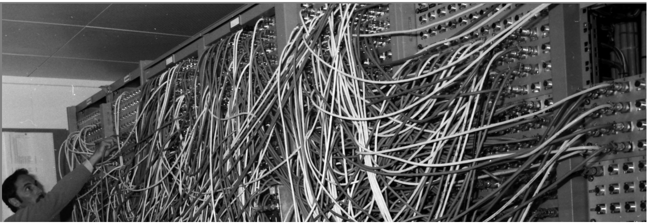


Calcolo Parallelo : Lezione 1

Fabio Durastante

Consiglio Nazionale delle Ricerche - Istituto per Le Applicazioni del Calcolo “M. Picone”

Master in Scienze e Tecnologie Spaziali, 2020

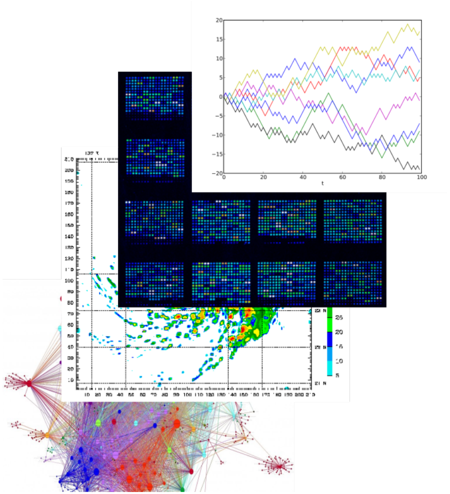
Scientific and parallel computing

"**Computational science** (also **scientific computing** or **scientific computation** (SC)) is a rapidly growing multidisciplinary field that uses advanced computing capabilities to *understand and solve complex problems*. It is an area of science which spans many disciplines, but at its core it involves the development of *models and simulations to understand natural systems*."

Wikipedia

What are the applications?

- Computational finance,
- Computational biology,
- Simulation of complex systems,
- Network analysis
- Multi-physics simulations,
- Weather and climate models,
- ...



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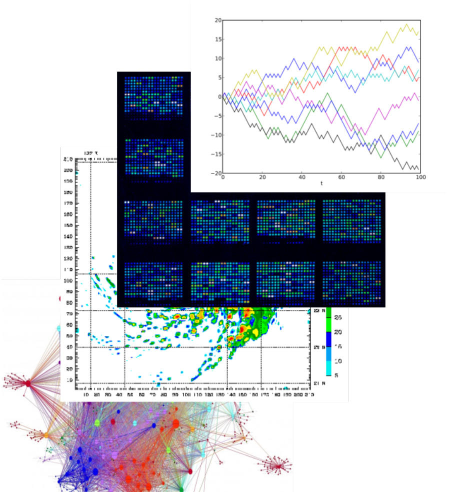
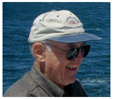


Why the need for parallelism?

Moore's law



"The complexity for minimum component costs has increased at a rate of roughly a factor of two per year. Certainly over the short term this rate can be expected to continue, if not to increase. Over the longer term, the rate of increase is a bit more uncertain, although there is no reason to believe it will not remain nearly constant for at least 10 years."

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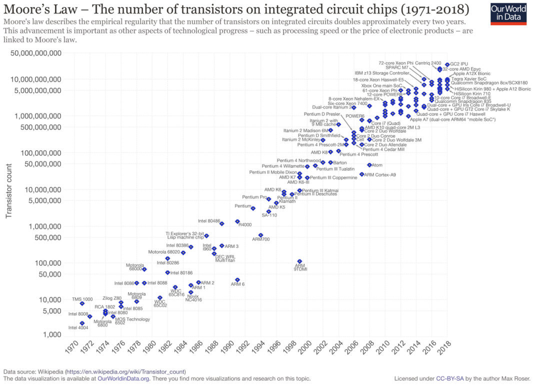

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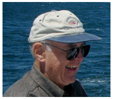

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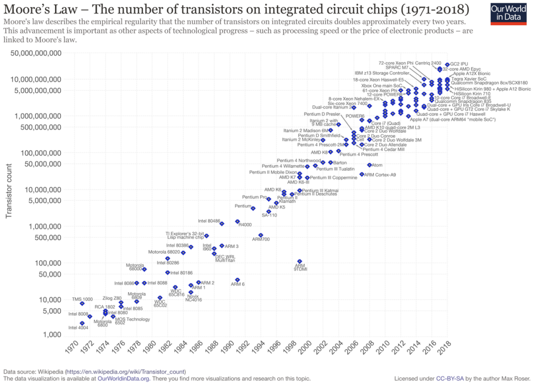

Computers *should* reach the physical limits of Moore’s Law at some point in the 2020s...exponential functions saturates physical capabilities!

Motivations for parallel computing

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Therefore, we need

- Algorithms that can work in parallel,
- A communications protocol for parallel computation integrated with our programming languages
- Parallel machines that can actually run this code

Parallel computers: Flynn’s Taxonomy

Let us start from the bottom: the machines.

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  - Multi-core computing
  - Symmetric multiprocessing
  - Distributed computing
  - Cluster computing
  - Massively parallel computing
  - Grid computing
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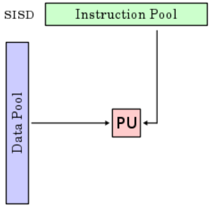
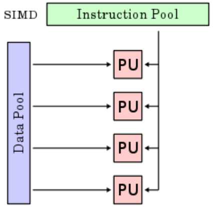
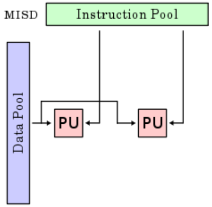


Single instruction stream, single data stream
SISD



Single instruction stream, multiple data streams
SIMD



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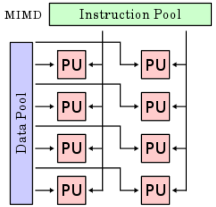

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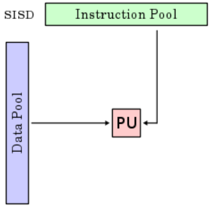

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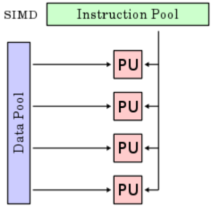

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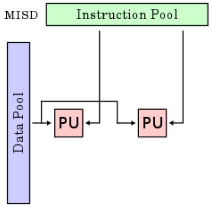

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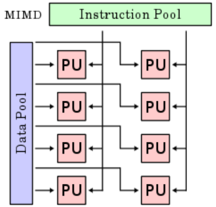

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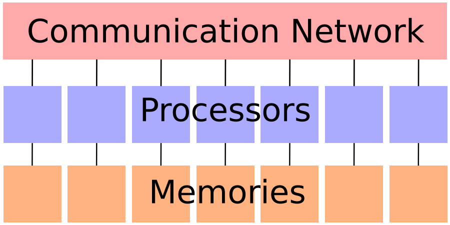
Parallel Computers: our computer model

For our task of introducing parallel computations we need to fix a **specific multiprocessor model**, i.e., a specific generalization of the sequential RAM model in which there is more than one processor.

Since we want to stay in a SIMD/MIMD model, we focus on a *local memory machine model*, i.e., a set of M processors each with its own local memory that are attached to a common communication network.



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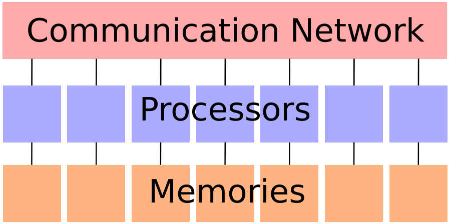

- We can be more precise about the connection between processors, one can consider a network (a collection of switches connected by communication channels) and delve in a detailed way into its pattern of interconnection, i.e., into what is called the network topology.

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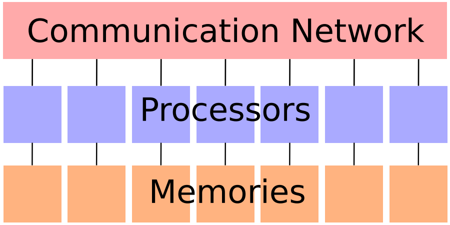

- An alternative is to summarize the network properties in terms of two parameters: latency and bandwidth

Latency	the time it takes for a message to traverse the network;
Bandwidth	the rate at which a processor can inject data into the network.

The TOP500 List – https://www.top500.org/

"...we have decided in 1993 to assemble and maintain a list of the 500 most powerful computer systems. Our list has been compiled twice a year since June 1993 with the help of high-performance computer experts, computational scientists, manufacturers, and the Internet community in general...
In the present list (which we call the TOP500), we list computers ranked by their performance on the LINPACK Benchmark."
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The LINPACK Benchmark.
Solution of a dense $n \times n$ system of linear equations $A\mathbf{x} = \mathbf{b}$, so that

- $\frac{\|A\mathbf{x}-\mathbf{b}\|}{\|A\|\|\mathbf{x}\|n\varepsilon} \leq O(1)$, for ε machine precision,
- It uses a specialized right–looking LU factorization with look–ahead
- Measuring
  - R_{max} the performance in GFLOPS for the largest problem run on a machine,
  - N_{max} the size of the largest problem run on a machine,
  - $N_{1/2}$ the size where half the R_{max} execution rate is achieved,
  - R_{peak} the theoretical peak performance GFLOPS for the machine.

Parallel Algorithms

In a fairly general way we can say that a **parallel algorithm** is an algorithm which can do *multiple operations* in a given time.

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$$\begin{array}{cl}
\mathbf{x} & = [x_1 \; x_2 \; \cdots \; x_i \quad x_{i+1} \; \cdots x_n] \\
+ & \\
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= & \\
\mathbf{x}+\mathbf{y} & = [x_1 + y_1 \; x_2 + y_2 \; \cdots \; x_i + y_i \quad \cdots x_n + y_n]
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- If we do the operation sequentially we do $O(n)$ operations in T_n
- If we split the operation among 2 processors, one summing up the entries between $1,\ldots,i$, and one summing up the entries between $i+1,\ldots,n$ we take T_i time for the first part and T_{n-i} time for the second, therefore the overall time is $\max(T_i, T_{n-i})$ for doing always $O(n)$ operations.

Parallel Algorithms: *speedup*

Let us try to think again in an abstract way and to quantify the overall speed gain for a given gain in a subset of a process.

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Amdahl's Law

Then the overall speedup for $\mathbf{P} = (P_1, \ldots, P_N)$, $\mathbf{S} = (S_1, \ldots, S_{N-1})$ is:

$$S(\mathbf{P}, \mathbf{S}) = \left(P_N + \sum_{i=1}^{N-1} \frac{P_i}{S_i} \right)^{-1}.$$

Parallel Algorithms: *Amdahl's Law*

Let us make some observations on Amdahl's Law

- We are not assuming about whether the original completion time involves some optimization,
- We are not making any assumption on what our optimization process is,
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Amdahl's Law is a fairly general way of looking at how processes can be speed up by dividing them into sub-tasks with lower execution time.

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Amdahl's Law is a fairly general way of looking at how processes can be speed up by dividing them into sub-tasks with lower execution time. Moreover, it fixes the theoretical maximum speedup in various scenarios.

- If we allow all components S_i to grow unbounded then the upper bound on all scenario si $S_{\mathsf{max}} = 1/P_N$.

Let us decline it in the context of the potential utility of *parallel hardware*.

Parallel Algorithms: *Amdahl's Law* for *parallel hardware*

Consider now having a parallel machine that permits us dividing the execution of code across M hardware units, then the problem independent maximum speedup that such hardware can provide is M.

Parallel Efficiency

We define the parallel efficiency E as

$$E \triangleq \frac{S_{\text{overall}}}{M},$$

where $E = 100\%$ correspond to the maximal use of the available hardware. When $S_{\text{max}} < M$, it is then impossible to take full advantage of all available execution units.

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<ins>Every dusty corner of a code must scale</ins>, any portion that doesn't becomes the rate-limiting step!

Parallel Algorithms: *Amdahl's Law* limitations

What we are neglecting and what we are tacitly assuming

- We are neglecting *overhead costs*, i.e., the cost associated with parallel execution such as
  - initializing (spawning) and joining of different computation threads,
  - communication between processes, data movement and memory allocation.
- We considered also the ideal case in which $S_i \to +\infty \ \forall i$, observe that with finite speedup on portions 1 through $N-1$, the S_{overall} might continue to improve with increasing number of execution units.
- We are assuming that the size of the problem remains fixed while the number of execution units increases, this is called the case of strong scalability. In some contexts, we need to turn instead to weak scalability in which the problem size grows proportionally to the number of execution units.

How do we realize practically this parallelism?

Let us focus on what we have discussed until now:

- We have "machines" with multiple processors and whose main memory is partitioned into fragmented components,
- We have algorithms that can divide a problem of size N among these processors so that they can run (almost) independently,
- With a certain degree of approximation, we know how to compute what is the *best improvement* we can expect from a parallel program with M processors on a problem of size N.

What we need to discuss now is then: "How can we actually implement these algorithms on real machines?"

- We need a way to define a parallel environment in which every processor is accounted for,
- We need to have data formats that are aware of the fact that we have a *distributed* memory,
- We need to exchange data between the various memory fragments.

Message Passing Interface – https://www.mpi-forum.org/

"MPI (Message Passing Interface) is a specification for a standard library for message passing that was defined by the MPI Forum, a broadly based group of parallel computer vendors, library writers, and applications specialists." – W. Gropp, E. Lusk, N. Doss, A. Skjellum, A high-performance, portable implementation of the MPI message passing interface standard, Parallel Computing, 22 (6), 1996.

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- MPI uses Language Independent Specifications for calls and language bindings;
- The MPI interface provides an essential *virtual* topology, synchronization, and communication functionality inside a set of processes.
- There exist many implementations of the MPI specification, e.g., MPICH, Open MPI, pyMPI

Hello (parallel) world!

In all the course we are going to use the MPI inside C programs.

```
#include"mpi.h"
#include<stdio.h>

int main(int argc,
^^Ichar **argv){
 MPI_Init( &argc, &argv);
 printf("Hello, world!\n");
 MPI_Finalize();
 return 0;
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We need now to *compile* and *link* the `helloworld.c` program, and we can do it simply by:

```
mpicc helloworld.c -o helloworld
```

Hello (parallel) world! – Compile, Link and Run

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- `mpicc` is a wrapper for a C compiler provided by the Open MPI implementation of MPI.
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Let us see what is happening behind the curtains

- you can first try to discover what compiler are you using by executing `mpicc --version`, that will give you something like
  ```
  icc (ICC) 17.0.4 20170411
  Copyright (C) 1985-2017 Intel Corporation.
  All rights reserved.
  ```
  for an Intel compiler, or maybe
  ```
  gcc (Ubuntu 7.4.0-1ubuntu1~18.04.1) 7.4.0
  Copyright (C) 2017 Free Software Foundation, Inc.
  ```

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- you can first try to discover what compiler are you using by executing `mpicc --version`,
- or discover what are the library inclusion and linking options by asking for `mpicc --showme:compile` and `mpicc --showme:link`, respectively.

Hello (parallel) world! – Compile, Link and Run

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- `mpicc` is a wrapper for a C compiler provided by the Open MPI implementation of MPI.
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“If you find yourself saying, ”But I don’t want to use wrapper compilers!”, please humor us and try them. See if they work for you. Be sure to let us know if they do not work for you. ” - https://www.open-mpi.org/faq/?category=mpi-apps

Hello (parallel) world! – Compile, Link and Run

A piece of advice: if your program is anything more realistic than a classroom exercise use `make`[1], and save yourself from writing painfully long compiling commands, and dealing with complex dependencies more than once.

> *"Make gets its knowledge of how to build your program from a file called the makefile, which lists each of the non-source files and how to compute it from other files."*

A very simple `Makefile` for our first test would be

```
MPICC = mpicc #The wrapper for the compiler
CFLAGS += -g  #Useful for debug symbols
all: helloworld
helloworld: helloworld.c
	$(MPICC) $(CFLAGS) $(LDFLAGS) $? $(LDLIBS) -o $@
clean:
	rm -f helloworld
```

[1] https://www.gnu.org/software/make/

Hello (parallel) world! – Compile, Link and Run

Let us run our first parallel program by doing:

```
mpirun [ -np X ] [ --hostfile <filename> ]  helloworld
```

or by using its synonym

```
mpiexec [ -np X ] [ --hostfile <filename> ]  helloworld
```

- `mpirun`/`mpiexec` will run `X` copies of `helloworld` in your current run-time environment, scheduling (by default) in a round-robin fashion by CPU slot.
- if running under a supported resource manager, Open MPI's `mpirun` will usually automatically use the corresponding resource manager process starter, as opposed to, for example, rsh or ssh, which require the use of a hostfile, or will default to running all `X` copies on the localhost

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- as always, look at the manual, by doing `man mpirun`.

Hello (parallel) world! – Compile, Link and Run

If we now run

```
mpirun -np 6 helloworld
```

we get the following output:

```
Hello, world!
Hello, world!
Hello, world!
Hello, world!
Hello, world!
Hello, world!
```

Every process executes the line

```
printf("Hello, world!\n");
```

that it is a local routine!

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local vs non-local procedure

A procedure is **local** if completion of the procedure depends only on the local executing process.
A procedure is **non-local** if completion of the operation may require the execution of some MPI procedure on another process. Such an operation *may require communication* occurring with another user process.

The MPI parallel environment

Let us modify our `helloworld` to investigate the MPI parallel environment. Specifically, we want to answer, from within the program, to the questions:

1. How many processes are there?
2. Who am I?

```c
#include "mpi.h"
#include <stdio.h>
int main( int argc, char **argv ){
 int rank, size;
 MPI_Init( &argc, &argv );
 MPI_Comm_rank( MPI_COMM_WORLD, &rank );
 MPI_Comm_size( MPI_COMM_WORLD, &size );
 printf( "Hello world! I'm process %d of %d\n",rank, size );
 MPI_Finalize();
 return 0;
}
```

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- How many is answered by a call to `MPI_Comm_size` as an `int` value,
- Who am I? Is answered by a call to `MPI_Comm_rank` as an `int` value that is conventionally called `rank` and is a number between `0` and `size-1`.

The MPI parallel environment

The last keyword we need to describe is the `MPI_COMM_WORLD`, this is the standard Communicator object.

Communicator

A Communicator object connects a group of processes in one MPI session. There can be more than one communicator in an MPI session, each of them gives each contained process an independent identifier and arranges its contained processes in an ordered topology.

This provides

- a safe communication space, that guarantees that the code can communicate as they need to, without conflicting with communication extraneous to the present code, e.g., if other parallel libraries are in use,
- a unified object for conveniently denoting communication context, the group of communicating processes and to house abstract process naming.

The MPI parallel environment

If we have saved our inquiring MPI program in the file `hamlet.c`, we can then modify our `Makefile` by modifying/adding the lines

```
all: helloworld hamlet
hamlet: hamlet.c
 $(MPICC) $(CFLAGS) $(LDFLAGS) $? $(LDLIBS) -o $@
clean:
 rm -f helloworld hamlet
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Then, we compile everything by doing `make hamlet` (or, simply, `make`).

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- Every processor answers the call,
- But it answers it as soon as he has done doing the computation! There is no synchronization.

A word of advice

When should you **not** write parallel code with MPI?

- The effort of writing optimized and scalable MPI codes is not negligible, therefore a direct usage of it its usually best suited for developing *libraries for scientific computations*.

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- Sometimes it happens, you are using a library based on MPI and some function that you truly need is not included.
- To develop new and better libraries for your scientific challenge!

References

There are more books, notes, tutorials, online courses and oral tradition on scientific and parallel computing than we would have time to read and listen in a life. Pretty much everything that contains the words Parallel Programming and Scientific Computing is good...
I suggest here the book

Rouson, D., Xia, J., & Xu, X. (2011). Scientific software design: the object-oriented way. Cambridge University Press.

that discusses general aspect of scientific computing (not perfectly related to parallel computing), and to have on your bedside

Message Passing Interface Forum. MPI: A Message-Passing Interface Standard, Version 3.1. https://www.mpi-forum.org/docs/mpi-3.1/mpi31-report.pdf, High Performance Computing Center Stuttgart (HLRS).