Master in High Performance Computing

Continuum mechanics and fluid-structure interaction problems: mathematical modelling and numerical approximation

Course Presentation

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SISSA

Luca Heltai: minimal BIO

- Visiting professor @ KAUST
- Director of the **Master in High Performance Computing**
- Associate Professor of **Numerical Analysis** @ SISSA
- **Math PhD** @ University of Pavia & Courant Institute, NYU
- BsC in **Electronic Engineering** @ University of Pavia

Research Interests

- Finite Element Methods
- Boundary Element Methods
- Non-matching Discretisation Methods
- Error analysis
- High Performance Computing
- Open Source Software Development (www.dealii.org)
- Machine Learning and Artificial Intelligence

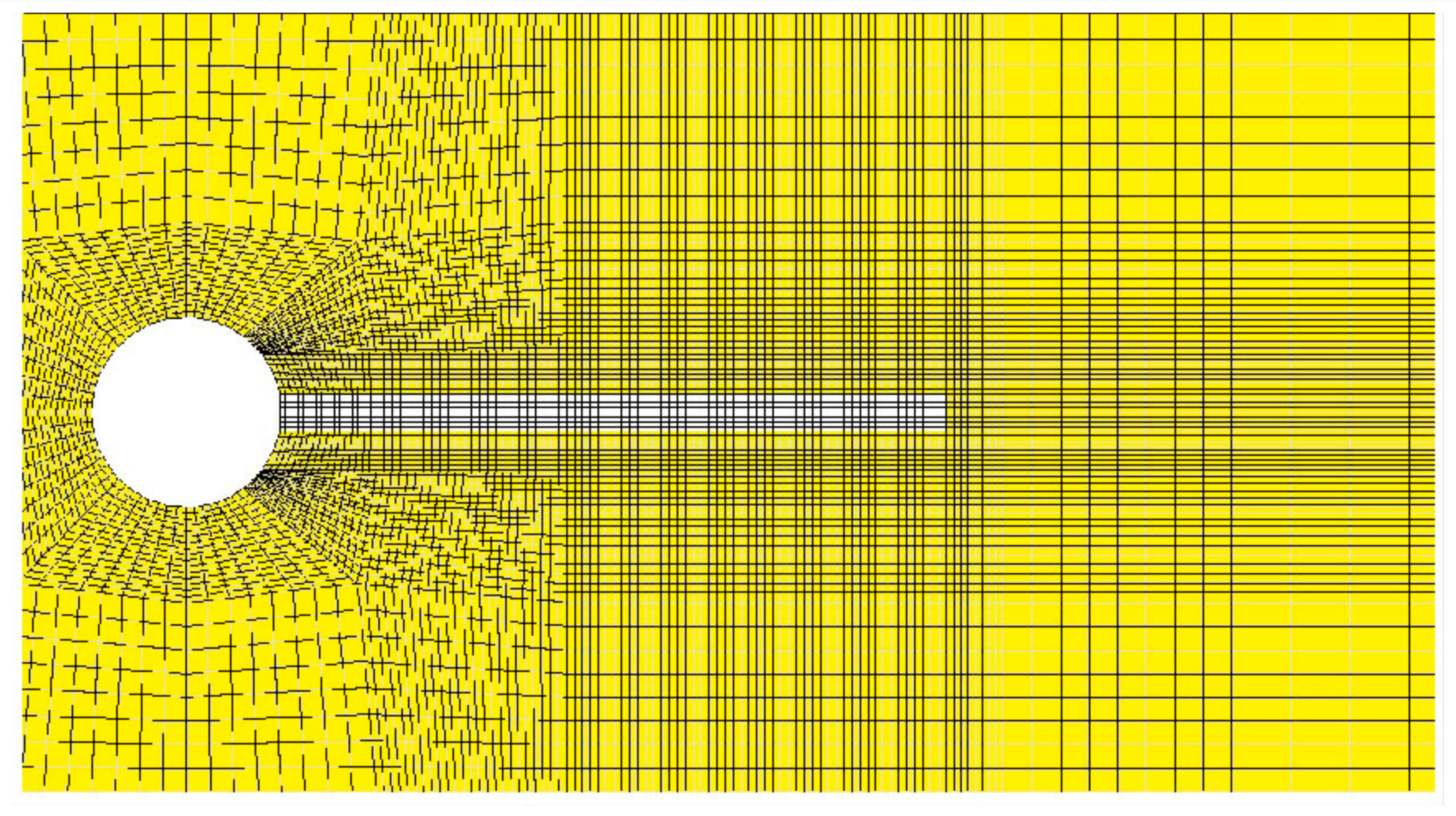
Fields of application

- Fluid structure interaction problems
  - Microswimmers
  - Naval hydro-dynamics
  - Brain bio-mechanics
- Micro and nano electronic devices
  - "quantum reinforced" continuum models
  - non-matching discretisation of defects and interfaces

Course content: three parallel paths

- basics of continuum mechanics
  - kinematics, dynamics, conservation equations, and PDEs
- mathematical modelling of FSI problems
  - Lagrangian, Eulerian, arbitrary Lagrangian Eulerian, non-matching, distributed Lagrange multipliers
- numerical implementations based on the finite element method
  - git, docker, visual studio code, and deal.II

Course objectives



In collaboration with D.Boffi, L.Gastaldi, F.Costanzo

In collaboration with Michal Wichrowski

Course objectives

- What you will learn:
  - Basics of continuum mechanics
  - Basic theory of Finite Elements
  - Fluid structure interaction
  - State-of-the-art implementation of FEM codes for FSI/continuum mechanics
  - How to use a modern C++ IDE, to build and debug your codes
  - How to use a large FEM library to solve complex PDE problems
  - How to properly document your code using Doxygen
  - How to use a proper Git workflow to develop your applications
  - How to leverage GitHub actions, google tests, and docker images to test and deploy your application
  - How hybrid parallelisation (threads + MPI + GPU) works in real life FEM applications

Outcome of the course — Theory

- You will learn how to model and study coupled problems of continuum mechanics, i.e.,
  - solid mechanics
  - fluid dynamics
  - everything in between

Outcome of the course — Practice

- You will learn how to use and develop FEM applications based on deal.II which:
  - Solve coupled, geometrically non-linear, physically non-linear, time dependent partial differential equations, on adaptively refined grids, in parallel
  - Uses modern version control tools (on GitHub)
  - Is tested automatically (through GitHub actions) every time you push a commit, or open a pull request
  - Is documented using Doxygen, and its web page is updated and deployed automatically every time you merge to master a new branch

Prerequisites

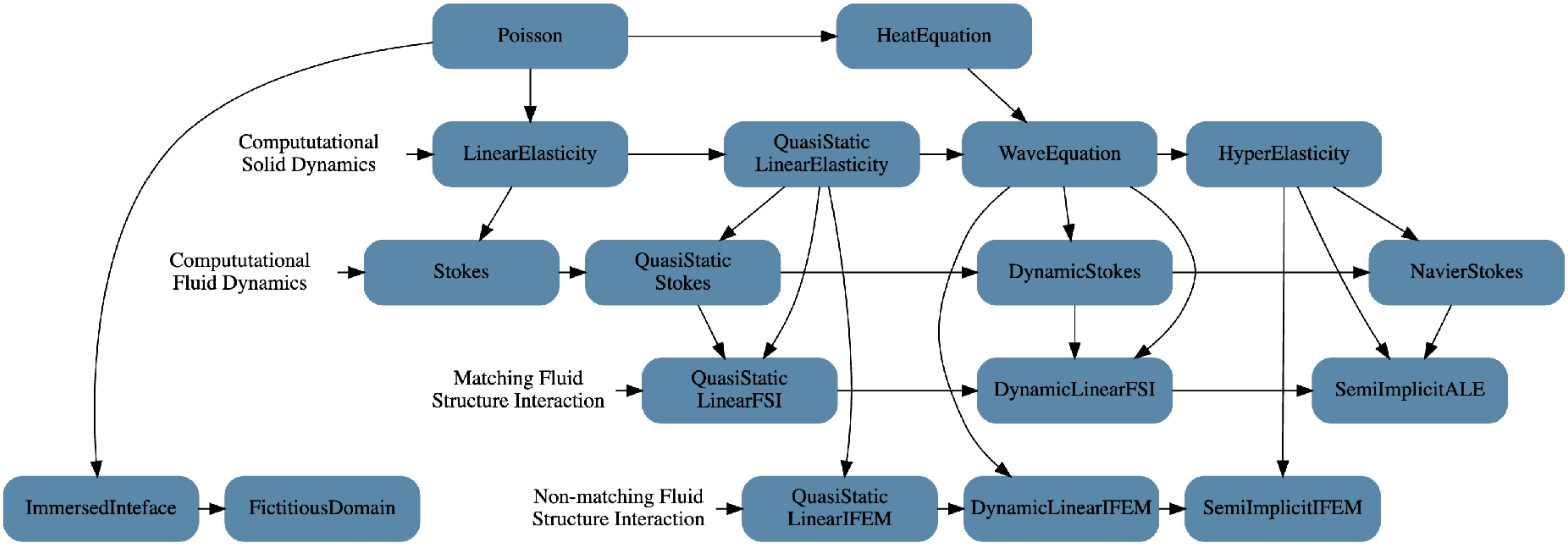
- Theory:
  - Some knowledge of Sobolev Spaces
    - Linear operators, Banach and Hilbert spaces, duality, etc.
  - Some knowledge on Numerical Analysis and Finite Elements
    - Quadrature, interpolation, Taylor expansions, Lagrangian Finite Elements, etc.

- Practice:
  - Some knowledge of C/C++
  - To run out of the box:
    - a machine with Visual Studio Code installed
    - Docker
    - A GitHub account
  - Do it yourself strategy:
    - deal.II with all its dependencies
    -

More Info

- Course pages:
  - Official Github course page (the most up to date information is found here): https://github.com/luca-heltai/fsi-suite
    - Course slides
    - Programs
  - Course recordings: https://bit.ly/2NY46LZ
  - Email:
    prof. Luca Heltai <luca.heltai@sissa.it>

Plan of the course (don't panic!)



Why deal.II (or any other Finite Element library)

- The numerical solution of partial differential equations is an immensely vast field!
- It requires us to know about:
  - Partial differential equations
  - Methods for discretizations, solvers, preconditioners
  - Programming
  - Adequate tools
  - **This course will cover all of this to some degree!**

Numerics of PDEs

There are 3 standard tools for the numerical solution of PDEs:

Finite element method (FEM)

Finite volume method (FVM)

Finite difference method (FDM)

Common features:

Split the domain into small volumes (cells)

Define balance relations on each cell

Obtain and solve very large (non-)linear systems

Problems:

Every code has to implement these steps

There is only so much time in a day

There is only so much expertise anyone can have

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In addition:

We don't just want a simple algorithm

We want state-of-the-art methods for everything

Numerics of PDEs

Examples of what we would like to have:

Adaptive meshes

Realistic, complex geometries

Quadratic or even higher order elements

Multigrid solvers

Scalability to 1000s of processors

Efficient use of current hardware

Graphical output suitable for high quality rendering

Q: How can we make all of this happen in a single code?

The hard reality

- Most research software today:
  - **Written by graduate students**
    - without a good overview of existing software
    - with little software experience
    - with little incentive to write high quality code
  - **Maintained by postdocs**
    - with little time
    - who need to consider the software primarily as a tool to publish papers
  - **Advised by faculty**
    - with no time
    - oftentimes also with little software experience

How we develop Software

Q: How can we make all of this happen in a single code?

Not a question of feasibility but of how we develop software:
Is every student developing their own software?
Or are we re-using what others have done?

Do we insist on implementing everything from scratch?
Or do we build our software on existing libraries?

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There has been a major shift on how we approach the second question in scientific computing over the past 10-15 years!

The secret to good scientific software is (re)using existing libraries!

Existing Software

There is excellent software for almost every purpose!

Basic linear algebra (dense vectors, matrices):
BLAS
LAPACK

Parallel linear algebra (vectors, sparse matrices, solvers):
PETSc
Trilinos

Meshes, finite elements, etc:
deal.II – the topic of this class
…

Visualization, dealing with parameter files, ...

Our experience

It is realistic for a student developing numerical methods using external libraries to have a code at the end of a PhD time that:

- Works in 2d and 3d
- On complex geometries
- Uses higher order finite element methods
- Uses multigrid solvers or preconditioners
- Solves a nonlinear, time dependent problem

Doing this from scratch would take 10+ years.

Common arguments…

Arguments against using other people's packages:

I would need to learn a new piece of software, how it works, its conventions. I would have to find my way around its documentation. Etc.

I think I'll be faster writing the code I want myself!

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Answers:

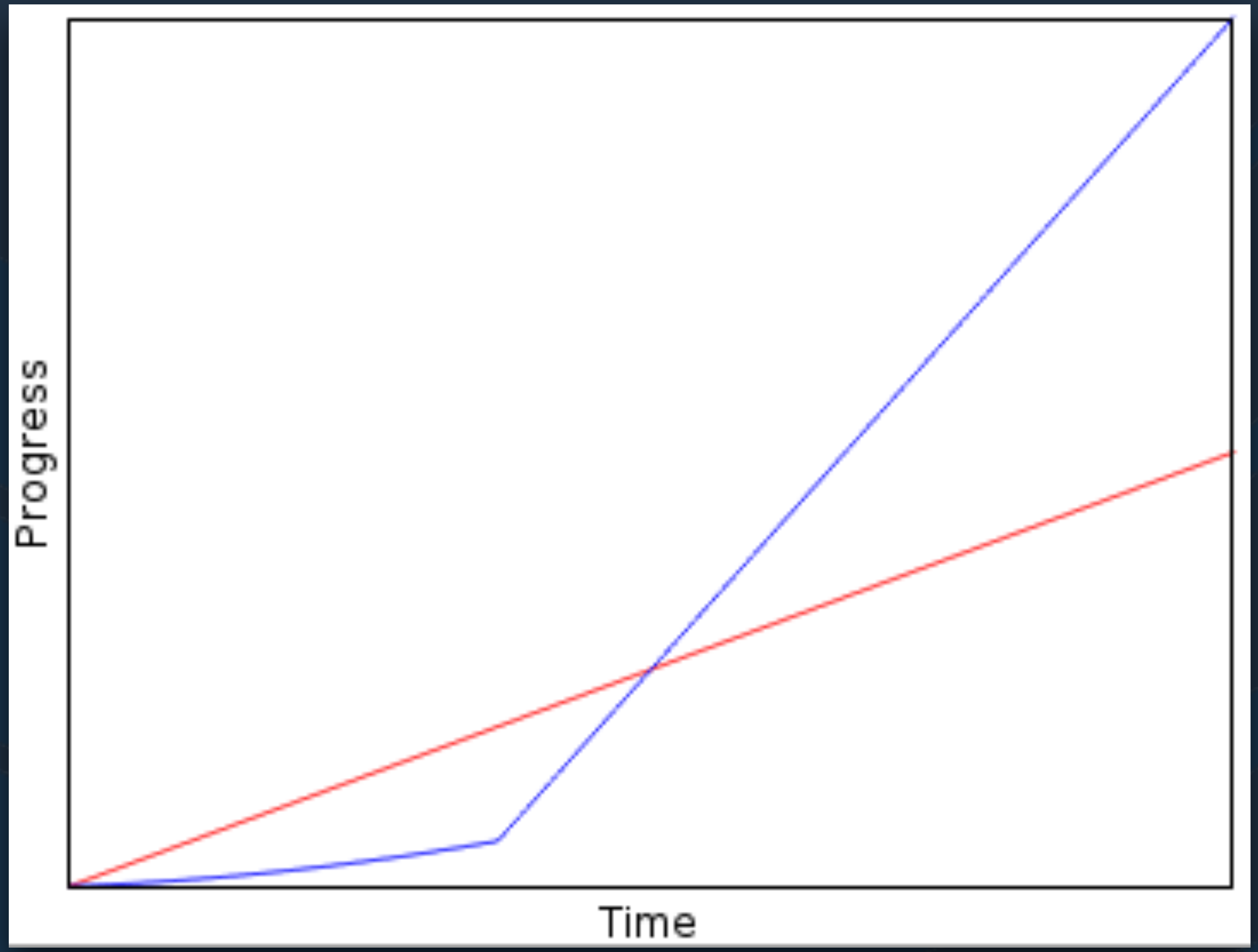
The first part is true.

The second is not!

You get to use a lot of functionality you could never in a lifetime implement yourself.

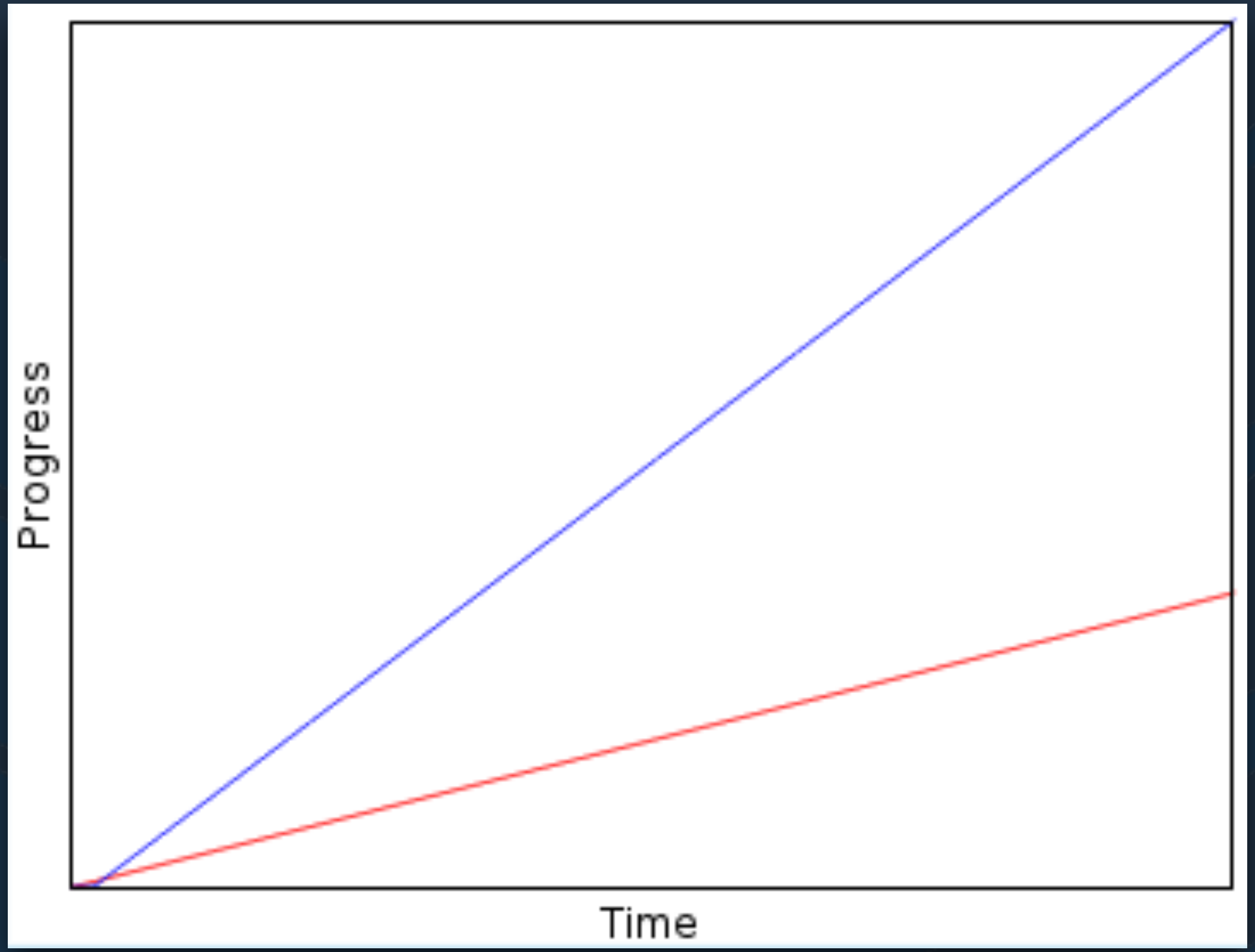
Think of how we use Matlab today!

I’m faster!



Blue: use external libraries
Red: do it yourself

The real picture…



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Answers:

Yes, there is value to that.

But: if you know quadrature in 2d, why implement it again in 3d?

So let them write a toy code and throw it away after 3 months and do it right based on existing software.

Common Arguments…

Arguments against using other people's packages:

How do I know that that software I'm supposed to use doesn't have bugs? How can I *trust* other people's software?

With my own software, at least I know that I don't have bugs!

Answer 1:

You can't be serious to think that your own software has no bugs!

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Answer 2:

The packages I will talk about are developed by professionals with a lot of experience

They have extensive testsuites

For example, deal.II runs 3,000+ tests **after every single change**

Bottomline:

When having to implement software for a particular problem, re-use what others have done already

There are many high-quality, open source software libraries for every purpose in scientific computing

Use them:
– You will be far more **productive**
– You will be able to use **state-of-the-art** methods
– You will have far **fewer bugs** in your code

If you are a graduate student:

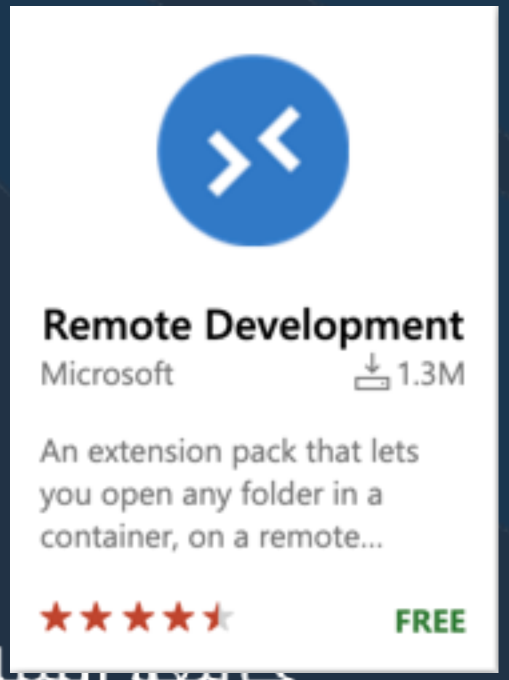
Use them because you will be able to impress your advisor with quick results!

Roadmap for next lectures:

- Recap on Sobolev spaces, and basic tensor analysis
- Recap on the Finite Element Method
- Familiarising with the tools:
  - Version control system (git)
  - Modern IDEs (VSCode)
  - Remote development using Docker inside VSCode
- “Road to Poisson”

Setting up VSCode

- Download and install **Docker**: https://www.docker.com/products/docker-desktop
  - Read some doc: https://www.docker.com/get-started
- Download and install: https://code.visualstudio.com/download
  - Read some doc: https://code.visualstudio.com/docs
  - Install the following extension:



Open the course repository

- Clone the repository of the course to a directory of your liking
- Open the directory containing the repository with Visual Studio Code (the directory contains a hidden folder, called “.**devcontainer”,** used by VSCode to understand the
- VSCode should ask you if you want to reopen the folder within a container. Say yes.
- VSCode will now download a docker image. The first time around, this will take some time.