

### Calcolo Parallelo dall'Infrastruttura alla Matematica

Calcolo parallelo: perché, quali infrastratture, quali problemi?

Laurea Triennale e Magistrale in Matematica

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**Dipartimento di Matematica** Università di Pisa



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#### Scientific computing 1 Parallel computing: why?

"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."



Leonardo, CINECA

Wikipedia



## What are the applications?

1 Parallel computing: why?

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

...



## What are the applications?

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Why the need for parallelism?



#### Moore's law 1 Parallel computing: why?



"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."



G. Moore, 1975



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1. Floating-point operation: A floating-point operation (FLOP) is a type of computer operation. One FLOP is equivalent to one addition, subtraction, multiplication, or division of two decimal numbers.

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

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1 Parallel computing: why?

• We are hitting the wall of single processor transistor count/computing capabilities,



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" $\delta\iota\alpha i\rho\epsilon\iota\kappa\alpha i\beta\alpha\sigma i\lambda\epsilon\nu\epsilon$ " (diáirei kái basíleue)



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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.



### The philosophy behind the effort

1 Parallel computing: why?



C. E. Leiserson, N. C. Thompson, J. S. Emer, B. C. Kuszmaul, B. W. Lampson, D. Sanchez, and T. B. Schardl, "There's plenty of room at the Top: What will drive computer performance after Moore's law?", *Science* (2020)

"As miniaturization wanes, the silicon-fabrication improvements at the Bottom will no longer provide the predictable, broad-based gains in computer performance that society has enjoyed for more than 50 years. Software performance engineering, development of algorithms, and hardware streamlining at the Top can continue to make computer applications faster in the post-Moore era."



Solve :  $A\mathbf{x} = \mathbf{b}$ ,

where

- $A \in \mathbb{R}^{n \times n}$  is a very large and sparse matrix nnz(A) = O(n),
- $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$ ,

is often the most time consuming computational kernel in many areas of computational science and engineering problems.



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"In a ground wire problem involving a large number of ground conductors, 13 simultaneous equations were solved..." – Dwight (1930)"
"The second machine, now in operation, was designed for the direct solution of nine or fewer simultaneous equations." – Wilbur, J. B. (1936)



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"Finally, though the labour of relaxation in three dimensions is prohibitively great, the future use of the new electronic calculating machines in this connexion is a distinct possibility" – Fox, L. (1947)



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"The Ferranti PEGASUS computer, with a main store of 4096 words, can solve a maximum of 86 simultaneous equations by its standard subroutine and takes about 45 minutes to complete this calculation." – Wilson, L. B. (1959)



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"...the bound imposed by this is  $m + n \le 474$ . In addition, this number of equations would fill one standard (1.800ft) reel of magnetic tape, and the fifty-odd hours taken in the calculation might be thought excessive." – Barron, Swinnerton-Dyer (1960)



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"...handling problems involving sets of simultaneous equations of two-thousandth order, and SAMIS available through "Cosmic" at the University of Georgia, which can treat up to 10,000 simultaneous equations." – Melosh, Schmele (1969)



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"The mini-computer cost algorithm is applied to the same complex shell problem used previously, with 9120 degrees of freedom [...]. The running times, however, are 40 and 70 hr, respectively! It would appear that improvement of mini-computer speeds is required..." – Kamel, McCabe (1978)



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"For instance, Pomerell in 1994 reports on successful application of preconditioned Krylov methods for very ill-conditioned unstructured finite element systems of order up to 210,000 that arise in semiconductor device modeling." – Saad Y., van der Vorst, H.A. (2000)



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"As a second example, we show results (Table VIII) for a problem arising in ocean modeling (barotropic equation) with n = 370,000 unknowns and approximately 3.3 million nonzero entries..." – Benzi, M. (2002)



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"Problem: Large, mesh size:  $180 \times 60 \times 30$ ,  $\ddagger$  unknowns (in simulation): 1,010,160, Solution time 45.7 h" – Wang, de Sturler, Paulino (2006)



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"The parallel GMRES was tested on the Tesla T10P GPU using a set of matrix data from the oil field simulation data of Conoco Phillips. The order of the system ranges from  $\sim 2000$  to  $\sim 1.1$  million." – M. Wang, H. Klie, M. Parashar, H. Sudan (2009)



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The exascale challenge, using computer that do  $10^{15}$  Flops, targeting next-gen systems doing  $10^{18}$  Flops to solve problems with tens of billions of unknowns.



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2 Parallel computing: where?

Let us start from the bottom: the machines.



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- What is a parallel computer? well, it can be a certain number of different "things"
  - Multi-core computing
  - Symmetric multiprocessing
  - Distributed computing
  - Cluster computing
  - Massively parallel computing
  - Grid computing
  - General-purpose computing on graphics processing units (GPGPU)
  - Vector processors



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- What is a parallel computer?
- Let us abstract from the machine by describing Flynn's taxonomy





Single instruction stream, single data stream SISD Single instruction stream, multiple data streams SIMD Multiple instruction streams, single data stream MISD

Instruction Pool

MISD

Data Pool

DII



Multiple instruction streams, multiple data streams MIMD



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## Parallel Computers: our computer model

2 Parallel computing: where?

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.


#### **Parallel computing: where?** - https://www.top500.org/ 2 Parallel computing: where?

"...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."

http:

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//www.netlib.org/benchmark/hpl/
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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

- $\frac{\|\mathbf{A}\mathbf{x}-\mathbf{b}\|}{\|\mathbf{A}\|\|\|\mathbf{x}\|_{n\varepsilon}} \leq O(1)$ , for  $\varepsilon$  machine precision,
- It uses a specialized right-looking LU factorization with look-ahead



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- Measuring
  - $R_{\text{max}}$  the performance in GFLOPS for the largest problem run on a machine,
  - $N_{\text{max}}$  the size of the largest problem run on a machine,
  - $N_{1/2}$  the size where half the  $R_{\text{max}}$  execution rate is achieved,
  - $R_{\text{peak}}$  the theoretical peak performance GFLOPS for the machine.



#### **The TOP500 List** 2 Parallel computing: where?

**Rmax** (PFlop/s) **Rpeak** (PFlop/s) Power (kW) Rank System Cores Frontier 8,730,112 1,102.00 1,685.65 21,100 2 Supercomputer 7,630,848 442.01 537.21 29,899 Fugaku LUMI 2,220,288 428.70 309.10 6.016 Leonardo 1,463,616 174.70 255.75 5,610 4 Summit 148.60 5 2,414,592 200.79 10,096





# The machines we have in the department

2 Parallel computing: where?

The Toeplitz Cluster made of 5 nodes:

- 4 Nodes Intel

   Xeon
   CPU E5-2650
   v4 @ 2.20GHz with 2 threads per core, 12 cores per socket and 2 socket with 256 GB;
- 1 Node Intel

   Xeon
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The machine we will build here!



#### **Beowulf** 2 Parallel computing: where?

HWÆT: WE GAR-DENA IN GEARDAGUM beodcyninga brym gefrunon. Hu da æbelingas ellen fremedon! Oft Scyld Scefing sceabena breatum monegum mægbum meodosetla ofteah. egsode eorl. svððan ærest wearð feasceaft funden. He bæs frofre gebad. weox under wolcnum. weorðmyndum bah. oð bæt him æghwylc bara ymbsittendra ofer hronrade hyran scolde, gomban gyldan. Þæt wæs god cyning.





# **Beowulf** 2 Parallel computing: where?

"Bēowulf is a multi-computer architecture which can be used for parallel computations. It is a system which usually consists of one server node, and one or more client nodes connected via Ethernet or some other network. It is a system built using commodity hardware components, like any PC capable of running a Unix-like operating system, with standard Ethernet adapters, and switches."

> Radajewski, Radajewski; Eadline, Douglas (22 November 1998). "Beowulf HOWTO". ibiblio.org. v1.1.1





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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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**Example:** the sum of two vectors  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ 

.

$$\mathbf{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_i & x_{i+1} & \cdots & x_n \end{bmatrix} \\ + \\ \mathbf{y} = \begin{bmatrix} y_1 & y_2 & \cdots & y_i & y_{i+1} & \cdots & y_n \end{bmatrix} \\ = \\ \mathbf{x} + \mathbf{y} = \begin{bmatrix} x_1 + y_1 & x_2 + y_2 & \cdots & x_i + y_i & \cdots & x_n + y_n \end{bmatrix}$$

• If we do the operation sequentially we do O(n) operations in  $T_n$ 



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**Example:** the sum of two vectors  $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ 

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$$\mathbf{x} = [x_1 \ x_2 \ \cdots \ x_i \ | \ x_{i+1} \ \cdots \ x_n]$$

$$+$$

$$\mathbf{y} = [y_1 \ y_2 \ \cdots \ y_i \ | \ y_{i+1} \ \cdots \ y_n]$$

$$=$$

$$\mathbf{x} + \mathbf{y} = [x_1 + y_1 \ x_2 + y_2 \ \cdots \ x_i + y_i \ | \ \cdots \ x_n + y_n]$$

- 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  $17/37 \max(T_i, T_{n-i})$  for doing always O(n) operations.



Let us think again abstractly and quantify the overall speed gain for a given gain in a subset of a process.

• We break a process into *N* distinct portions with the *i*th portion occupying the *P<sub>i</sub>* fraction of the overall completion time,



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- order the portions in such a way that the *N*th portion subsumes all the parts of the overall processes with fixed costs.
- The speedup of the *i*th portion can then be defined as

$$S_i \triangleq rac{t_{ ext{original}}}{t_{ ext{optimized}}}, \quad i = 1, \dots, N-1$$

where the numerator and denominator are the original and optimized completion time.



Let us think again abstractly and quantify the overall speed gain for a given gain in a subset of a process.

Amdahl's Law
Then the overall speedup for $\mathbf{P}=(P_1,\ldots,P_N), \mathbf{S}=(S_1,\ldots,S_{N-1})$ is:
$\mathcal{S}(\mathbf{P},\mathbf{S}) = \left(P_N + \sum_{i=1}^{N-1} rac{P_i}{S_i} ight)^{-1}.$



# Parallel Algorithms: Amdahl's Law 3 Parallel computing: how?

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,
- We are not even saying that the process in question involves a computer!

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<sub>i</sub>* to grow unbounded then the upper bound on all scenario si *S*<sub>max</sub> = 1/*P<sub>N</sub>*.

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



# **Parallel Algorithms:** Amdahl's Law for parallel hardware <sup>3</sup> Parallel computing: how?

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

$$E \triangleq rac{S_{ ext{overall}}}{M},$$

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



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



# **Parallel Algorithms:** Amdahl's Law limitations 3 Parallel computing: how?

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  $S_{\text{overall}}$  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.



#### In the weak scalability case the right framework is to use Gustafson's law

## Gustafson's law

$$S = s + p \times N = s + (1 - s) \times N = N + (1 - N) \times s$$

where

- *S* is the theoretical speedup of the program with parallelism (scaled speedup),
- *N* is the number of computing units,
- *s* and *p* are the fractions of time spent executing the serial parts and the parallel parts of the program on the parallel system, i.e., *s* + *p* = 1.



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"Solving a larger problem in the same amount of time should be possible by using more computing units"



**Test Case** 3 Parallel computing: how?

# **Poisson equation**

 $-\Delta f = 1$  on unit cube, with Dirichlet Boundary Conditions

- 7-point finite-difference discretization
- cartesian grid with uniform refinement along the coordinates for increasing mesh size







## **Test Case** 3 Parallel computing: how?

# Solver/preconditioner settings

• AMG as preconditioner of Flexible CG, stopped when  $\|\mathbf{r}^k\|_2 / \|\mathbf{b}\|_2 \le 10^{-6}$ , or itmax = 500

KCMATCH K-cycle with 2 inner iterations, CMATCH building aggregates of max size 8, unsmoothed prolongators

VSCMATCH V-cycle, CMATCH building aggregates of max size 8, smoothed prolongators VSDVB V-cycle for decoupled classic smoothed aggregation

- 1 sweep of forward/backward Hybrid Gauss-Seidel smoother, parallel CG preconditioned with Block-Jacobi and ILU(0) at the coarsest level
- coarsest matrix size  $n_c \leq 200 np$ , with np number of cores

An example from: P. D'Ambra, F. Durastante, and S. Filippone, "AMG preconditioners for linear solvers towards extreme scale", *SIAM J. Sci. Comput.* (2021).



# Experimental environment & Comparison

3 Parallel computing: how?

# **Piz Daint - Swiss National Supercomputing Center by PRACE**

- Cray Model XC40/Cray XC50 architecture with 5704 hybrid compute nodes (Intel Xeon E5-2690 v3 with Nvidia Tesla P100 accelerator)
- Cray Aries routing and communications ASIC with Dragonfly network topology
- GNU compiler rel. 8, Cray MPI 7, Cray-libsci 20.09.1
- PSBLAS 3.7, AMG4PSBLAS 1.0 (See: psctoolkit.github.io)





# Experimental environment & Comparison

3 Parallel computing: how?

# Hypre: Scalable Linear Solvers and Multigrid Methods by LLNL

- BoomerAMG as preconditioner of CG, stopped when  $\|\mathbf{r}^k\|_2 / \|\mathbf{b}\|_2 \le 10^{-6}$ , or itmax = 500
- V-cycle with 1 sweep of forward/backward Hybrid Gauss-Seidel smoother, LU factorization at the coarsest level
- 3 coarsening schemes: hybrid RS/CLJP (Flg), Hybrid Maximal Independent Set (HMIS), HMIS with first level of aggressive coarsening (HMIS1); default parameters for coarsest matrix size  $1 \le n_c \le 9$ , coupled with modified (long-range) classical interpolation



# Weak scaling (256K dofs $\times$ core): Iteration number

3 Parallel computing: how?

		AMG4PSBLAS			Hypre			
np	$n/10^6$	KCMATCH	VSCMATCH	VSDVB	Flg	HMIS	HMIS1	
1	0.256	12	7	11	6	6	12	
2	0.512	12	7	12	7	9	15	
$2^2$	1.036	12	7	13	7	12	17	
$2^3$	2.048	12	7	14	8	13	17	
$2^4$	4.075	12	8	14	8	14	20	
$2^{5}$	8.049	13	9	15	8	14	20	
$2^{6}$	16.384	12	8	15	9	16	22	
$2^{7}$	32.604	12	8	15	10	18	25	
$2^{8}$	63.917	13	9	16	10	20	27	
$2^{9}$	131,072	14	8	18	11	22	29	
$2^{10}$	256,000	15	8	17	12	25	32	
$2^{11}$	511,335	16	12	21	13	29	37	
$2^{12}$	1024,192	15	8	26	13	35	40	
$2^{13}$	2097,152	16	9	27	14	37	44	

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## Weak scaling (256K dofs × core): operator complexity 3 Parallel computing: how?



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# Weak scaling (256K dofs $\times$ core): solve time <sup>3</sup> Parallel computing: how?





## **Results at extreme scale: MPI vs hybrid MPI-CUDA** 3 Parallel computing: how?





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- Parallel computing: why?
   Linear Systems, mon amour
- Parallel computing: where?
   Flynn's Taxonomy
   Bēowulf
- Parallel computing: how?
   An example of contemporary application
- ► First order of business: GIT
- ► Exercises



#### **Software Version Control: GIT** 4 First order of business: GIT

In software engineering, version control is a class of systems responsible for managing changes to **computer programs**, **documents**, large web sites, or other *collections of information*. Version control is a component of software configuration management.



- We are going to use GIT: https://git-scm.com/,
- Specifically, the Gitea instance run by the PHC: https://git.phc.dm.unipi.it/.



## Getting an up-and-running GIT account <sup>4</sup> First order of business: GIT

- 1. Go to: https://git.phc.dm.unipi.it/,
- 2. Click on: [ Accedi (top right of the screen),
- 3. Then: Accedi con G,
- 4. Use UNIPI credentials to login.


### Getting an up-and-running GIT account <sup>4</sup> First order of business: GIT

- 1. Go to: https://git.phc.dm.unipi.it/,
- 2. Click on: [ Accedi (top right of the screen),
- 3. Then: Accedi con G,
- 4. Use UNIPI credentials to login.

Create an SSH key:

- 1. Open a terminal (CTRL+ALT+T),
- 3. Press ENTER to confirm default file location ( $\sim$ /.ssh),
- 4. At the prompt, type a secure passphrase (you have to remember it!),
- 5. Run: eval "\$(ssh-agent -s)" and then ssh-add  $\sim/.ssh/id_ed25519.$



4 First order of business: GIT

From the settings menu you have access to the configurations of the Git service.





4 First order of business: GIT

From the settings menu you have access to the configurations of the Git service.



### • SSH key entry:

	Profilo	Account	Appearance	Sicurezza	Applicazioni	Chiavi SSH / GPG	Organizzazioni	Repository	
Gestisci chiavi 55H									Aggivingl Chiave
Queste chiavi SSH p	ubbliche sor	no associate c	on il tuo account.	Le corrispond	lenti chiavi privat	e consentono l'accesso	completo alle tue re	epositories.	
Hai bisogno di aluto?	Dai un'occhi	iata alla guida	di GitHub percre	a le tue chiavi	SSH o risolvere p	robiemi comuni che po	tresti trovare utilizz	ando SSH.	
Gestisci Chiavi GP	5								Aggiungi Chiave
Queste chiavi GPG p	ubbliche so	no associate o	on il tuo account	Proteggi le tu	ve chiavi private j	perché permettono di v	erificare i commits.		
Hai bisogno di aluto?	Dai un'occh	iata alla guida	di GitHub riguer	do il GPG.					



4 First order of business: GIT

From the settings menu you have access to the configurations of the Git service.







4 First order of business: GIT

From the settings menu you have access to the configurations of the Git service.



• SSH key entry

#### Chiavi SSH / GPG

- Which inserts similarly:

#### Nome della Chiave

Chiave

#### Contenuto

Inizia con 'ssh-ed25519', 'ssh-rsa', 'ecdsa-sha2-nistp256', ed25519@openssh.com'



4 First order of business: GIT

From the settings menu you have access to the configurations of the Git service.



• SSH key entry

#### Chiavi SSH / GPG

- Which inserts similarly:







• You can create a new repository easily.





• You can create a new repository easily.

	Nuovo Repository	
Un repository contiene tutti i file de	el progetto, inclusa la cronologia delle revisioni. Lo hai già altro repository.	ve? Migrare il
Proprietario *	fdurastante -	
	Alcune organizzazioni potrebbero non essere visualizzate nel causa di un limite massimo al numero di repository.	menu a discesa a
Nome Repository *		
	Un buon nome per un repository è costituito da parole chiave ricordare e uniche.	corte, facili da
Visibilità	Rendi privato il repository Solo il proprietario o i membri dell'organizzazione se hanno d grado di vederlo.	iritti, saranno in
Descrizione	Inserisci una breve descrizione (opzionale)	





- You can create a new repository easily.
- And then: Crea Repository

	Nuovo Repository
Un repository contiene tutti i file d	el progetto, inclusa la cronologia delle revisioni. Lo hai già altrove? Migrare il repository.
Proprietario *	fdurastante -
	Alcune organizzazioni potrebbero non essere visualizzate nel menu a discesa a causa di un limite massimo al numero di repository.
Nome Repository*	
	Un buon nome per un repository è costituito da parole chiave corte, facili da ricordare e uniche.
Visibilità	<ul> <li>Rendi privato il repository</li> <li>Solo il proprietario o i membri dell'organizzazione se hanno diritti, saranno in grado di vederlo.</li> </ul>
Descrizione	Inserisci una breve descrizione (opzionale)





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Descrizione	Inserisci una breve descrizione (opzionale)



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   + Nuova Repository

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- You can create a new repository easily.
- And then: Cres Repository

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git clone git@git.phc.dm.unipi.it:fdurastante/cpar2023.git cd cpar2023

The folder will contain these slides, and – in the future – the other material we will use.

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Local

We will use GIT to exchange files and working on writing code.



The **repository** is where files' current and historical data are stored, often on a server. checkout To check out is to create a local working copy from the repository,

pull, push Copy revisions from one repository into another. Pull is initiated by the receiving repository, while push is initiated by the source.

commit To commit is to write or merge the changes made in the working copy back to the repository. A commit contains metadata, typically the author information and a commit message that describes the change.

merge is an operation in which two sets of changes are applied to a file or set of files.

Central

Cit cane



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### ► Exercises



- Review the slides at least once to get used to the vocabulary.
- Make working in a Linux shell comfortable, *e.g.*, ls, cd, ssh, mkdir, mv, cp, rm, grep, diff;
- Follow this GIT tutorial to familiarize yourself with the commands and workflow: https://git-scm.com/docs/gittutorial
- Propose a name for our Beowulf machine:

https://forms.gle/F9XtvAWmVqv6jD5f7

• Have fun.



# Calcolo Parallelo dall'Infrastruttura alla Matematica Thank you for listening!

Any questions?