

Software Sustainability

The why and the how

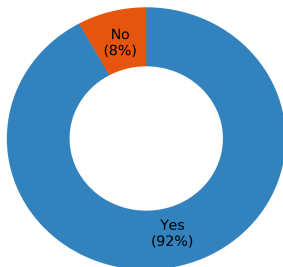
Phil Tooley
University of Sheffield

Cardiovascular Fluids Modelling SIG
20 September 2018

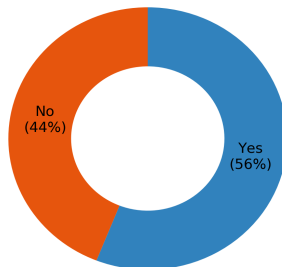
Science relies on research software

2014 UK Research Software Survey¹

Do you use research software?



Do you develop your own research software?



It must be *good* research software



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

Software Sustainability Institute²

- ▶ Funded in 2010 by EPSRC to promote sustainable development of research software and now a collaborative effort by multiple research councils
- ▶ Provide training and support for developers of scientific software
- ▶ Focus on reproducible research and recognising software as a research output
- ▶ “Better software, better research”



²www.software.ac.uk

My first research code experience



My first research code experience

 `README.txt`

```
1 Dear Phil,  
2  
3 This is a copy of the code WAKE, which is written by Mora and Antonsen.  
4 There is also a photon-kinetic version of it, QWAKE. If anyone can read  
5 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?

The code I actually used

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>

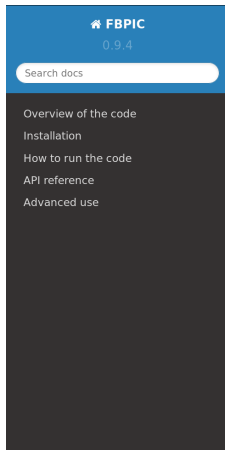
Support: [Join slack](#)

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.

The code I actually used



FBPIC documentation

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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:

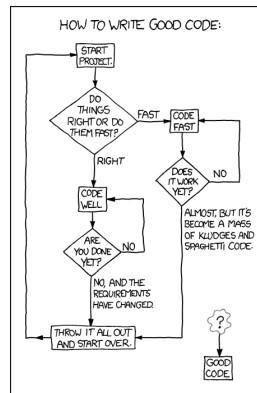
- Moving window
- Calculation of **space-charge fields** at the beginning of the simulation
- Intrinsic **mitigation of Numerical Cherenkov Radiation** (NCR) from relativistic bunches
- **Field ionization** module (ADK model)
- Support for **boosted-frame simulations** (see [Running boosted-frame simulations](#))

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

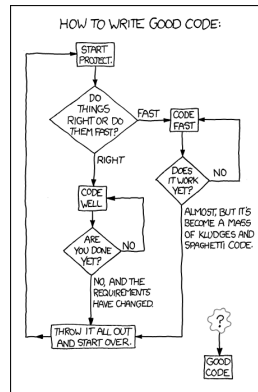
Symptoms of unsustainable software or development practices include:

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



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

“**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

Well structured code is:

- ▶ Easy to understand
 - ▷ Consistent code style
 - ▷ Names should explain what things do
 - ▷ Use more, simpler, statements
 - ▷ Comments explain design decisions

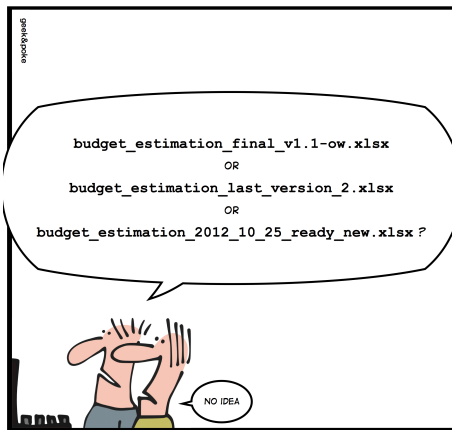
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 - ▷ Don't hardcode variables, use a configuration file
- ▶ Necessary
 - ▷ Use existing libraries where you can
 - ▷ Don't invent your own data formats

Keeping Code Organised



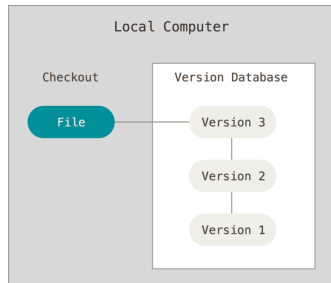
Have you ever

- ▶ Had files with names like “awesomocode_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

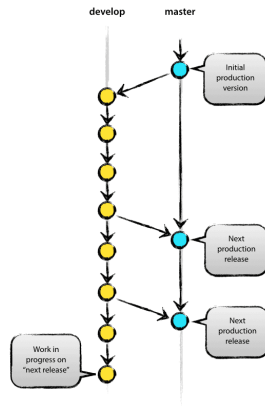
Version Control Systems (VCS)

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



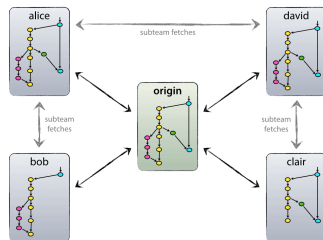
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- ▶ Try things out without consequences



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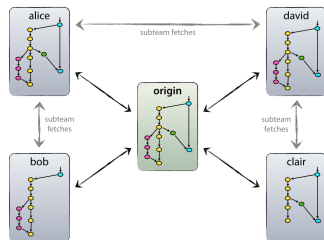
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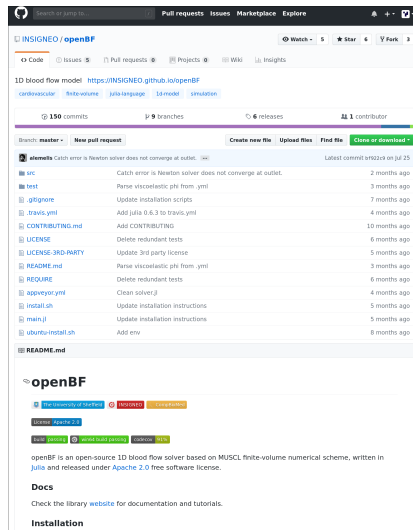
Most commonly used VCS is git

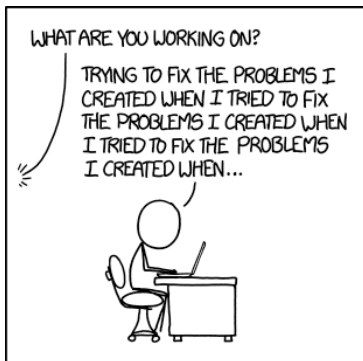


Keeping Code Organised

Github

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





Testing and Benchmarking



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
 - ▷ These should be run every time the code is changed

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Lots of tools to help automate this

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 $
```

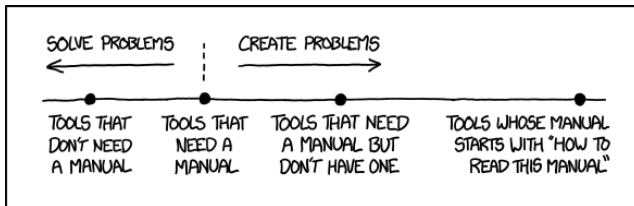
Continuous Integration

- ▶ 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

INSIGNEO / openBF  build: passing

Current Branches Build History Pull Requests More options

 julia7	Remove installation scripts (not needed)	 #85 passed	 11 min 26 sec
 Alessandro Melis		 c37c40d 	 about a month ago
 julia7	Fix compbiomed badge	 #84 passed	 11 min 19 sec
 Alessandro Melis		 9a7105e 	 about a month ago
 julia7	Fix badges	 #83 passed	 11 min 23 sec
 Alessandro Melis		 32b04b0 	 about a month ago
 julia7	direct clone YAML and Codecs	 #81 failed	 6 min 4 sec
 Alessandro Melis		 4bfefae 	 about a month ago



Getting Users Started

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

User Manual

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

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 5 years?)

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

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



We all need to:

- ▶ Structure projects carefully
 - ▶ Keep code safe with version control
 - ▶ Backup to Github etc.
 - ▶ Test everything!
-
- ▶ Lots of tools available to help
 - ▶ Building a user community shares the burden
 - ▶ Lots of help out there:
 - ▷ Software Sustainability Institute
 - ▷ Research Software Engineers
 - ▷ Software Carpentry
 - ▷ (Google!)



- ▶ **Software Sustainability**
 - ▷ 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>