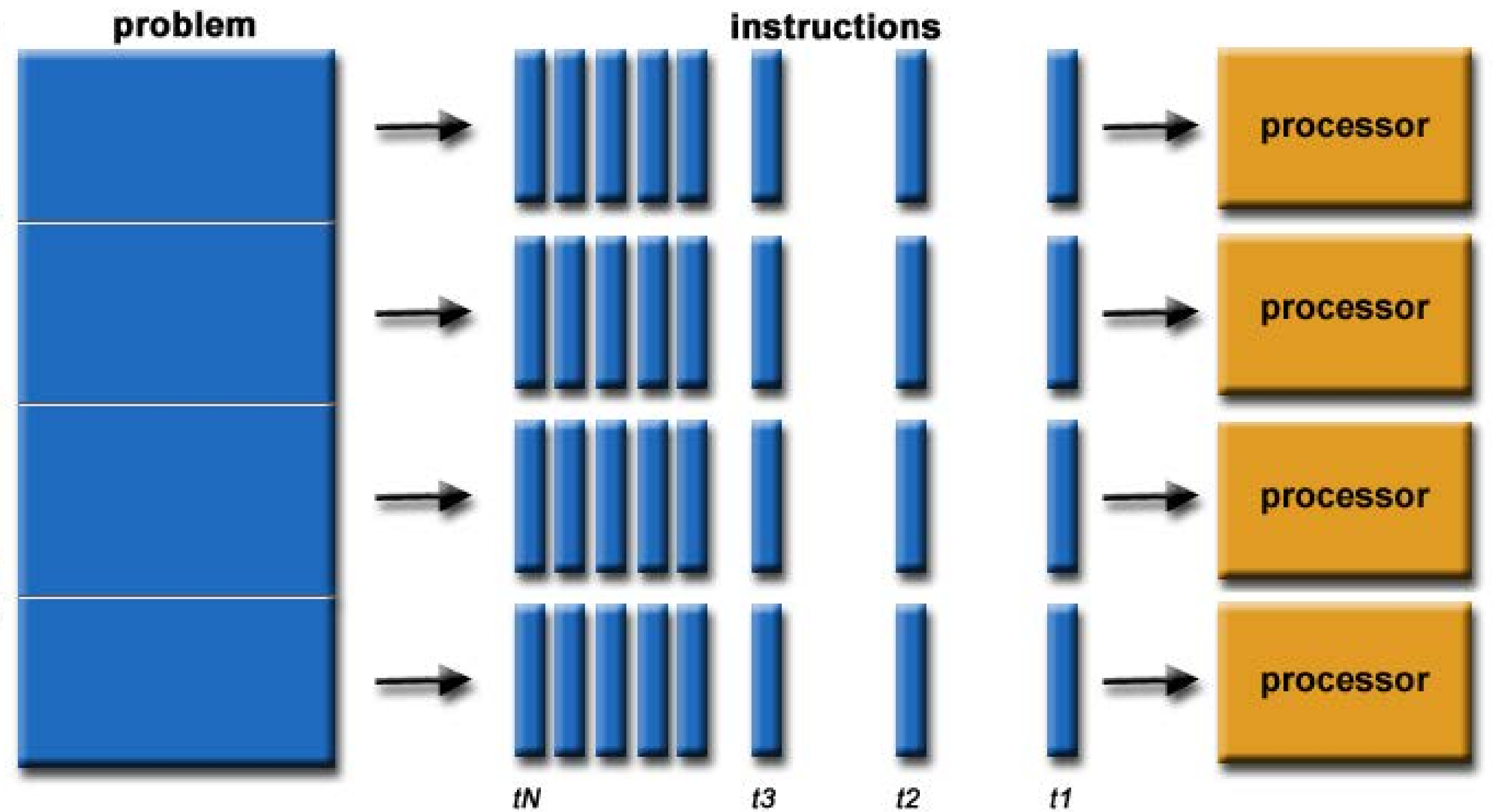
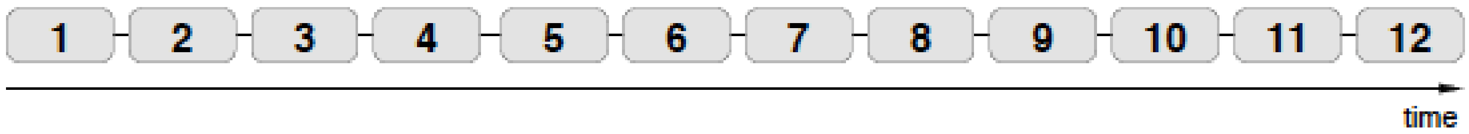
Serial execution

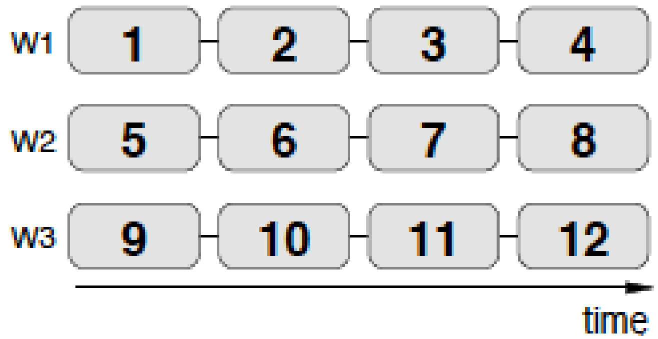


Parallel execution



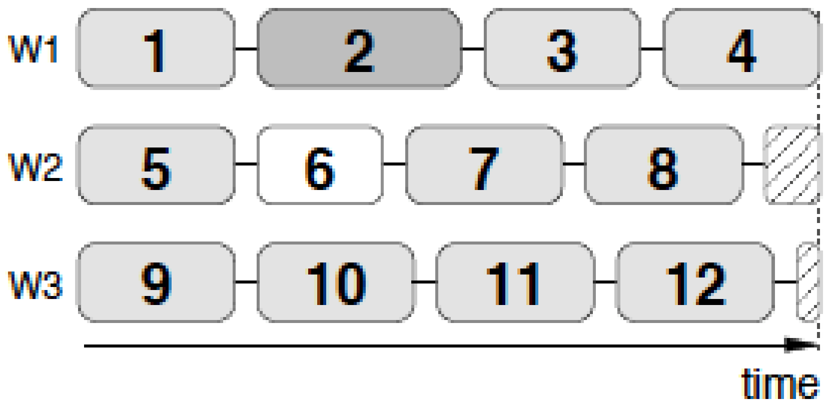
Running in parallel





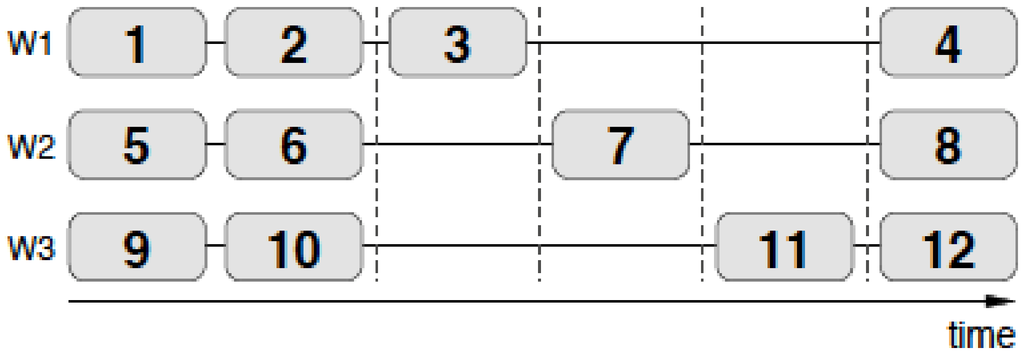
- Execution time reduces from 12 secs to 4 secs!

Load imbalance..



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

Dependency among tasks



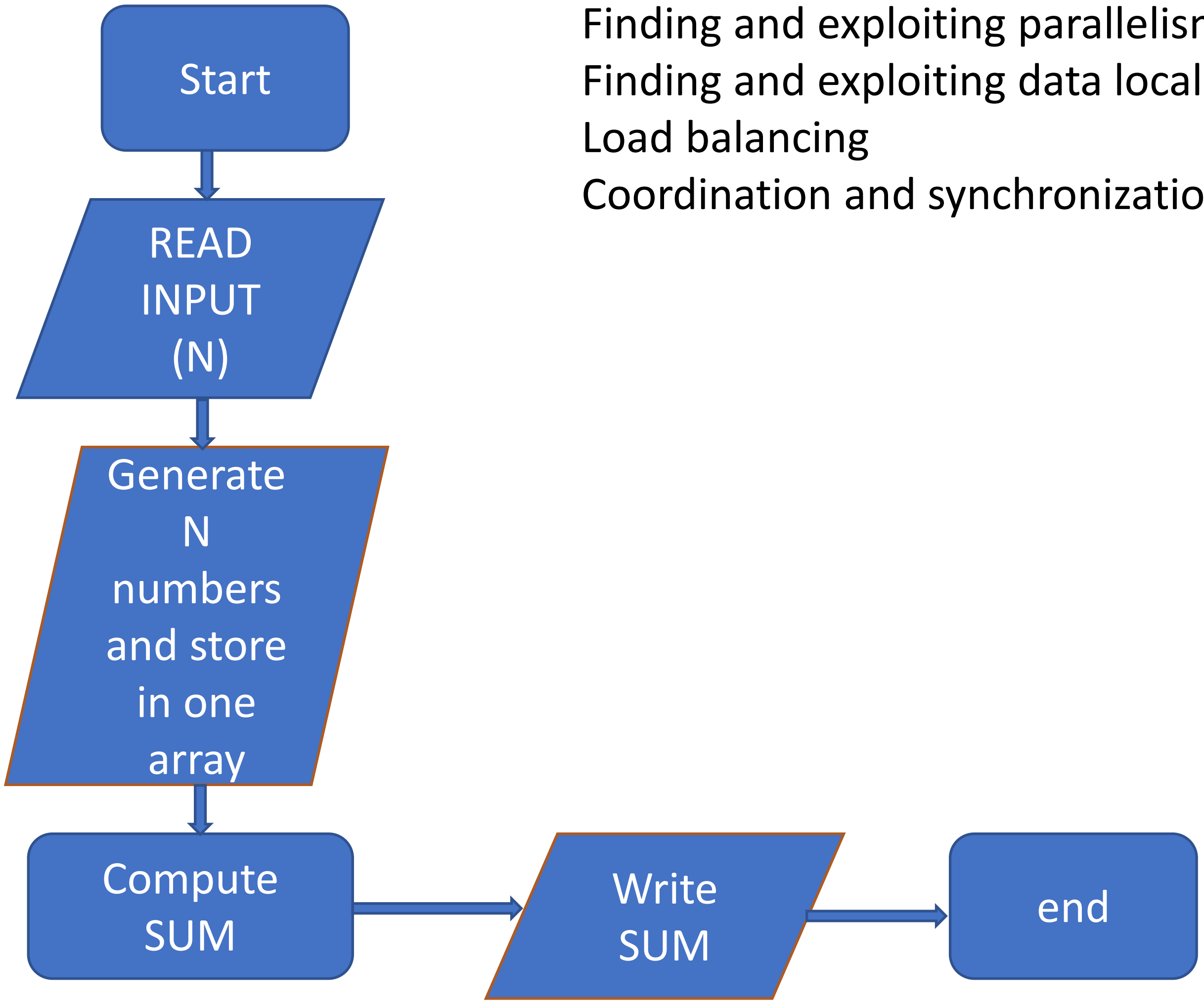
- What if section 11 depends on section 7 that depends on section 3 ?
- Time increase from 4 to 6 !

Principle of parallel computing

- Finding and exploiting parallelism
- Finding and exploiting data locality
- Load balancing
- Coordination and synchronization
- Parallel performance
  - Speedup, efficiency
  - Ahmdal Law/Gustafson Law
  - Performance modeling

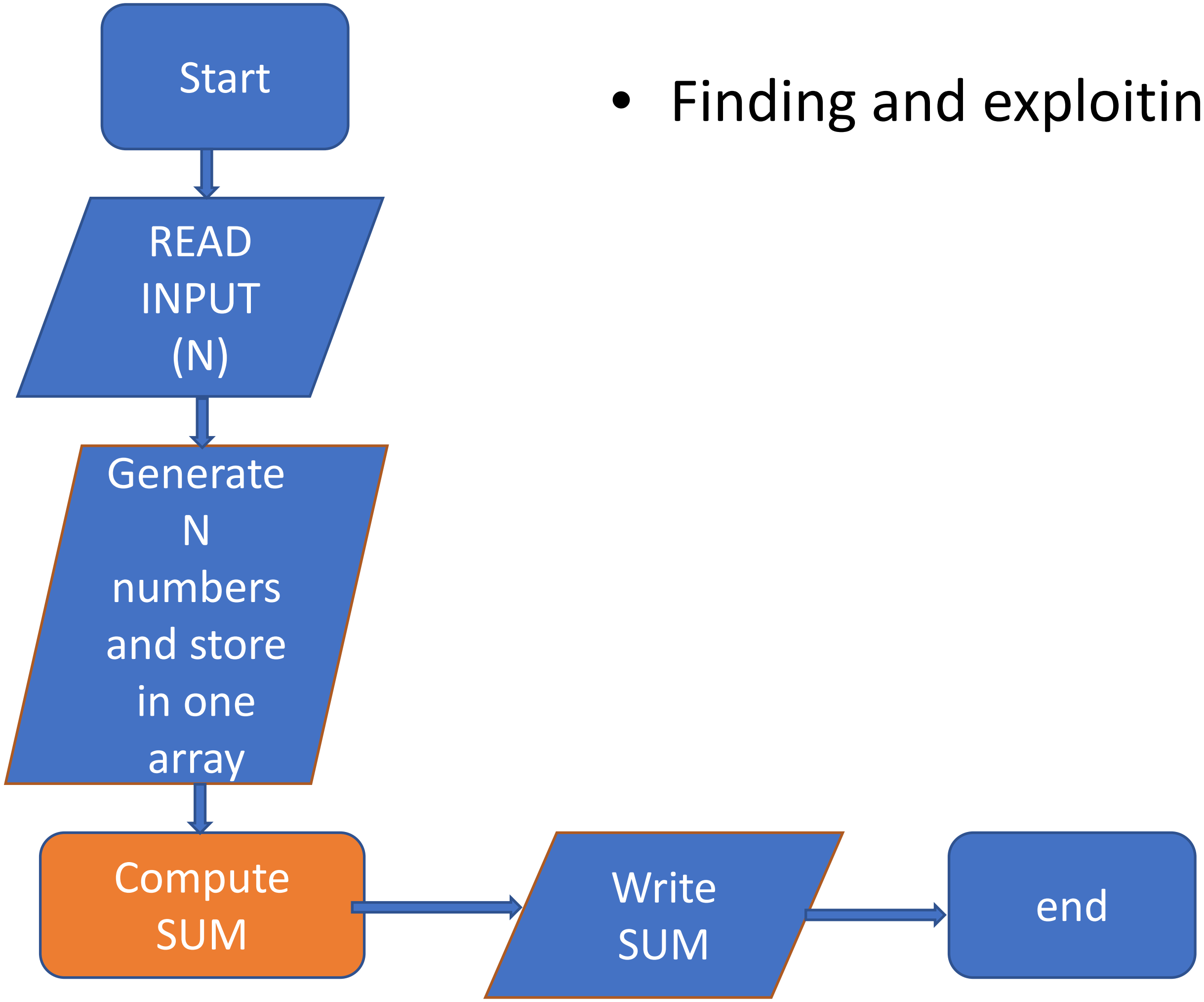
All of these things make parallel
programming more difficult
than sequential programming.

The simplest algorithm: sum of N numbers



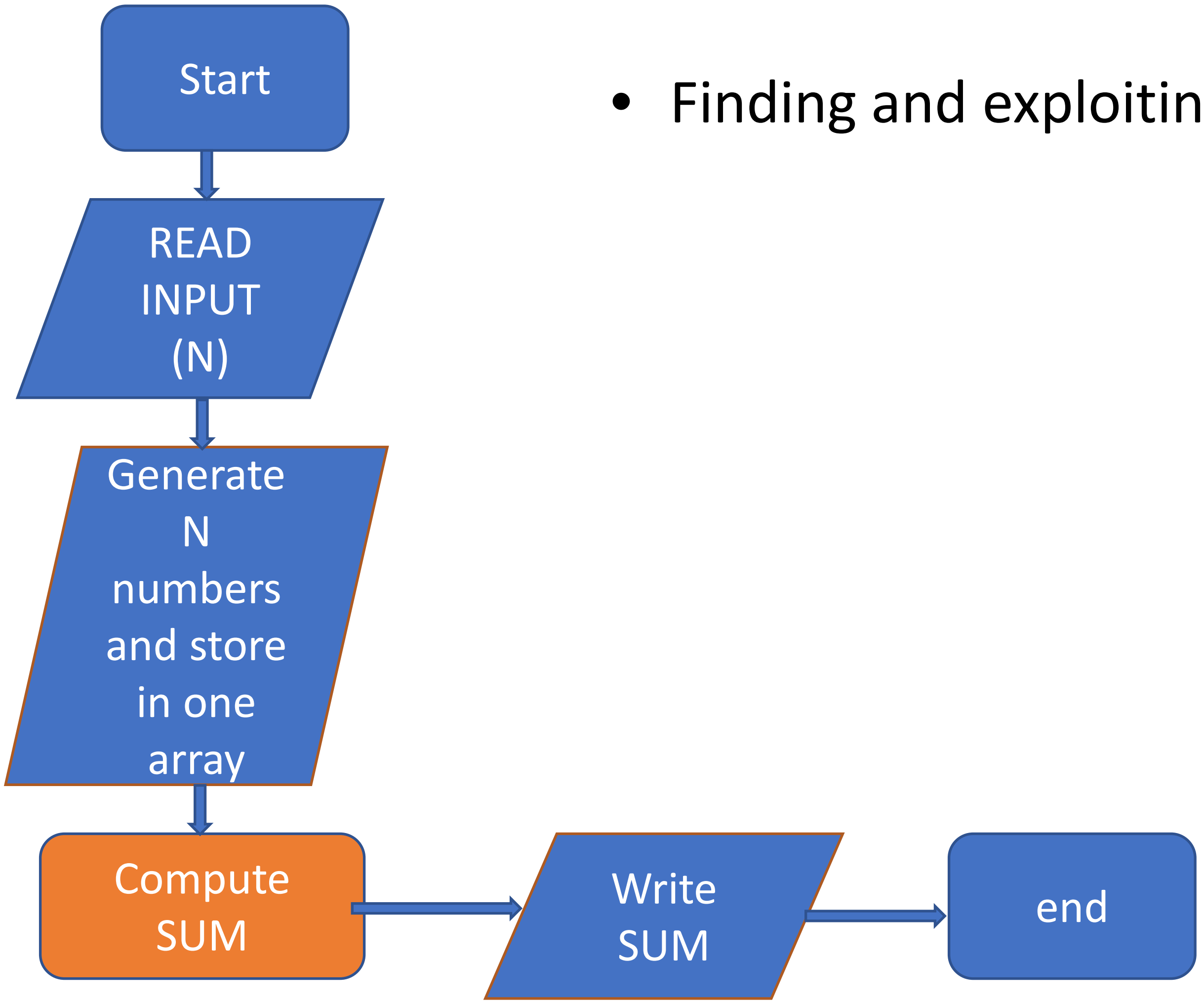
Finding and exploiting parallelism
Finding and exploiting data locality
Load balancing
Coordination and synchronization

The simplest algorithm: sum of N numbers



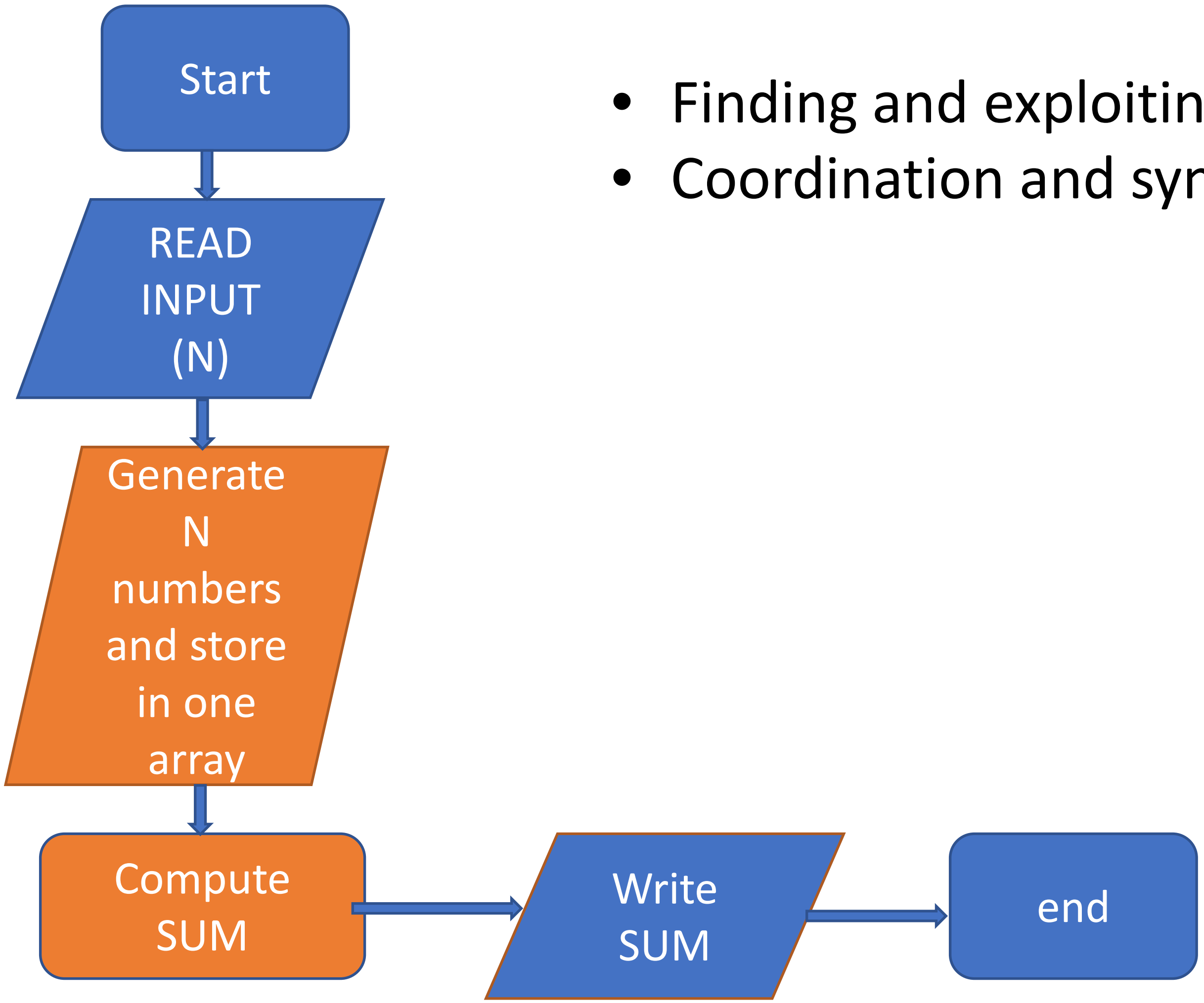
- Finding and exploiting parallelism

The simplest algorithm: sum of N numbers



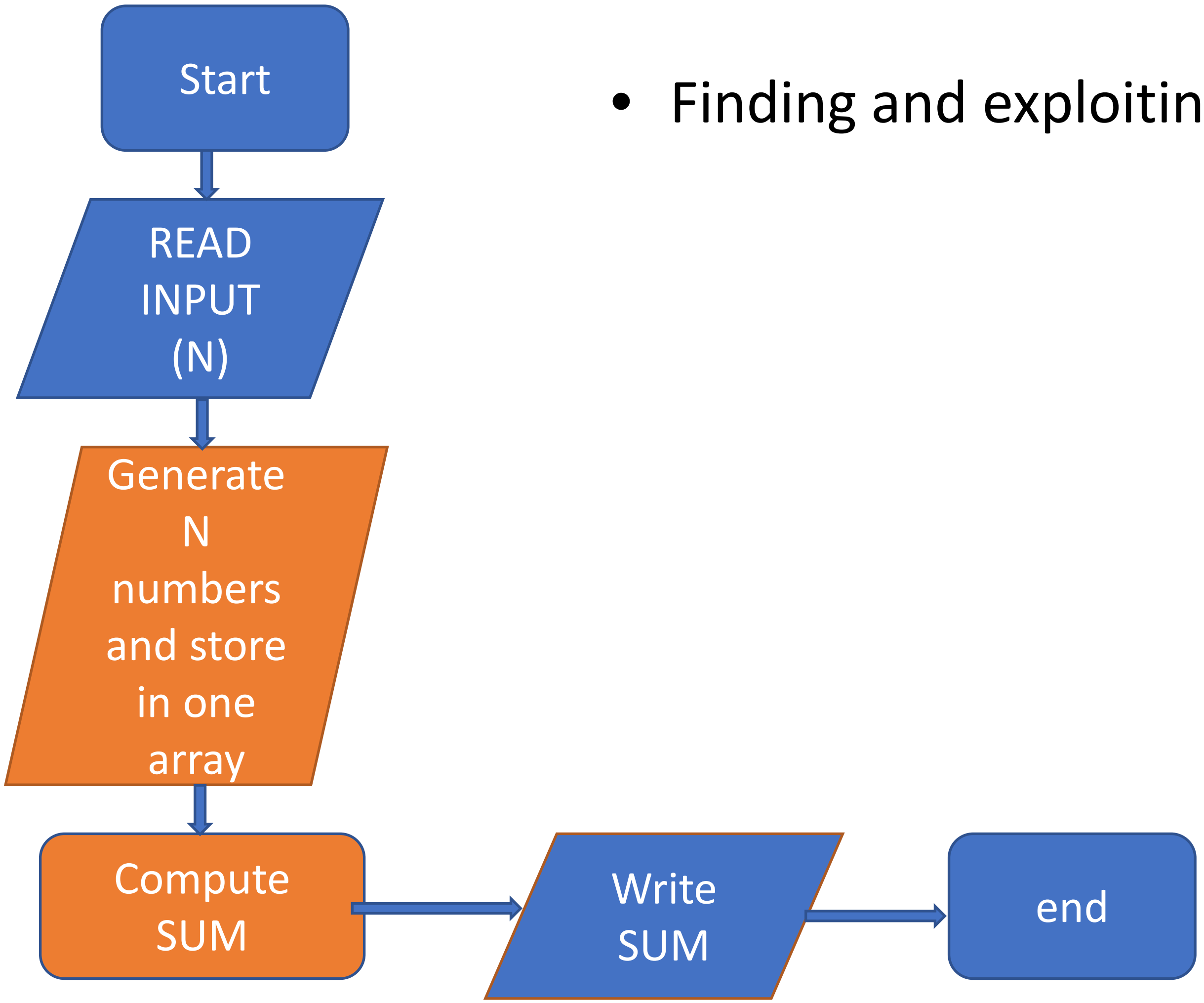
- Finding and exploiting parallelism

The simplest algorithm: sum of N numbers



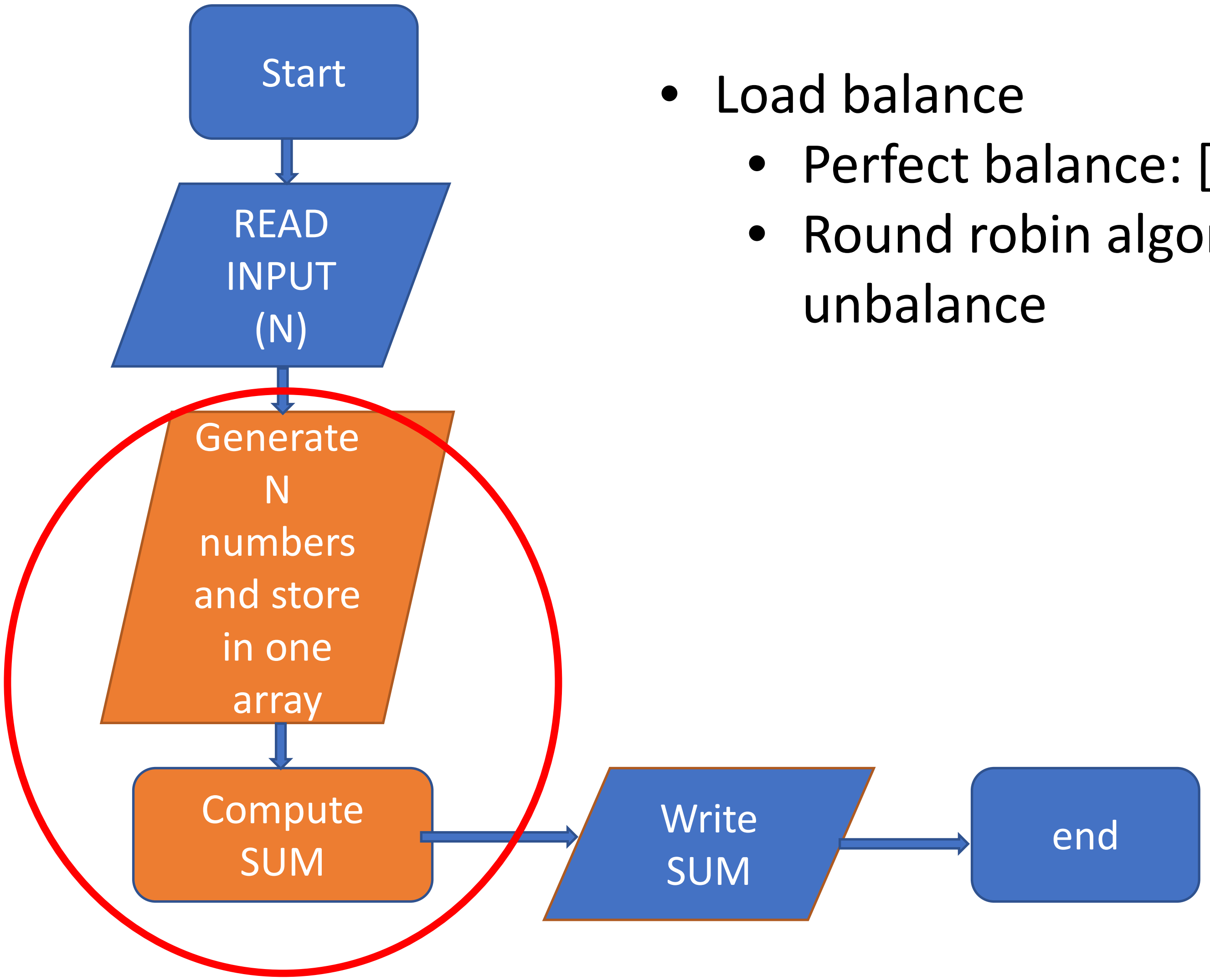
- Finding and exploiting data locality
- Coordination and synchronization

The simplest algorithm: sum of N numbers



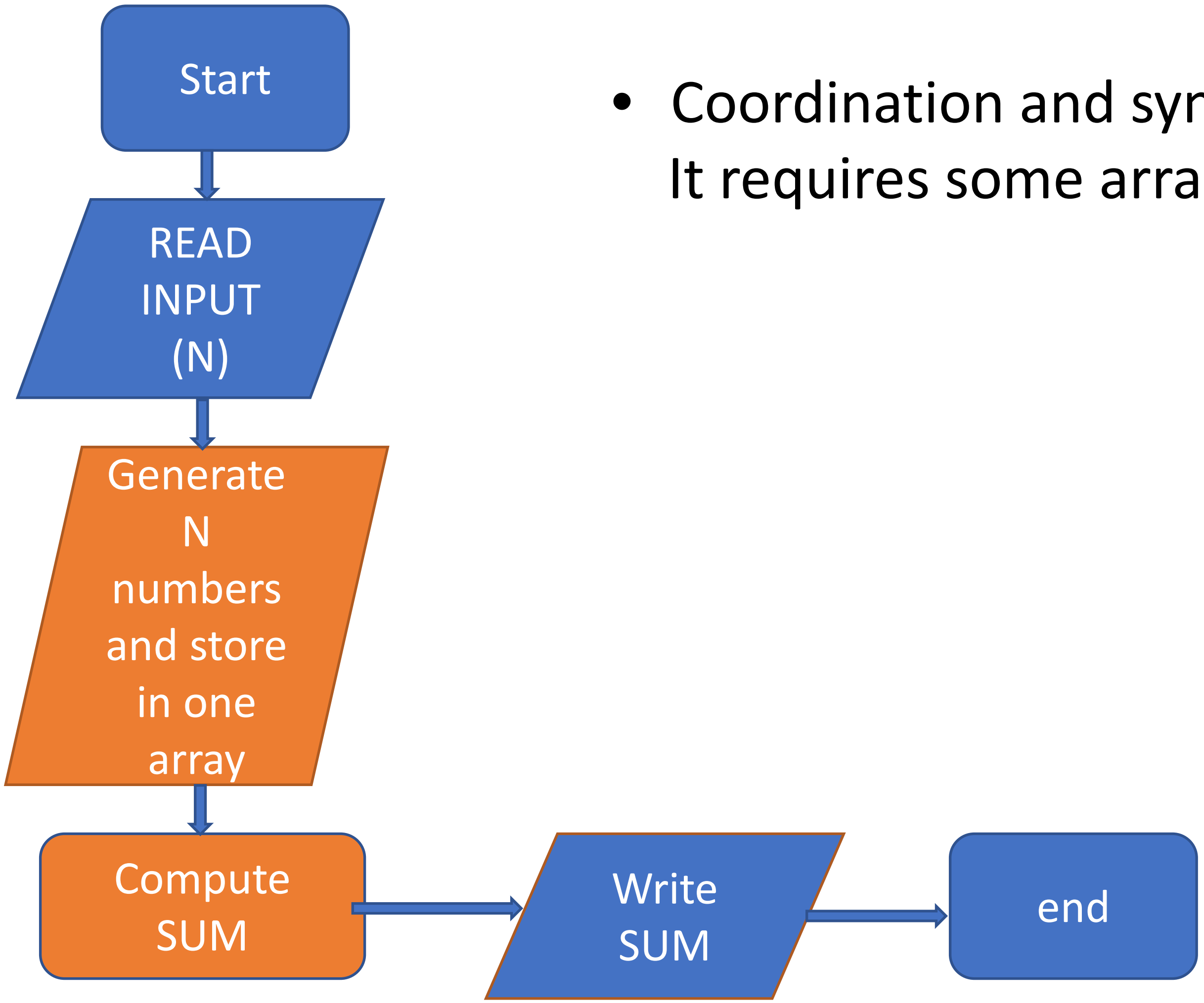
- Finding and exploiting data locality

The simplest algorithm: sum of N numbers



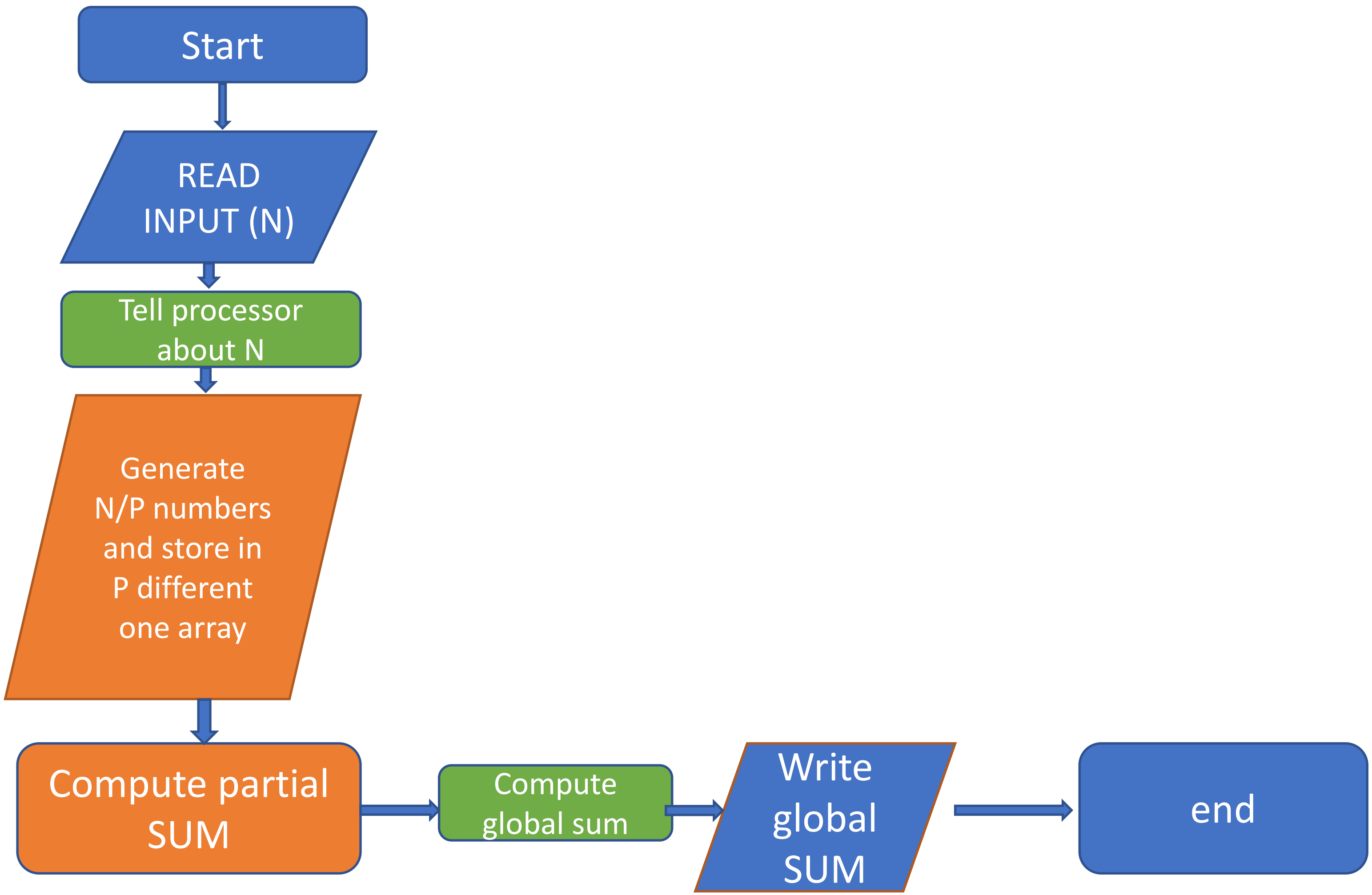
- Load balance
  - Perfect balance: [N/P]=0
  - Round robin algorithms minimize unbalance

The simplest algorithm: sum of N numbers



- Coordination and synchronization
  It requires some arrangements …

The simplest algorithm: sum of N numbers



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Scaling…

- Scaling or scalability: some sort of ratio 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
  - The ability to for some application to solve larger problems when the size of the HPC increases..

Some more specific questions on 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?

Identify basic limitations of code implementations or algorithms for parallel processing

Assumptions

- Underlying hardware is perfectly scalable
- Basic workload may have pure serial and pure parallel contributions
- P „workers“ have to perform either
  - Fixed amount of work as fast as possible Amdahl‘s law
  - Increasing amount of work (~P) in constant time Gustfson‘s law
- Time based view:
  - Time to execute the serial(P=1) workload on one worker: $T(1)=1$
  - Basic assumption(serial/parallel workload):

$$T(1)= s + p =1$$

No way to parallelise

Perfecly parallelisible

Speed-up and efficiency

- T(P) is the time to execute „some workload“ with P workers
- Parallel Speed-Up: How much faster do I execute the given workload on P workers?

Parallel Speed-Up: S(P)=T(1)/T(P)

- Efficiency: How efficient do I use the workers in average?

Parallel Efficiency: ε(P)=S(P)/P

- Warning: These metrics are relative to the time (performance) of a single worker → These metrics are not performance metrics!

Some observations

- If Speedup(p) = p we have perfect speedup (also called linear scaling)
  - For perfect speedup Efficiency (p) = 1
  - Ideal case: holy grail for all HPC users..
- speedup compares an application with itself on one and on p processors
  - Sometimes more useful to compare:

    The execution time of the best serial application on 1 processor against the execution time of best parallel algorithm on p processors

Understanding why an application is not scaling linearly will help finding ways improving the applications performance on parallel computers.

Superlinear speed-up

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

Speedup(p) > p ?

Choosing a bad "baseline" for T(1)
- Old serial code has not been updated with optimizations
- Parallel code on one processor does much more work

Shrinking the problem size per processor
- May allow it to fit in small fast memory (cache)

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Ahmdal's law

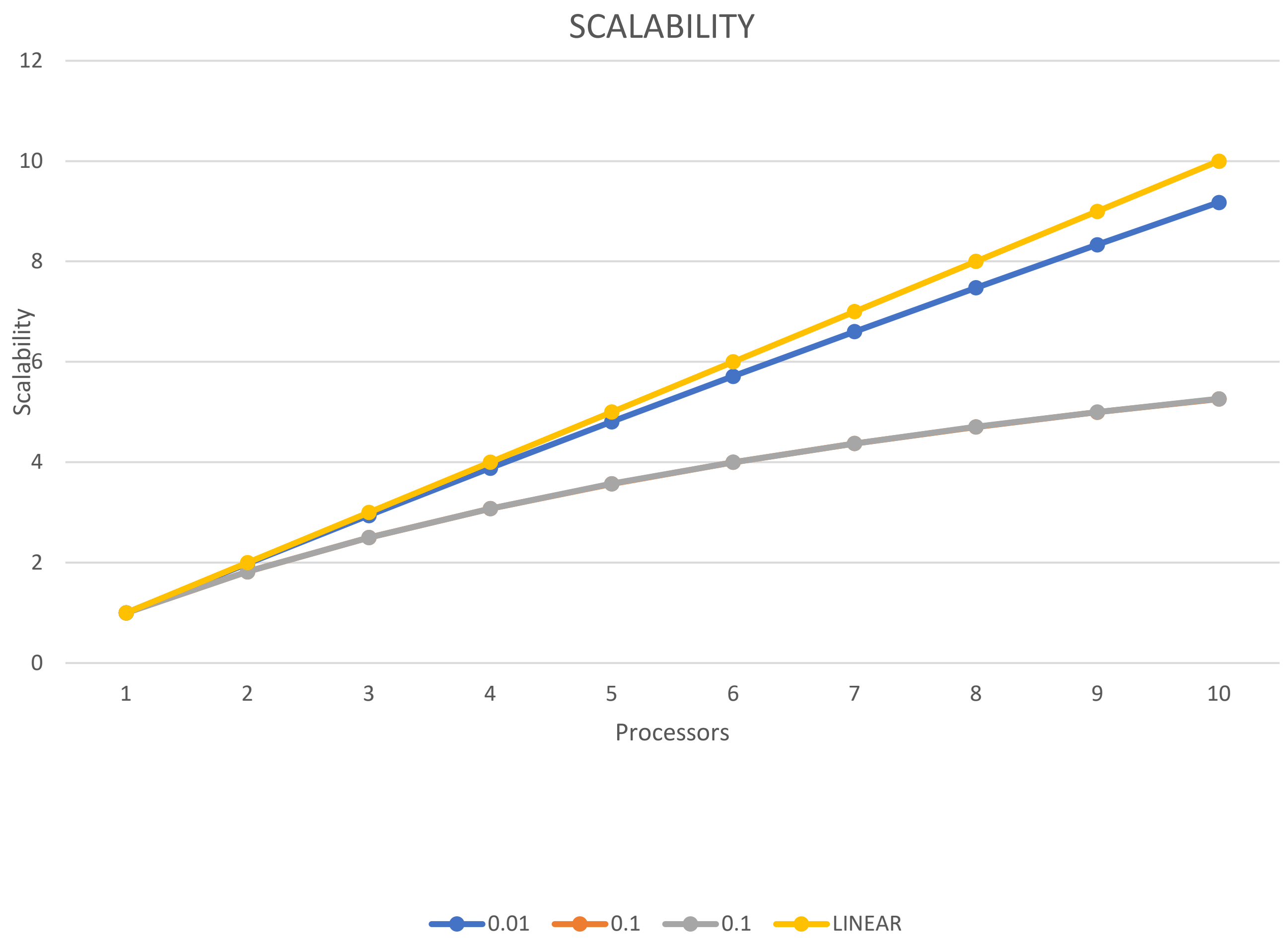
- $S(P) = T(1)/T(P)$
- $T(1) = s + p = 1$
- $T(P) = s + p/P$
- After a little bit of basic math:

$$S(P) = 1/(s + (p/N)$$

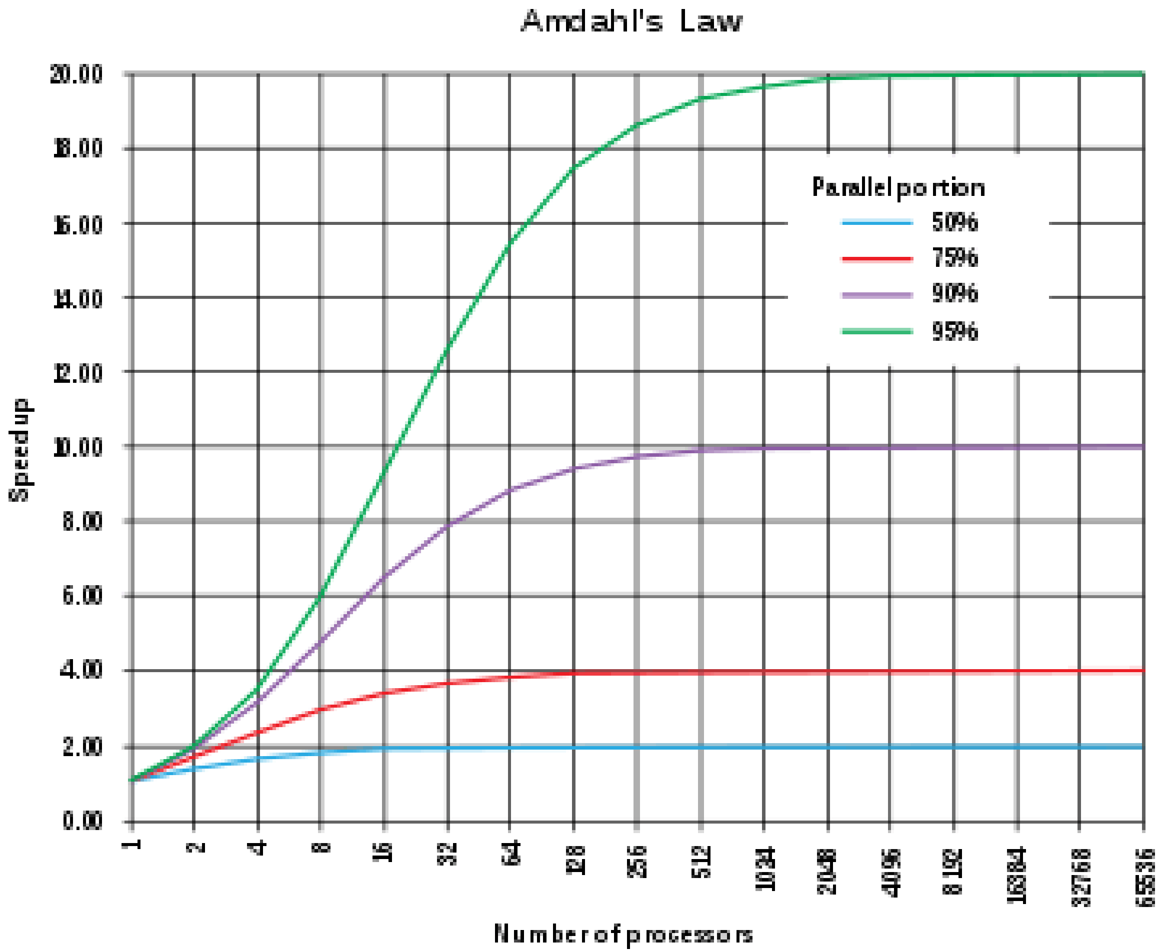
For P → infinity S → $1/s$

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

Which fraction of serial code ?



Which fraction of serial code is allowed ?



Ahmdal law: communication overhead

- Assume that c(P) the communication time when using P processors with c(1)=0

$$\to \quad T(P)=s + p/P+c(P)$$

- Communication time may depend on many factors:
  - Network topology
  - Communication pattern
  - Message sizes
- Typical scaling of communication times:
  - Global communication, e.g. barrier: $c(p)=k\log P$
  - Every process sending message over bus based network or serialization of communication in application code: c(P)=kP

What does it means k * P ?

T(1) = *p + s*

Communication model: constant fraction k for each communication among Processors

Let consider P=4
T(4)= p/4 + s + k*4

$$S = \frac{1}{s + \boxed{\frac{1-s}{4}} + \boxed{4k}}$$

Ahmdal’s law with simple communication model

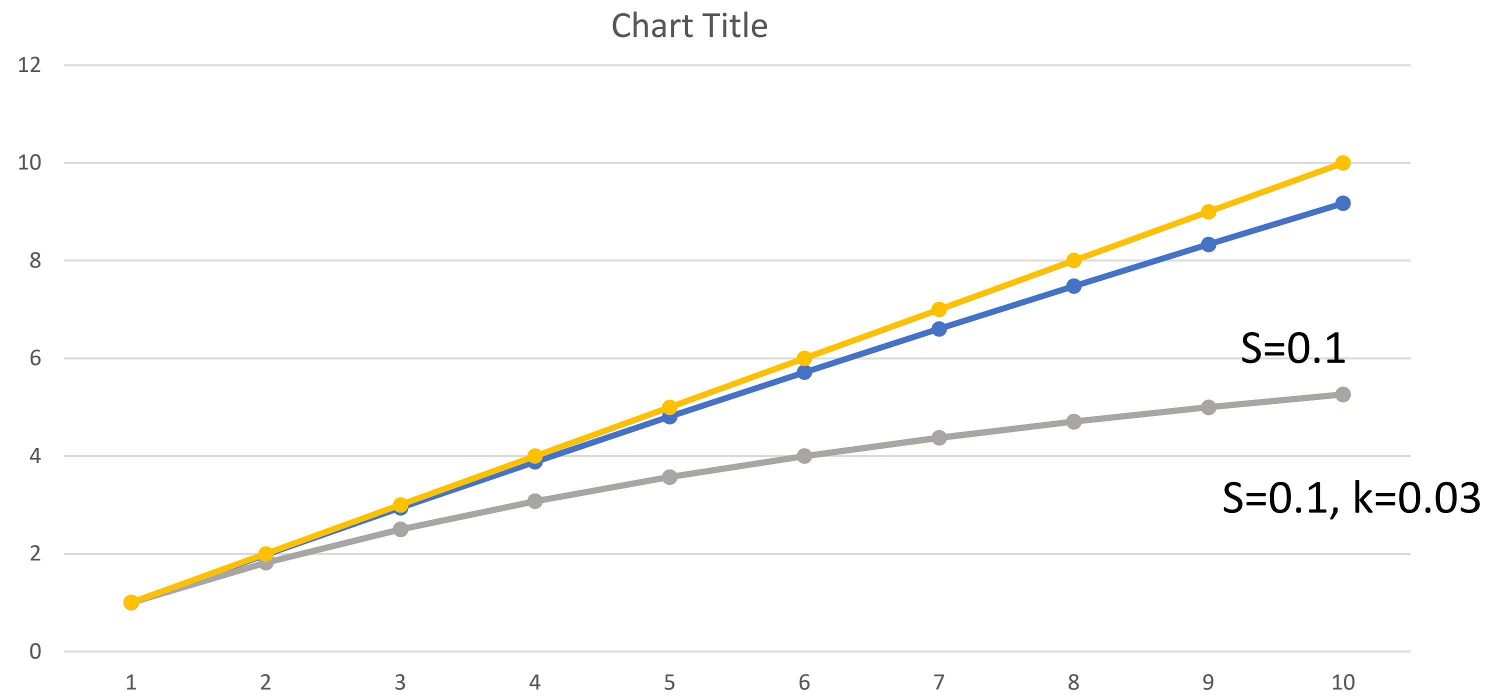
- Communication model: constant fraction k for each «communication» among processors

$$T(P) = s + p/P + kP$$

$$S(k,p) = T(1)/T(P)$$

$$S = \frac{1}{s + \frac{1-s}{P} + Pk}$$

Which fraction of communication ?



Large P limits

for P >> 1

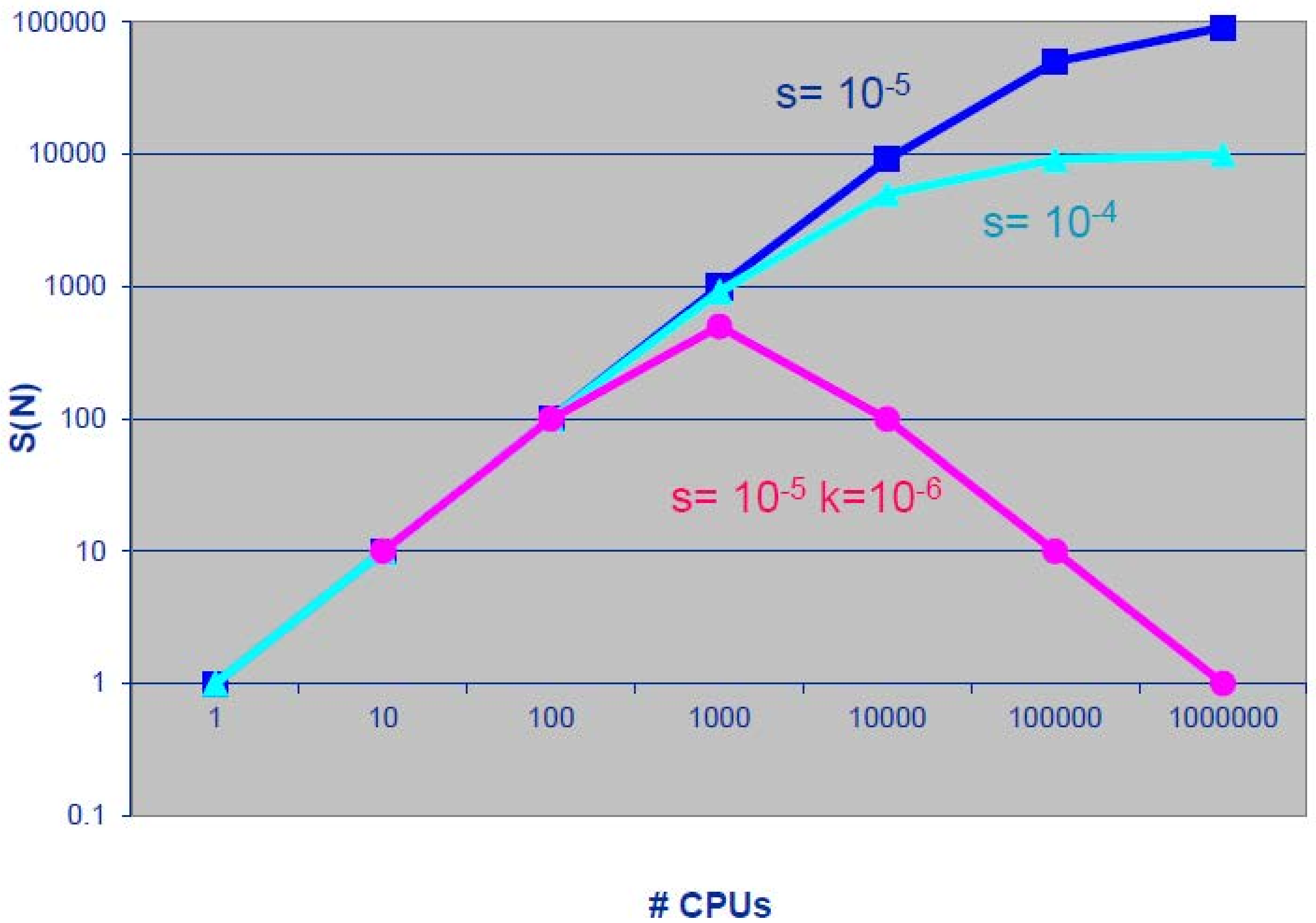
- Pure Ahmdal law :

$$S \rightarrow 1/s \quad \text{(Independent of P)}$$

- for k different from zero:

$$S \rightarrow 1/Pk$$

For smaller values and large P

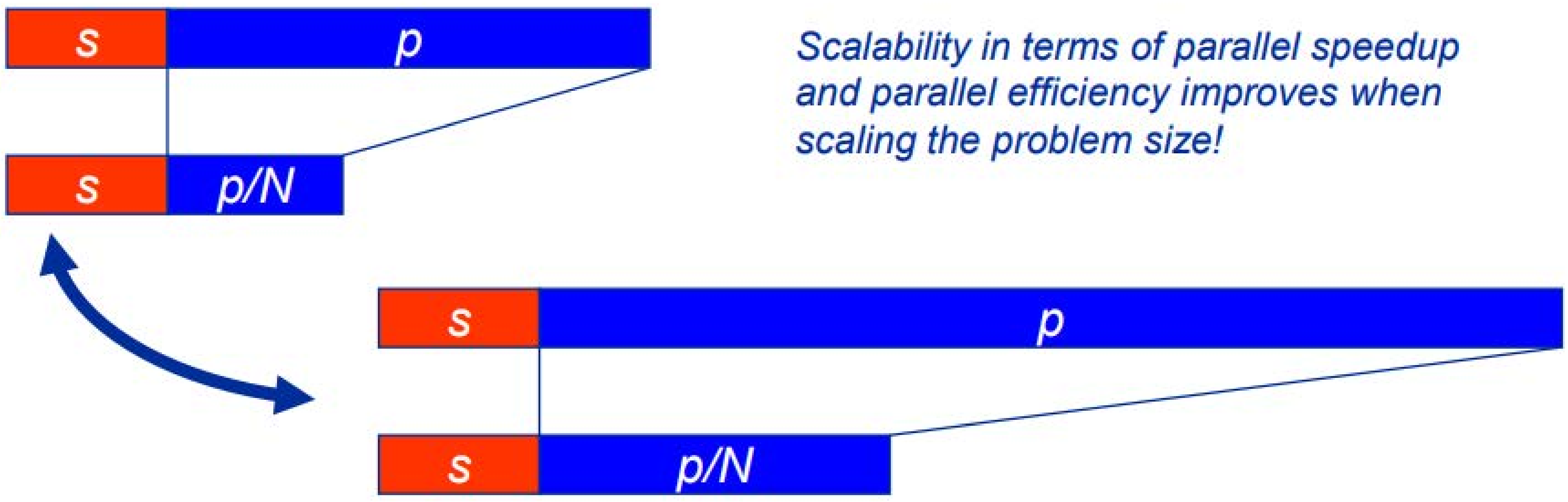


Problem scaling

- 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)

The „weak scaling“ scenario

- Increasing problem size often mainly enlarges „parallel“ workload p Then Speed-up increases with



Scalability in terms of parallel speedup and parallel efficiency improves when scaling the problem size!

Gustafson law

- Optimistic scenario:
  - Parallel workload increases linearly with P:

$$p \rightarrow \mathrm{P}p$$

$$\mathrm{T(P)} = s + p\mathrm{P}/\mathrm{P}$$
$$\mathrm{T(P)} = s + p$$

This means:

- Time remains constant when increasing parallel workload.
- Performance increase linearly with P.

Gustafsons law

How much does it take to solve the workload of P processor on 1 processor ?

$$T_P(1) = s + Pp$$

And then:

$$S(P) = \frac{T_p(1)}{T(p)} = \frac{s+Pp}{s+p} = s + Pp = s + P(1-s)$$

$$\boxed{S(P) = P - (P-1)*s}$$

Sustained Peak performance on real scientific codes

- Blue-waters at NCSA: 22,640 AMD 6276 processors
- Theoretical peak performance: 13 Petaflops
- Sustained performance on real scientific codes:..

Scientific code	Number of cores	Performance achieved(PF)	runtime (hour)
VPIC	22528	1.25	2.5
PPM	21417	1.23	~ 1
QMCPACK	22500	1.037	~1
SPECF3MD	21675	>1	Not reported
WRF	8192	0,160	<0.50

Why performance degradation ?

- HPC system is unable to exploit all the resources all of the time
- Many different causes and many parts of the HPC are responsible all together
- At abstract level four important factors:
  - Starvation
  - Latency
  - Overhead
  - Waiting for Contention =>SLOW

Starvation

- Happens when sufficient work is not available at any instance in
- time to support issuing instructions to all functional units every cycle.
- Typical case:
  - Not enough parallel work for all processors/components
  - Parallel work not evenly distributed among all processors/components (load is not balanced)

Latency

- Time it takes for information to move from one part of the system to the other.
- Typical cases:
  - Memory access
  - Data transfer between separate nodes
- Lot of tricks to hide latency (see next lectures)

Overhead

- The amount of additional work needed beyond that which is actually required to perform the computation.
- Typical cases:
  - Time to spawn and synchronize parallel tasks
  - Other kind of operation not directly associated to the computation
- The above operations steals resources to the computation and should be minimized

Waiting for contention

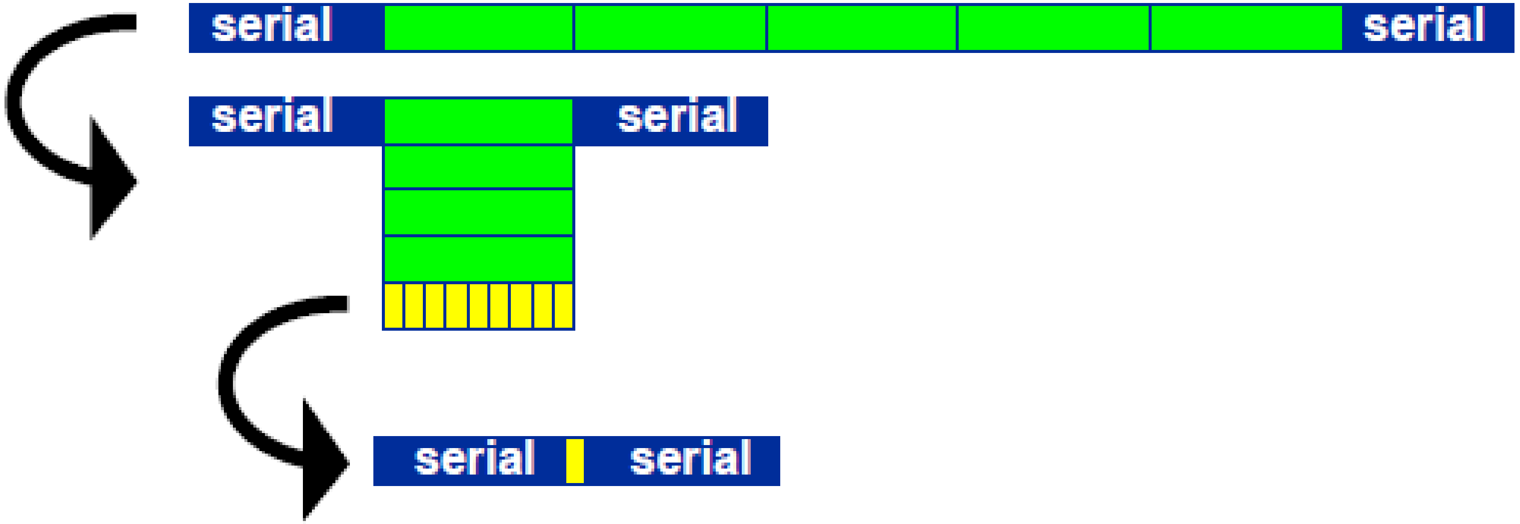
- Two or more request are made at the same time on the same resource (either HW or SW)..
- Typical cases:
  - Two task writing on the same disk and/or sending message to the same memory location at the same time
  - Generally such events are not predictable and so difficult to avoid and to optimize.

From Ideal world …

- All Work can be done in parallel !

First correction..

- Serial parts limit maximum speedup



Ugly Reality....

- Communication/synchronization /load imbalance..