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Software Sustainability

The why and the how

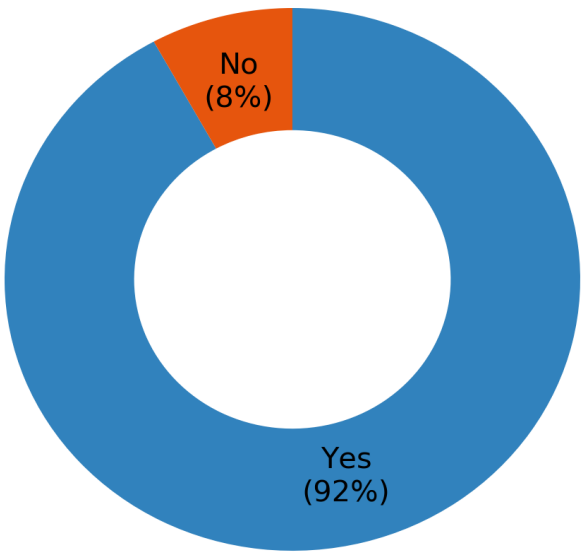
Phil Tooley
RSE@Sheffield

Cardiovascular Fluids Modelling SIG
20 September 2018

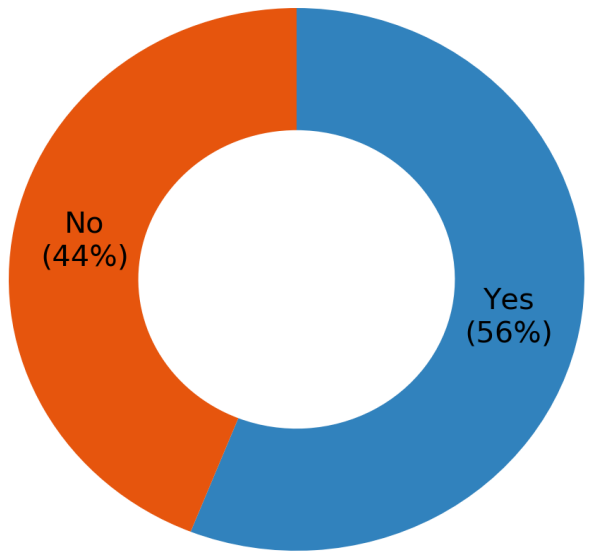
Science relies on research software

2014 UK Research Software Survey[1]

Do you use research software?



Do you develop your own research software?



[1] S.J. Hettrick et al, UK Research Software Survey 2014

It must be *good* research software

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The war over supercooled water

How a hidden coding error fueled a seven-year dispute between two of condensed matter's top theorists.

physicstoday.scitation.org

Source: Physics Today, DOI:10.1063/PT.6.1.20180822a

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Recognising the Problem

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Software Sustainability Institute[2]

- Funded in 2010 by EPSRC to promote sustainable development of research software and now a collaborative effort by multiple funders
- Focus on reproducible research and recognising software as a research output
- Encourage widespread recognition of research software engineer (RSE) role as experts in development of high quality software
- Provide training and support for developers of scientific software through RSEs (software/data carpentry)

Software Sustainability Institute

EPSRC Engineering and Physical Sciences Research Council

BBSRC bioscience for the future

E·S·R·C ECONOMIC & SOCIAL RESEARCH COUNCIL

Jisc

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[2] www.software.ac.uk

My first research code experience

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readme.txt

```
Dear Phil,

This is a copy of the code WAKE, which is written by Mora and Antonsen.
There is also a photon-kinetic version of it, QWAKE. If anyone can read
the comments (largely in French) they are welcome to use it, provided
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How do I run this?

What will it do?

How do I interpret the output?

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The code I actually used

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README.md

Fourier-Bessel Particle-In-Cell code (FBPIC)

master passing | dev passing | pypi v0.9.4 | license BSD-3-Clause-LBNL | DOI 10.5281/zenodo.1285993

Online documentation: http://fbpic.github.io
Support: Join slack

Overview

FBPIC is a Particle-In-Cell (PIC) code for relativistic plasma physics.

It is especially well-suited for physical simulations of **laser-wakefield acceleration** and **plasma-wakefield acceleration**, with close-to-cylindrical symmetry.

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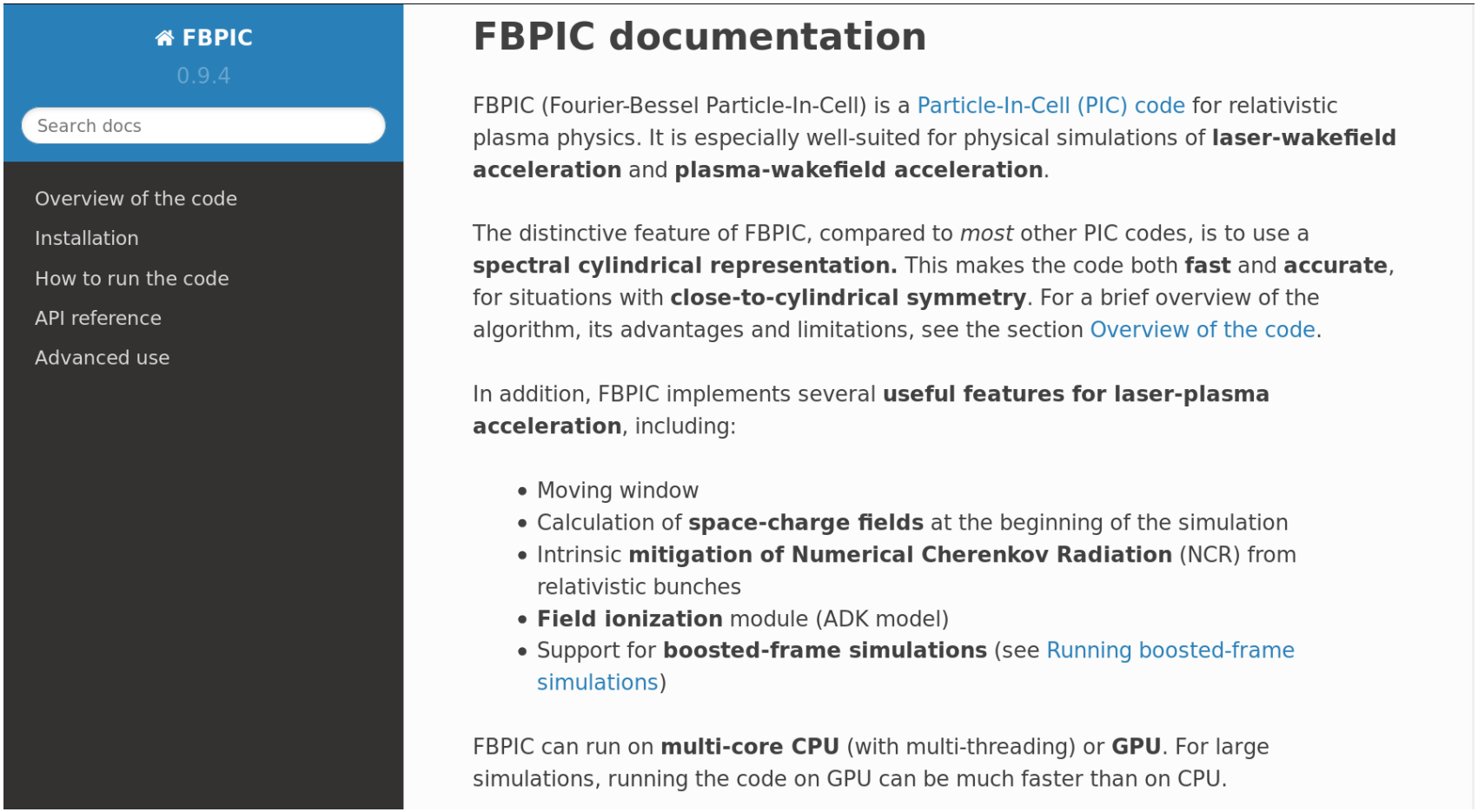
The code I actually used



FBPIC

0.9.4

Search docs

Overview of the code

Installation

How to run the code

API reference

Advanced use

FBPIC documentation

FBPIC (Fourier-Bessel Particle-In-Cell) is a Particle-In-Cell (PIC) code for relativistic plasma physics. It is especially well-suited for physical simulations of **laser-wakefield acceleration** and **plasma-wakefield acceleration**.

The distinctive feature of FBPIC, compared to *most* other PIC codes, is to use a **spectral cylindrical representation.** This makes the code both **fast** and **accurate**, for situations with **close-to-cylindrical symmetry**. For a brief overview of the algorithm, its advantages and limitations, see the section Overview of the code.

In addition, FBPIC implements several **useful features for laser-plasma acceleration**, including:

- Moving window
- Calculation of **space-charge fields** at the beginning of the simulation
- Intrinsic **mitigation of Numerical Cherenkov Radiation** (NCR) from relativistic bunches
- **Field ionization** module (ADK model)
- Support for **boosted-frame simulations** (see Running boosted-frame simulations)

FBPIC can run on **multi-core CPU** (with multi-threading) or **GPU**. For large simulations, running the code on GPU can be much faster than on CPU.

Unsustainable Software

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Symptoms of unsustainable software or development practices include:

- inherited magic/spaghetti code
- data hardcoded into software
- versioning hell
- lack of documentation
- no tests/benchmarks
- custom data formats
- hard to modify without breaking
- hard to install on new machines

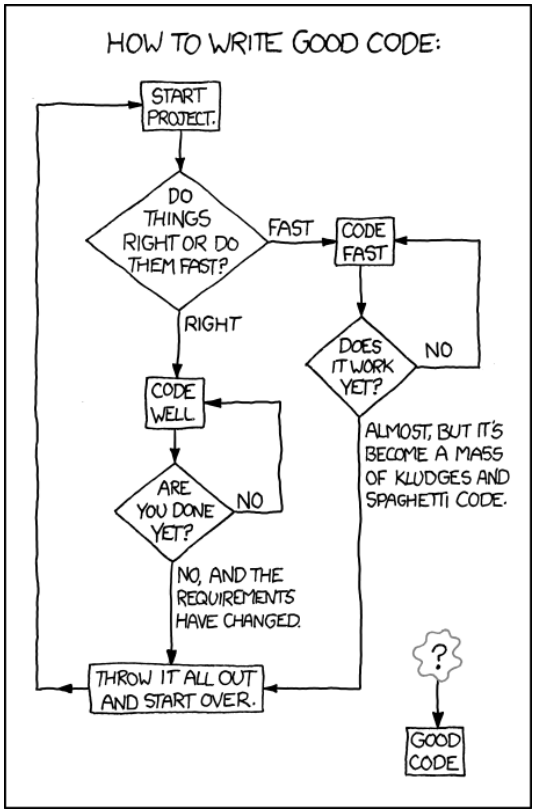

Image Source: Randall Munroe, XKCD (https://xkcd.com/844/)

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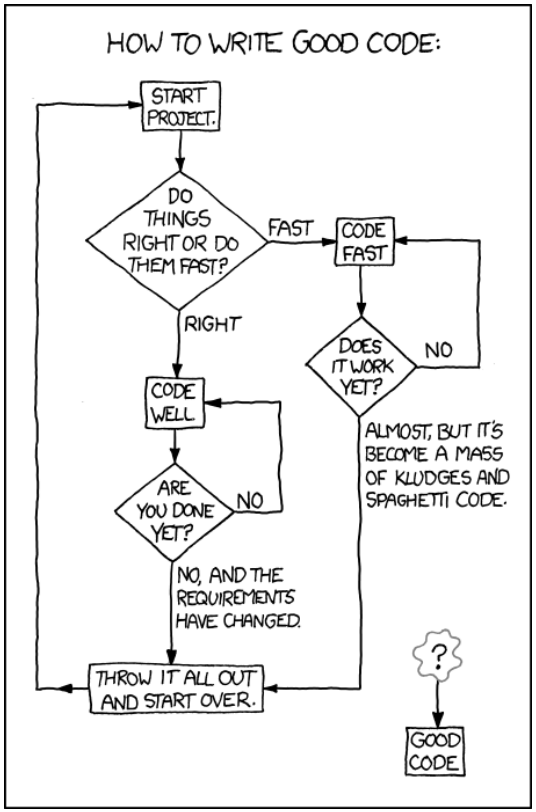

Writing good software is hard. Maintaining it can be even harder...

Image Source: Randall Munroe, XKCD (https://xkcd.com/844/)

How do we make sustainable software?

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"**Software sustainability** describes the practices, both technical and non-technical, that allow software to continue to operate as expected in the future. A constant level of effort is required to maintain the software's operation."[3]

Key Considerations

- Good organisation using version control
- Ensuring longevity of software, runnable on new hardware/OSes
- Testing and benchmarking to ensure valid results
- Documentation - both usage and technical
- Dissemination/sharing with wider community
- Community led maintainence effort

[3] S.J. Hettrick et al., UK Research Software Survey 2014, DOI:10.5281/zenodo.1183562

Good Code Structure

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Well structured code is:

- Easy to understand
  - Consistent code style
  - Names should explain what things do
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  - Don't hardcode variables, use a configuration file
  - Make use of existing language ecosystem
- Necessary
  - Use existing libraries where you can
  - Don't invent your own data formats

Keeping Code Organised

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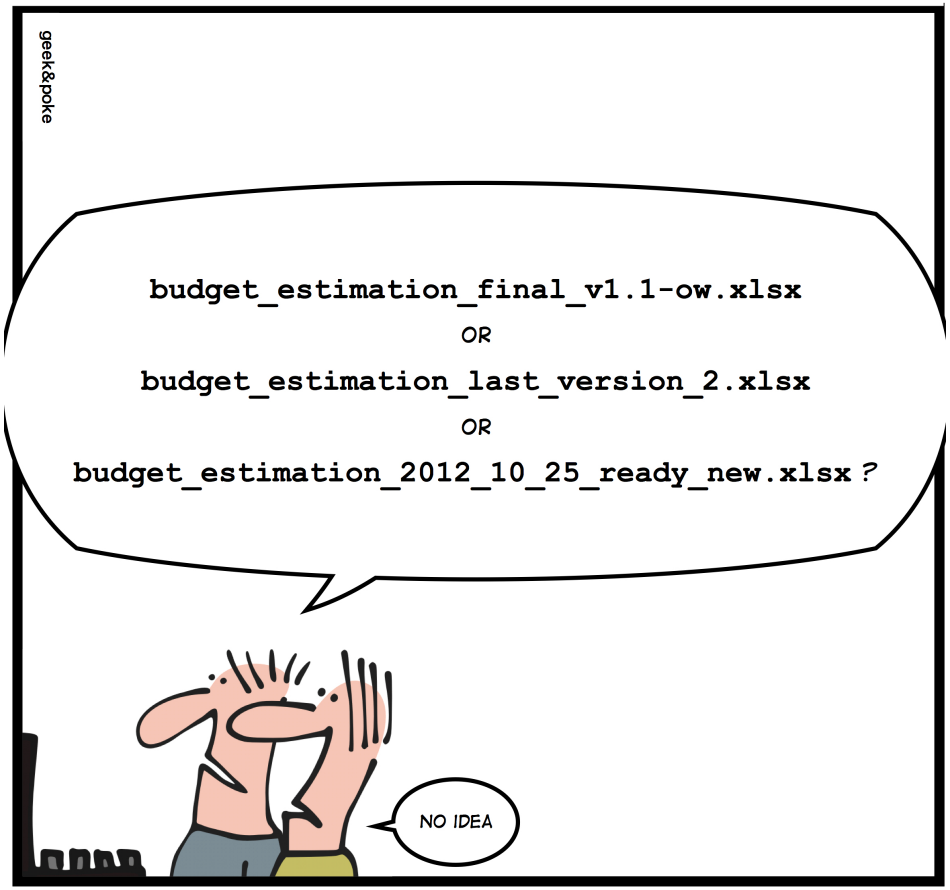

Image Source: http://geek-and-poke.com/2012/11/simply-explained.html

Keeping Code Organised

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Have you ever

- Had files with names like "awesomecode_v4_final_final.py"?
- Made a change to code, then wanted to change it back?
- Needed to compare two revisions of your code?
- Had to maintain different versions of your code?
- Wanted to develop code collaboratively?

Version control systems exist to help with this

Keeping Code Organised

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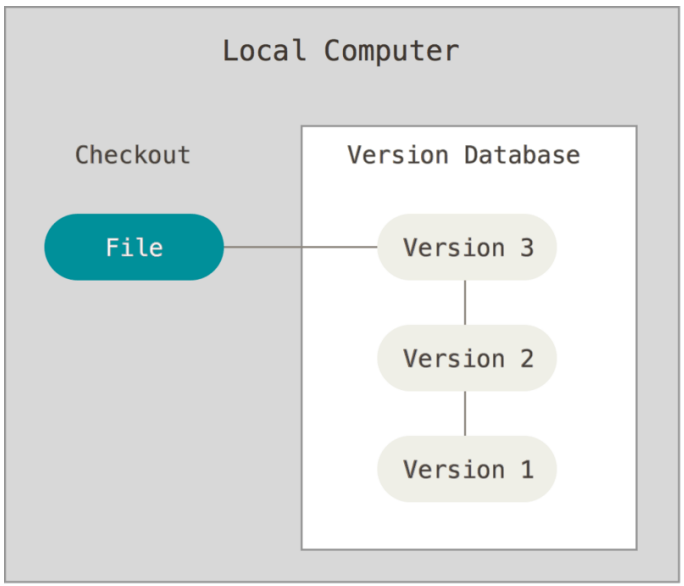
Version Control Systems (VCS)

- Keep a full history of changes
- Easily restore old versions



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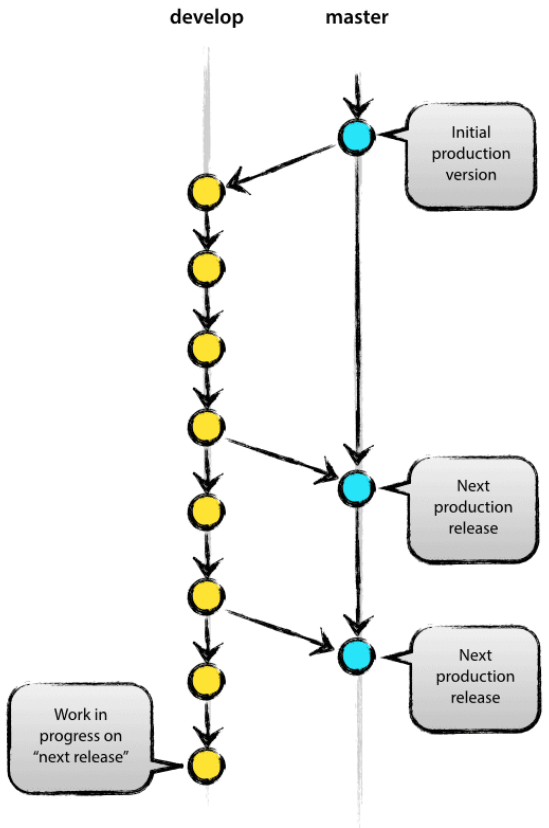

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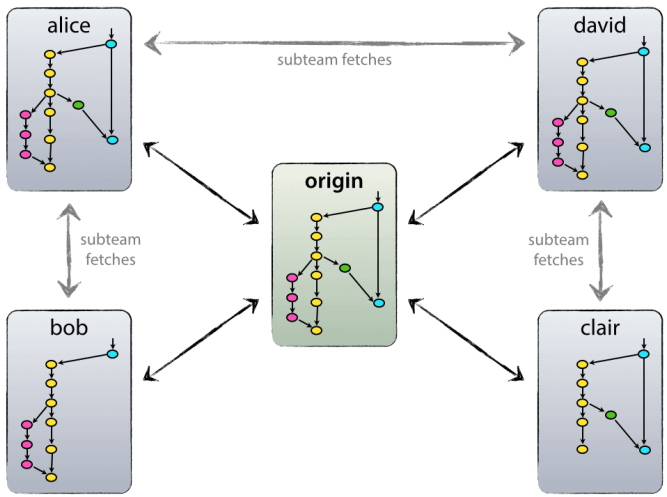

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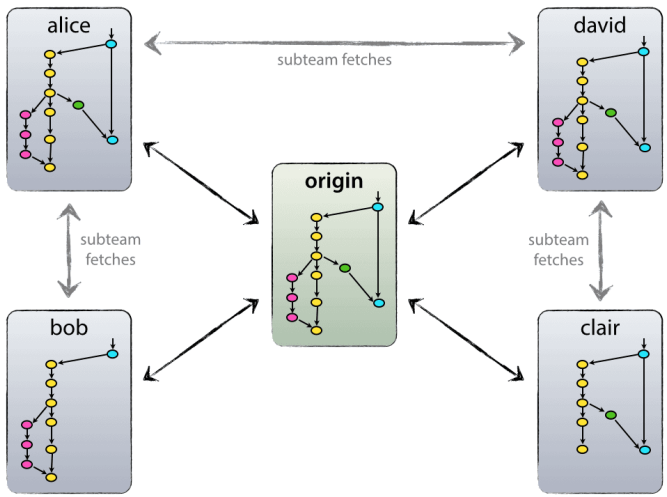

Most commonly used VCS is git

Keeping Code Organised

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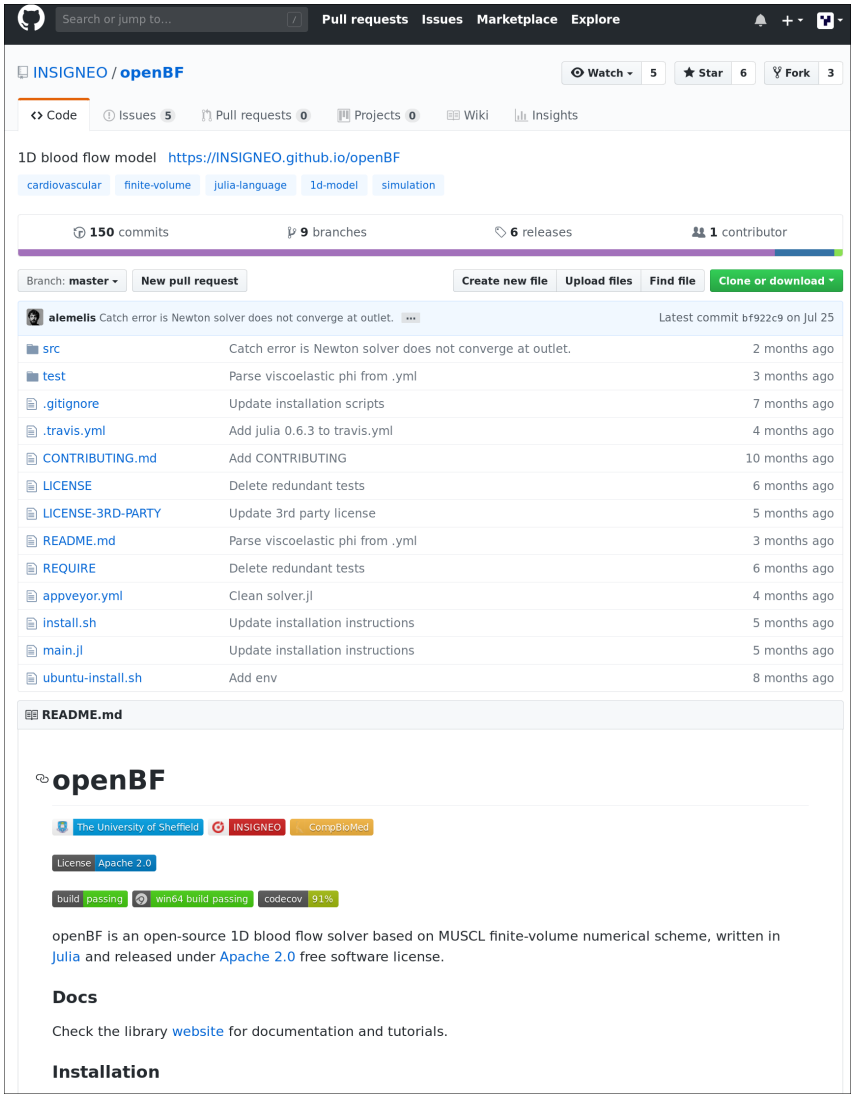
Github

- Store your git repositories online
- Public repos for open source software development
- Free private repos for education and research
- Impact and engagement tracking
- Community building tools:
  - Bug reporting/tracking
  - Documentation hosting
  - Project wikis



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Testing and Benchmarking

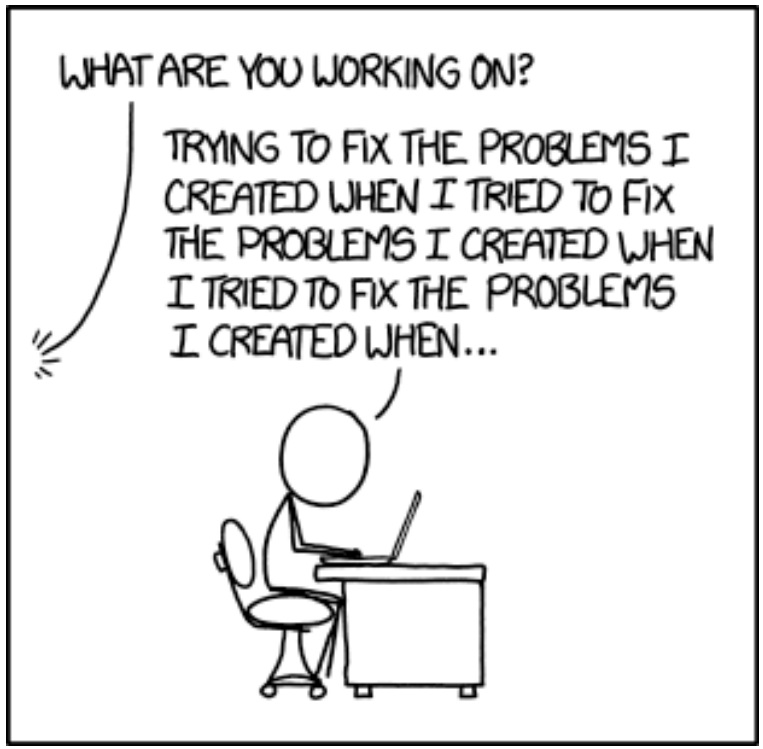

Image Source: Randall Munroe, XKCD (https://xkcd.com/1909/)

Testing and Benchmarking

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Testing early and often helps catch mistakes

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Ideally test at two different scales:

- Every function should have accompanying tests (unit tests):
  - Ensure functions give correct output for correct input
  - Graceful failures with invalid input
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Lots of tools to help automate this

Testing and Benchmarking

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Testing Frameworks

- Tools to automate running of tests
- Programmer writes test functions, provides expected output
- Framework runs all tests and provides report

```
phil@dva ~/philsniftycode $ pytest -v
==================================== test session starts ====================================
platform linux -- Python 3.6.6, pytest-3.6.3, py-1.5.4, pluggy-0.6.0 -- /usr/bin/python3.6
cachedir: .pytest_cache
rootdir: /home/phil/philsniftycode, inifile:
plugins: cov-2.5.1
collected 3 items

test_arrays.py::test_build_array PASSED                                              [ 33%]
test_arrays.py::test_copy_array PASSED                                               [ 66%]
test_arrays.py::test_multiply_array FAILED                                           [100%]

========================================= FAILURES ==========================================
_____________________________________ test_multiply_array _____________________________________

    def test_multiply_array():
>       raise ValueError("Wrong dimensions in array")
E       ValueError: Wrong dimensions in array

test_arrays.py:14: ValueError
========================== 1 failed, 2 passed in 0.03 seconds ===============================
phil@dva ~/philsniftycode $
```

Testing and Benchmarking

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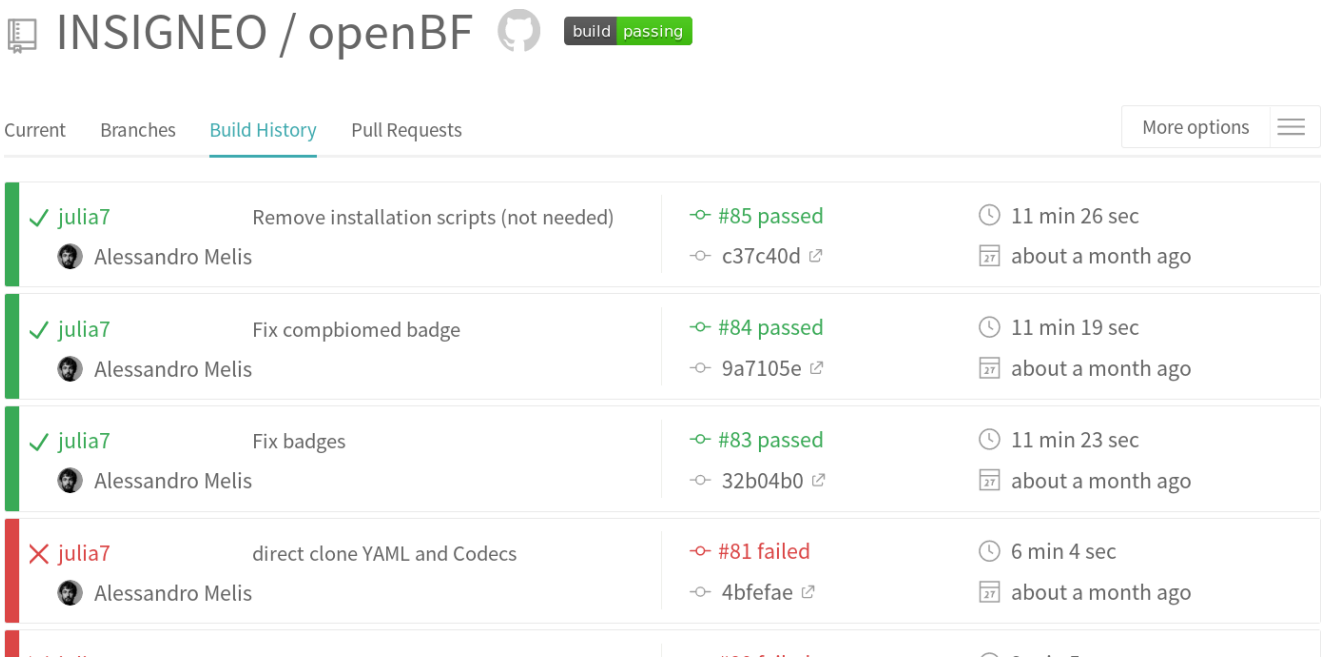
Continuous Integration

- Automatically build and test code after changes
- Test in different environments (linux/windows), compiler versions
- Free services for open source projects
- Immediate feedback on bugs/mistakes



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Documentation

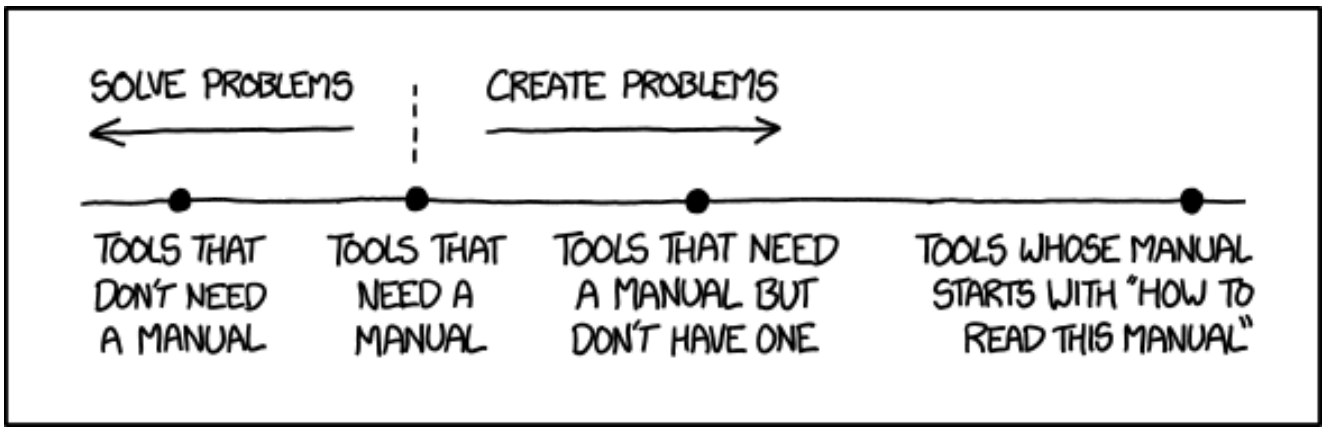

Image Source: Randall Munroe, XKCD (https://xkcd.com/1343/)

Documentation

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Getting Users Started

- Clear installation instructions
- Concise tutorial (with example data)
- Explanation of output
- Troubleshooting?

Documentation

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User Manual

- Document all features of the program
- Details of algorithms and maths used
- Advanced usage examples
- Test and benchmarking datasets
- Known issues, bugs?

Documentation

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API/Internal Documentation

- Application Programming Interface - functions for your users to call
- Document internal functions too
- Can be autogenerated from code and comments
- Crucial for future developers (you in 2 years?)

Documentation

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Documentation Generators

- Quickly create professional documentation pages or pdf
- Sphinx and Doxygen are most common
- Simple human readable format
- Build api docs from code and comments
- Use with continuous integration - build docs along with your code and host on github

Dissemination

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Citing

- Software now citable with DOI
- Publish on ORDA/Zenodo/Figshare

Licensing

- Publically available software should have a license
- Sustainable software should be open source
- University may have policy
- Research Councils may have requirements

Community Building

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Consumers or Collaborators?

- Sharing code exposes it to new users and use cases
- Bugs *will* be found, encourage reporting
- Open source allows users to engage with development
- More eyes on code means more issues found and fixed
- Contribution of new features
- Users help maintain code for you

Platforms like Github provide all this for minimal effort

Conclusion: producing good software is hard

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We all need to:

- Structure projects carefully
- Use version control to manage development
- Test everything!

- Lots of tools available to help
- Building a user community shares the burden
- Lots of help out there:
  - Software Sustainability Institute
  - University RSE groups
  - Software Carpentry courses
  - (Google!)

Software Sustainability Institute

Research Software Engineering Sheffield.

software carpentry

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Useful Resources

The University Of Sheffield.

- Best Practice Guidance
  - RSE@Sheffield https://rse.shef.ac.uk
  - SSI: https://software.ac.uk
  - Software Carpentry: https://software-carpentry.org
- Version Control
  - Github: https://github.com
  - Bitbucket: https://bitbucket.org
  - Git book: https://git-scm.com/book
- Continuous Integration
  - Travis: https://travis-ci.org
  - Appveyor: https://appveyor.com

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