Master in High Performance Computing

Theory and Practice of Finite Element Methods

Setting up a “best practice” FEM development environment
(some slides taken from prof. Wolfgang Bangerth)

Luca Heltai <luca.heltai@sissa.it>

International School for Advanced Studies (www.sissa.it)
Mathematical Analysis, Modeling, and Applications (math.sissa.it)
Master in High Performance Computing (www.mhpc.it)
SISSA mathLab (mathlab.sissa.it)

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ICTP The Abdus Salam International Centre for Theoretical Physics

SISSA

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:

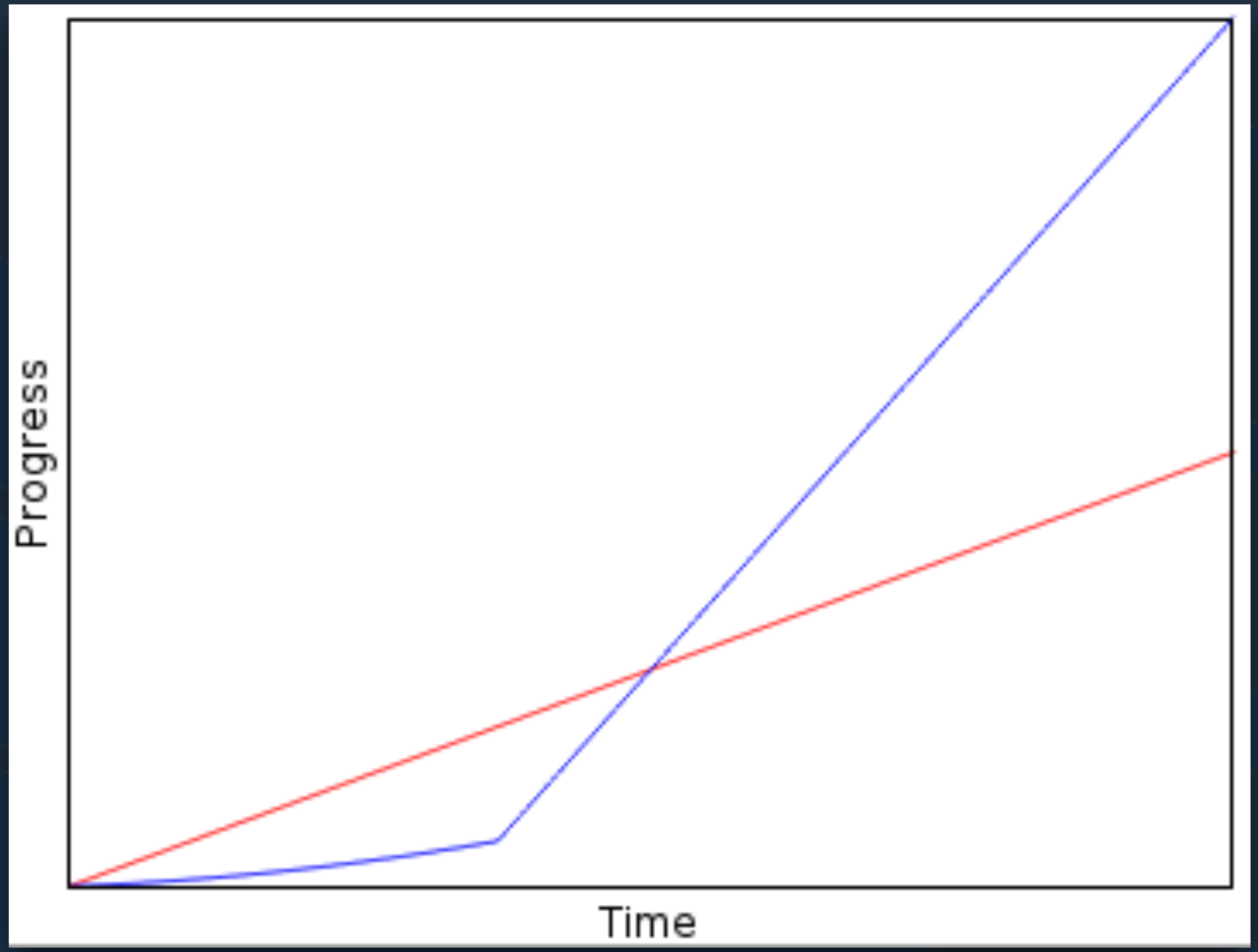
The first part is true.

The second is not!

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

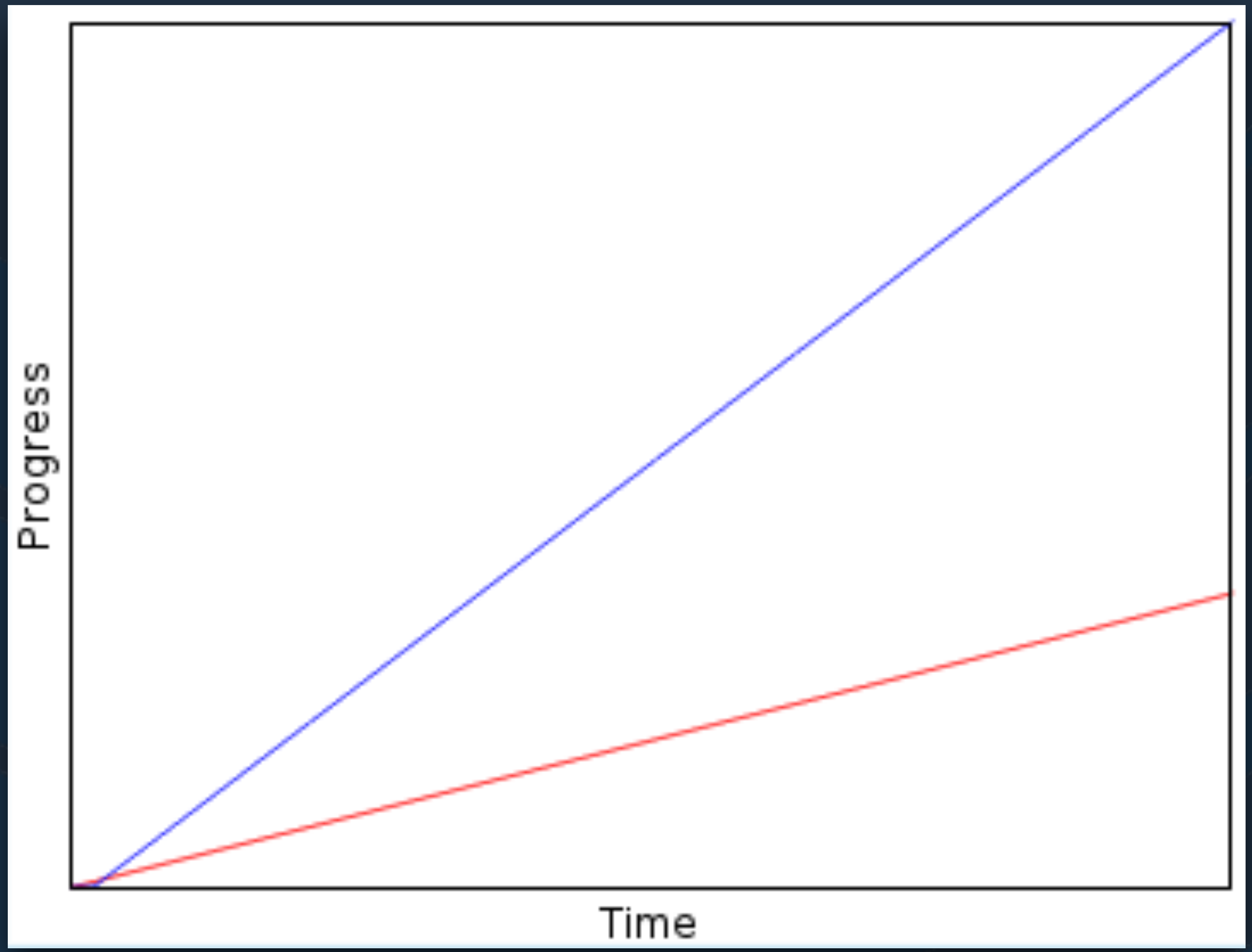
Think of how we use Matlab today!

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:

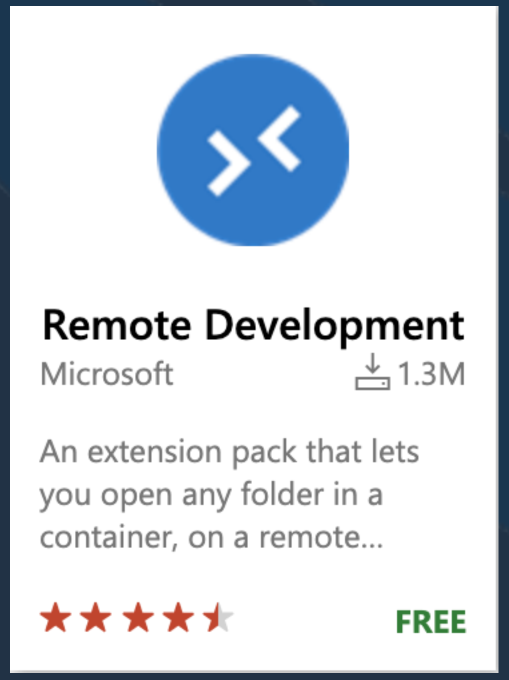
- Version control system (git)
- Modern IDE (VSCode)
- Cross platform build systems (cmake)
- Automatic formatting (clang-format)
- Test driven development (google test, deal.II testing framework)
- Inline documentation (doxygen)
- External visualisation tools (paraview)

Version control systems

- We'll use GitHub classrooms:
  - Understand how GitHub classrooms work
    https://github.com/jfiksel/github-classroom-for-students
    (the guide shows how to install R-Studio. We won't need that. Don't do that part.)
    After setting up git…
  - Accept the first assignment:
    https://classroom.github.com/a/SxO9Wq2M
  - If you are new to git, follow the tutorial at
    http://learngitbranching.js.org/
    to learn how to use git. I'll give a very short overview today.

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 assignment repo

- Open the directory containing the assignment. The directory contains a hidden folder, called “**.devcontainer**”
- VSCode should ask you if you want to run the folder in the container. Say yes.
- VSCode will now download a docker image. The first time around, this will take some time.