MÉTHODES ET PROGRAMMATION NUMÉRIQUES AVANCÉES

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Introduction

Advanced Numerical Methods and Programming

Goals are to master:

- the principles of modern numerical methods
- how to adapt them to new parallel and distributed architectures
- how to develop and optimize them according to execution time, memory, accuracy, energy consumption
- how they interact with various applications
- basics of machine learning and artificial intelligence

Motivations

Scientific simulations

Reproduce on a computer experiments that are impossible or too hard or too costly to only perform in real life.

- Physics
- Biology
- Demographics

Artificial Intelligence and Simulation

- Network analysis
- Statistics

From the problem to the computer

Theoretical part

- Model, for example physical equations
- Discretize, from a continuous physical space to a finite discrete domain
- Solve: design a method that solve the discrete model
  - Very often, rely on matrix computations

CS part

- Transform the method into algorithms
- Implement the algorithms
- Optimize and generate executable for the machine
- Run the program

Visible impact of why matrix computations are a key component

Several rankings mainly rely on matrix computations

- top500: Linpack, dense linear algebra
  - Very intensive for the hardware
- hpcg: sparse linear algebra
  - More realistic use of a supercomputer to run simulation codes
- graph500: graph algorithms, close to sparse linear algebra
- green500: top500 + energy consumption monitoring

TOP500, 2024-11

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)
1	El Capitan, LLNL (USA)	11,039,616	1,742.00	2,746.38
2	Frontier, ORNL (USA)	9,066,176	1,353.00	2,055.72
3	Aurora, ANL (USA)	9,264,128	1,012.00	1,980.01
4	Eagle, Microsoft NDv5 (USA)	2,073,600	561.20	846.84
5	HPC6, Eni (IT)	3,143,520	477.90	606.97
6	Fugaku, RIKEN (JP)	7,630,848	442.01	537.21
7	Alps, CSCS (CH)	2,121,600	434.90	574.84
8	LUMI, EuroHPC/CSC (FI)	2,752,704	379.70	531.51
9	Leonardo, CINECA (IT)	1,824,768	241.20	306.31
10	Tuolumne, LLNL (USA)	1,161,216	208.10	288.88

https://top500.org/lists/top500/2024/11/

HPCG, 2024-11

Rank	TOP500	System	Cores	Rmax (PFlop/s)	HPCG (TFlop/s)
1	6	Fugaku	7,630,848	442.01	16004.50
2	2	Frontier	9,066,176	1,353.00	14054.00
3	3	Aurora	9,264,128	1,012.00	5612.60
4	8	LUMI	2,752,704	379.70	4586.95
5	7	Alps	2,121,600	434.90	3671.32
6	9	Leonardo	1,824,768	241.20	3113.94
7	19	Perlmutter	888,832	79.23	1905.00
8	14	Sierra	1,572,480	94.64	1795.67
9	23	Selene	555,520	63.46	1622.51
10	33	JUWELS Booster	449,280	44.12	1275.36

https://top500.org/lists/hpcg/2024/11/

GREEN500

Rank	TOP500	System	Cores	Rmax (PFlop/s)	Power (kW)	Energy Eff. (GFlops/watts)
1	224	JEDI, Julich	19,584	4.50	67	72.733
2	122	ROMEO-2025, URCA	47,328	9.86	160	70.912
3	442	Adastra 2, CINES	16,128	2.53	37	69.098
4	155	Isambard-AI, Bristol	34,272	7.42	117	68.835
5	51	Capella, Dresden	85,248	24.06	445	68.053
6	18	JETI, Julich	391,680	83.14	1,311	67.963
7	69	Helios, Cyfronet	89,760	19.14	317	66.948
8	371	Henri, Flatiron inst.	8,288	2.88	44	65.396
9	340	HoreKa-Teal, KIT	13,616	3.12	50	62.964
10	49	rzAdams, LLNL	129,024	24.38	388	62.803

https://top500.org/lists/green500/2024/11/

Main points

- Dense linear algebra
- Sparse linear algebra
- Iterative solvers
- Eigen solvers
- Graph algorithms and their matrix formulations
- Applications

Dense linear algebra

Dense Matrix-Matrix multiplication

- Very important kernel in dense linear algebra
- Main contributor to Linpack's performances

Practical experiments

`https://github.com/cedricchevalier19/mpna`