Course description

TMA4280—Introduction to Supercomputing

Aurélien Larcher
NTNU, IMF

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Schedule

14 sessions: Week 2–12 then 14-16

Lectures	Friday 12–15	B1
Exercises	Wednesday 17–19	Banachrommet

Notes:

- Except the Curriculum presentation on Week 2, **all** Labs will be located at the computer room Banachrommet.
- Weeks 3 and 4 will serve as introduction and get everyone started with programming and numerics.
- Office hours are offered on:
  1. Thursday 17-19
  2. Friday 15-17
- Please book the office hours latest on Tuesday.

Evaluation

40%	Projects	1. Basic programming (10%)	2018-03-07
		2. MPI/OpenMP (30%)	2018-04-20
60%	Examination	Three problems	2018-05-16

Projects:

1. Delivery involves written report **and** source code.
2. Final handout consists of a commented project demo (approx. 5 min).
3. Other Labs are optional but obviously recommended.

Examination:

1. Small exercises during the Labs will cover most requirements.
2. Previous examination question studied during the lectures.
3. Repetition session scheduled at the end of the curriculum.

Course plan

Two main parts:

1. Computer architectures and programming models.
2. Application to numerical algorithms.

— The first part is usually easily understood by Computer Science students, but should not scare others away: the important is to understand the underling concepts. This is not a CS course.

— The second part is usually the other way around, but the mathematical requirements are kept at the application level.

Course plan: Part 1

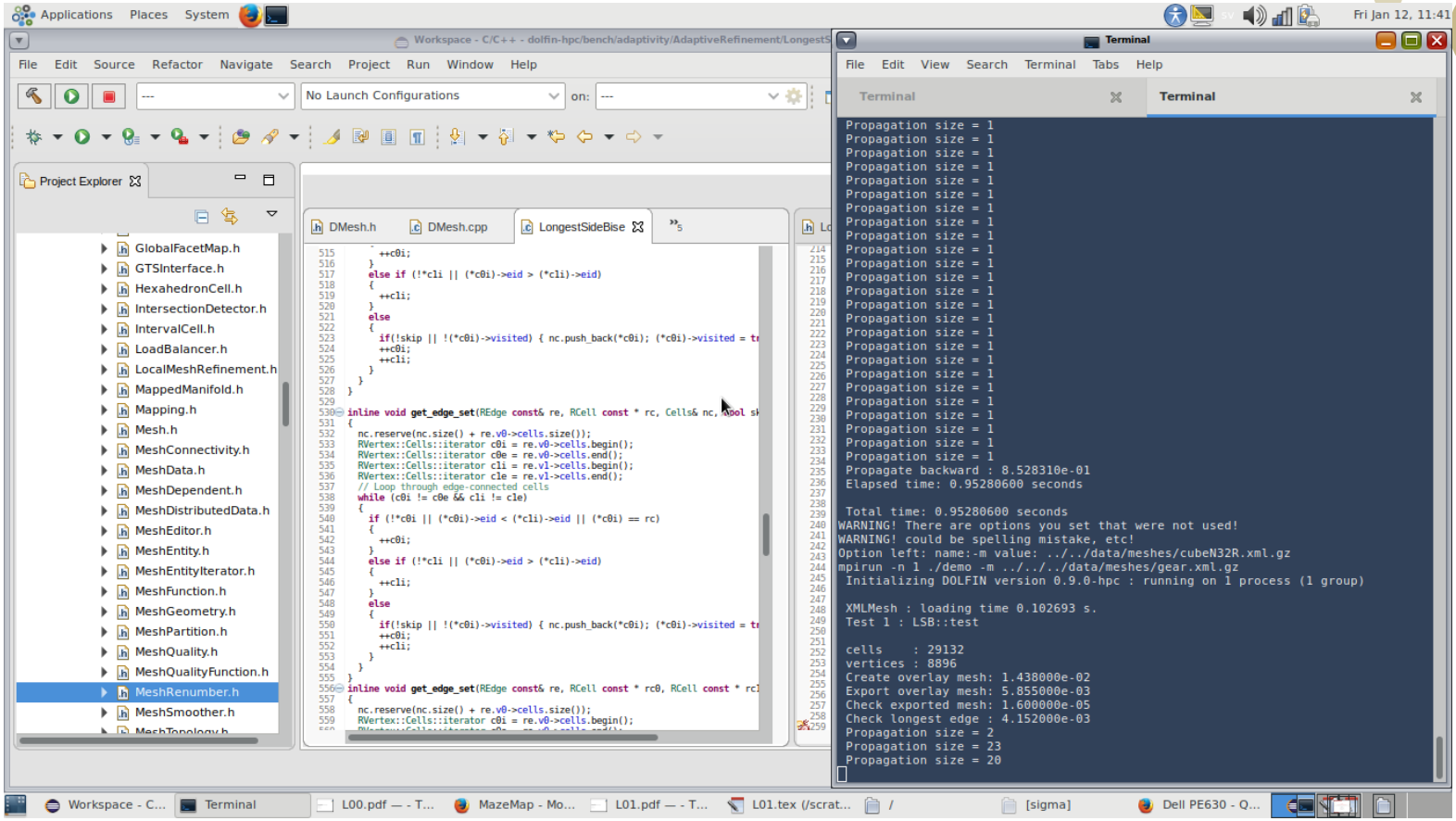
Computer architectures and programming models:

1. W2: Introduction to Supercomputing:
    - Why is Supercomputing needed?
    - What is the evolution of parallel computers and algorithms?
    - What is the future of Supercomputing?
2. W3: Computer architectures I : Single-Processor
    - What is the definition of a processing unit?
    - What are the different ways to take advantage of parallelism?
3. W4: Computer architectures II: Multi-Processor
    - What are the different possible extensions to multiprocessing?
    - What are the advantages and limits?
    - How to analyse the performance of an algorithm or a system?
4. W5-6: Distributed memory model: MPI (Message Passing)
5. W7-8: Shared memory model: OpenMP (Multithreading)

Supercomputing: history and trends

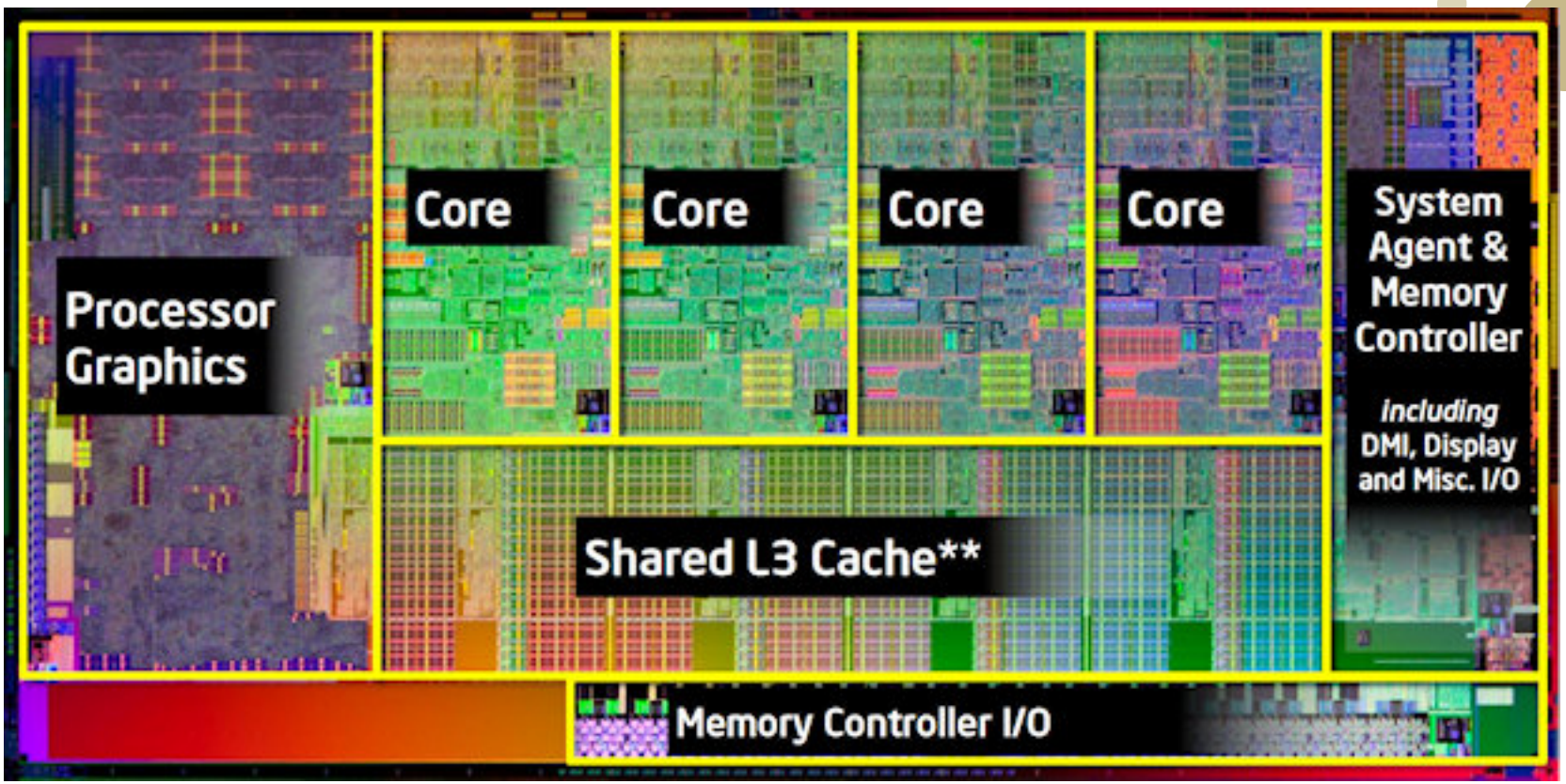
Past evolution, relation to numerical algorithms, and perspectives.

An introduction to UNIX and C/C++ Programming



Recommended practice to prepare for the projects.

Computing architectures



Introduction to floating-point computations and description of different levels of parallelism available on hardware.

Distributed memory programming with MPI

```
node 0:  Hello, world
node 1:  Hello, world
node 3:  Hello, world
node 2:  Hello, world
```

Development of parallel algorithms on distributed memory systems: message passing paradigm, performance analysis.

Shared memory programming with OpenMP

```
#pragma omp parallel for schedule(static)
```

Development of parallel algorithms on shared memory systems: thread model, concurrency, pitfalls.

Course plan: Part 2

Applications and libraries:

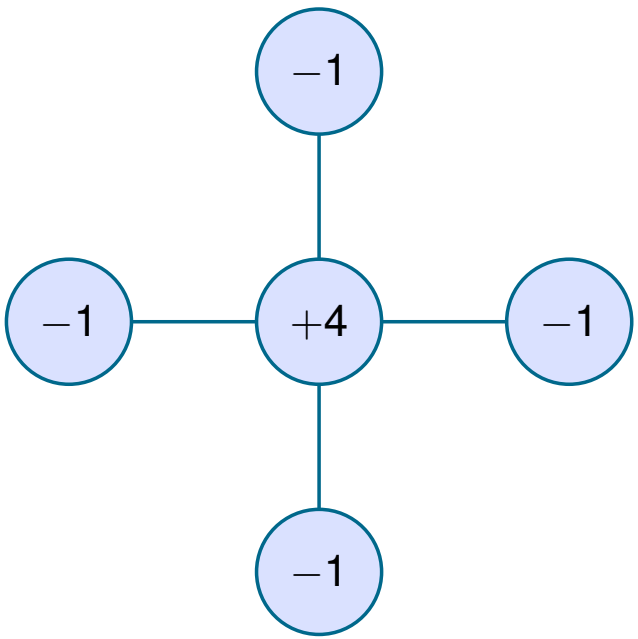
- W9: Poisson problem
  - How to define a discretization of a PDE problem?
  - What are the characteristics of numerical methods?
- W10: Direct linear solvers
- W11: Iterative linear solvers
  - How can a linear system be solved on a multiprocessor?
  - How to analyse the performance advantages and drawbacks?
- W12: Introduction to PETSc: the example of Finite Elements
- W14: Mesh generation, partitioning, and I/O with MPI-IO

W15: Guest lecture on Trends in Supercomputing

W16: Project demo and examination repetition.

Poisson problem: finite differences

$$-\nabla^2 u = f$$
$$u_{\partial\Omega} = g$$



Discretization and implementation of a solver.

Poisson problem: Diagonalization methods

1. Compute $\tilde{\boldsymbol{G}}$ using matrix-matrix products

$$\tilde{\boldsymbol{G}} = \boldsymbol{Q}^{\mathsf{T}} \boldsymbol{G} \boldsymbol{Q}.$$

2. Solve for $\tilde{\boldsymbol{U}}$.

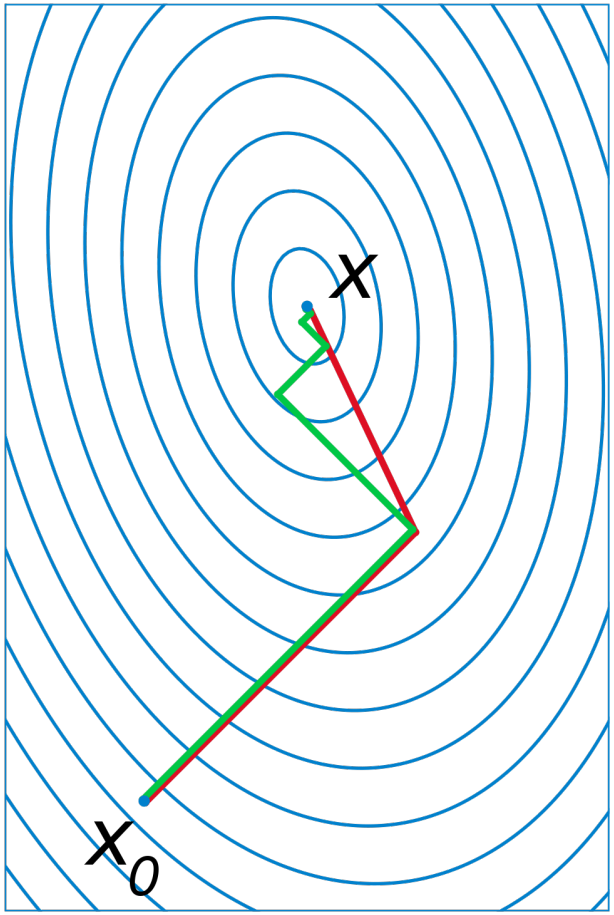
$$\boldsymbol{\Lambda}\tilde{\boldsymbol{U}} + \tilde{\boldsymbol{U}}\boldsymbol{\Lambda} = \tilde{\boldsymbol{G}}$$
$$\lambda_i \tilde{u}_{ij} + \tilde{u}_{ij}\lambda_j = \tilde{g}_{ij}$$
$$\tilde{u}_{ij} = \frac{\tilde{g}_{ij}}{\lambda_i + \lambda_j}$$

3. Compute $\boldsymbol{U}$ using matrix-matrix products

$$\boldsymbol{U} = \boldsymbol{Q}\tilde{\boldsymbol{U}}\boldsymbol{Q}^{\mathsf{T}}$$

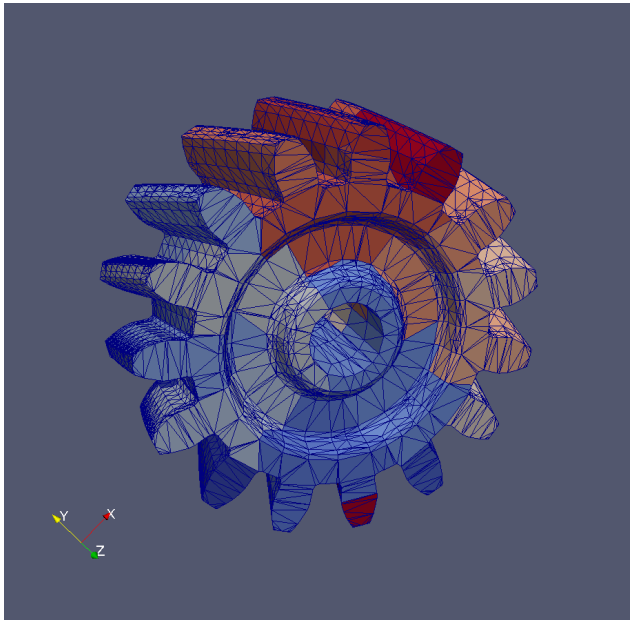
Parallelization of a Poisson solver.

Direct and iterative solvers



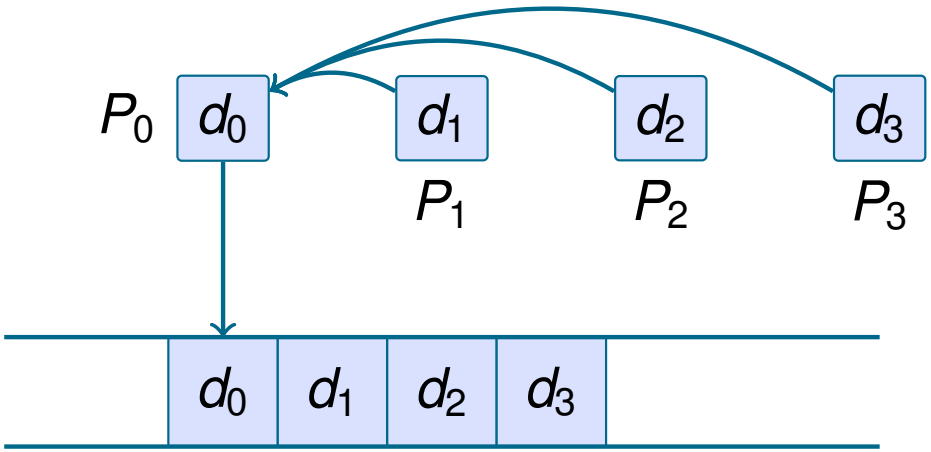
Overview and performance analysis of direct solvers, descent methods, and Krylov solvers.

Mesh distribution and domain decomposition



Review of partitioning techniques for computational meshes . . .

Parallell I/O with MPI-IO



. . . and implementation of I/O with MPI.

Practicalities: Programming, UNIX, Virtual Machine

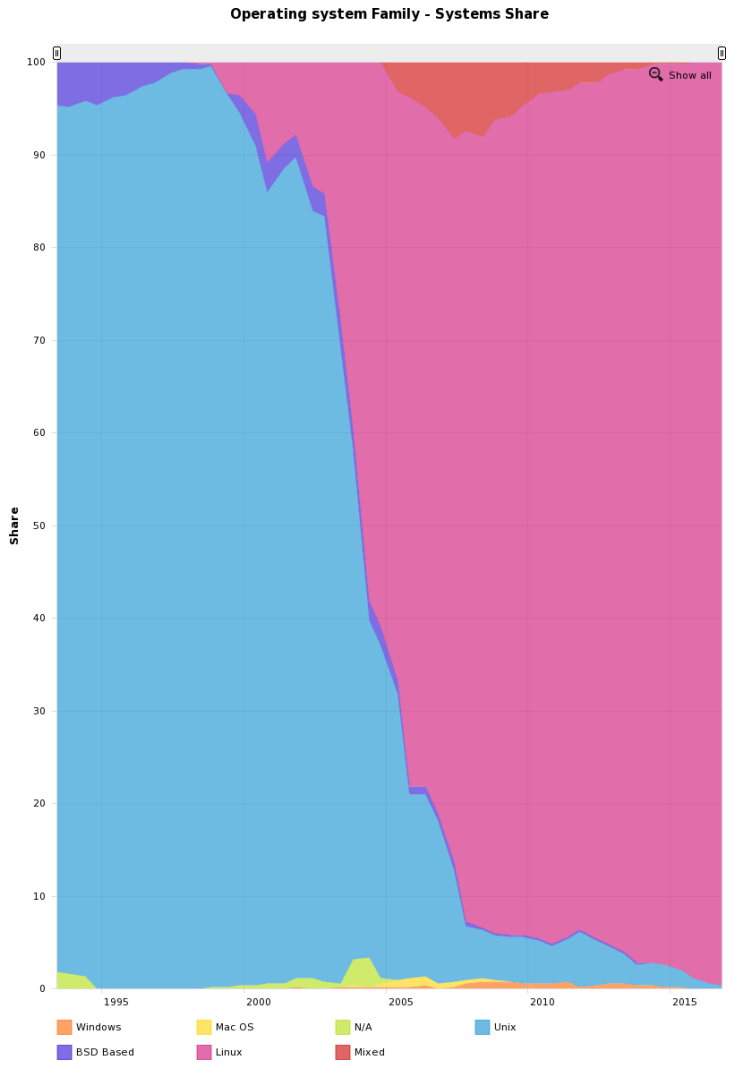


Figure: Top500: Operating System

Practicalities: Programming, UNIX, Virtual Machine

Introduction Survey: https://goo.gl/forms/Sh7nIVRbBo56lgnH3

- Most supercomputers run GNU/Linux or a flavour of UNIX
- Software written in C/C++ and FORTRAN mainly
- Use of Github for projects

- Introduction to UNIX on Wednesday January 17. 2018
- Installation of UNIX environment: virtual machine using Vagrant
- IRC Channel, ##tma4280 on Freenode

Practicalities: Access to IDUN/Lille

Form for access to supercomputing facilities:

- Faculty and institute are the ones you belong to, not (necessarily) IME and IMF.
- Your "local user name" is your NTNU username.
- Your personal ID is probably <username>@ntnu.no.
- Leave project number and manager fields blank.

Return to me or my mailbox at Sentralbygg II Floor 7 by January 26. 2018.

Introductory short courses

Why?

- Different programme/background with more or less experience with computers.
- While not a CS course, it is programming intensive.
- The time required by Projects will depend on your computer fluency.

Conclusion: better start getting used to Linux/UNIX as soon as possible!

Week 3-4 will not contain any compulsory tasks, but tutorials and training to get everyone onboard!