EPSRC and MRC Systems Approaches to Biomedical Science CDT

Introduction to Software Engineering Concepts

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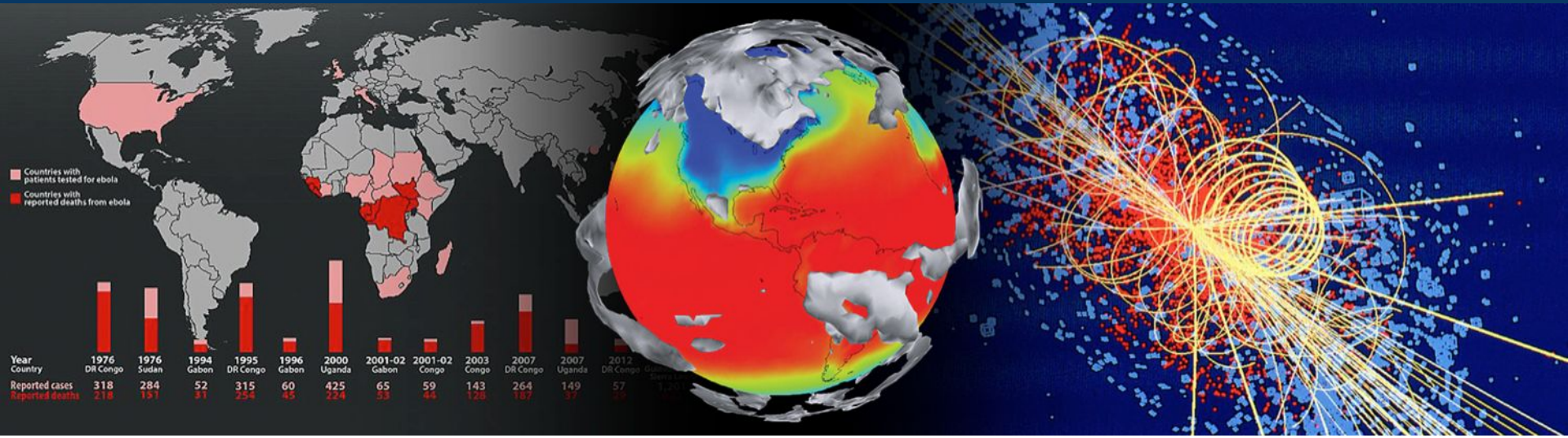
Modern research is impossible without software

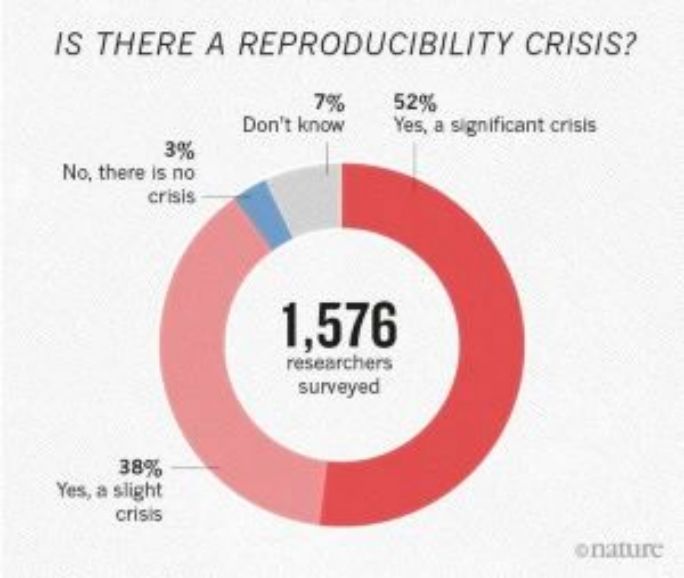


From thrown-together scripts, through an abundance of complex spreadsheets, to the millions of lines of code behind large-scale infrastructure, there are few areas where software does not play a fundamental part in research

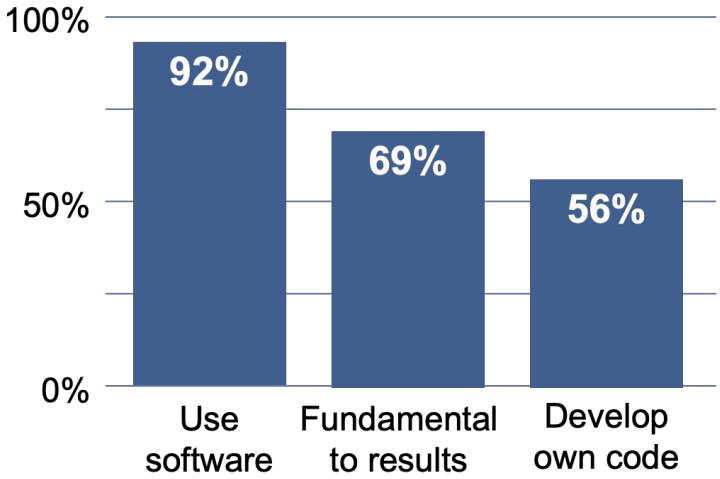
Why should we care about software?

"1,500 scientists lift the lid on reproducibility", Nature 2016[2]
Nature survey - 1,576 respondents

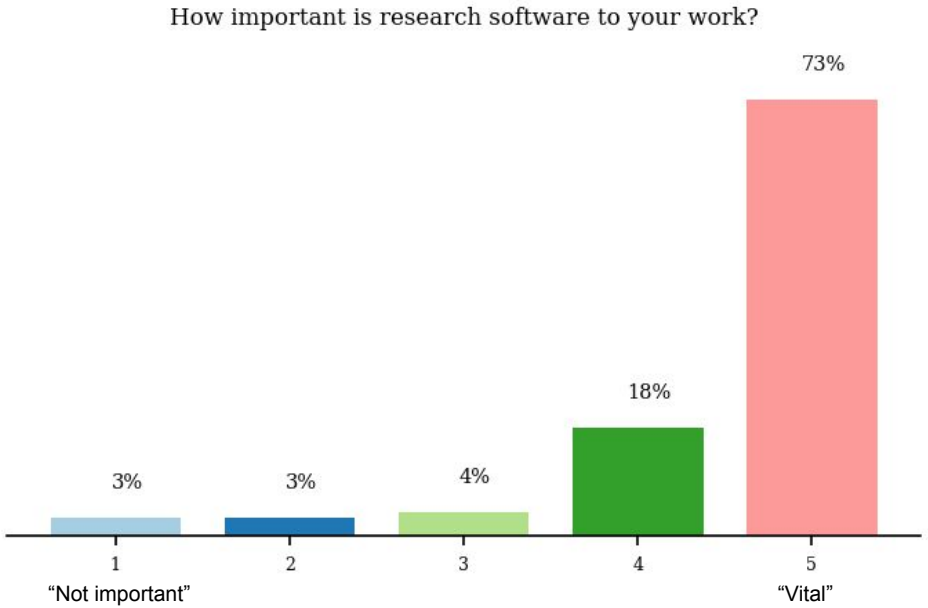
52%: a significant crisis of reproducibility
31%: think that failure to reproduce means wrong result



Why should we care about software?

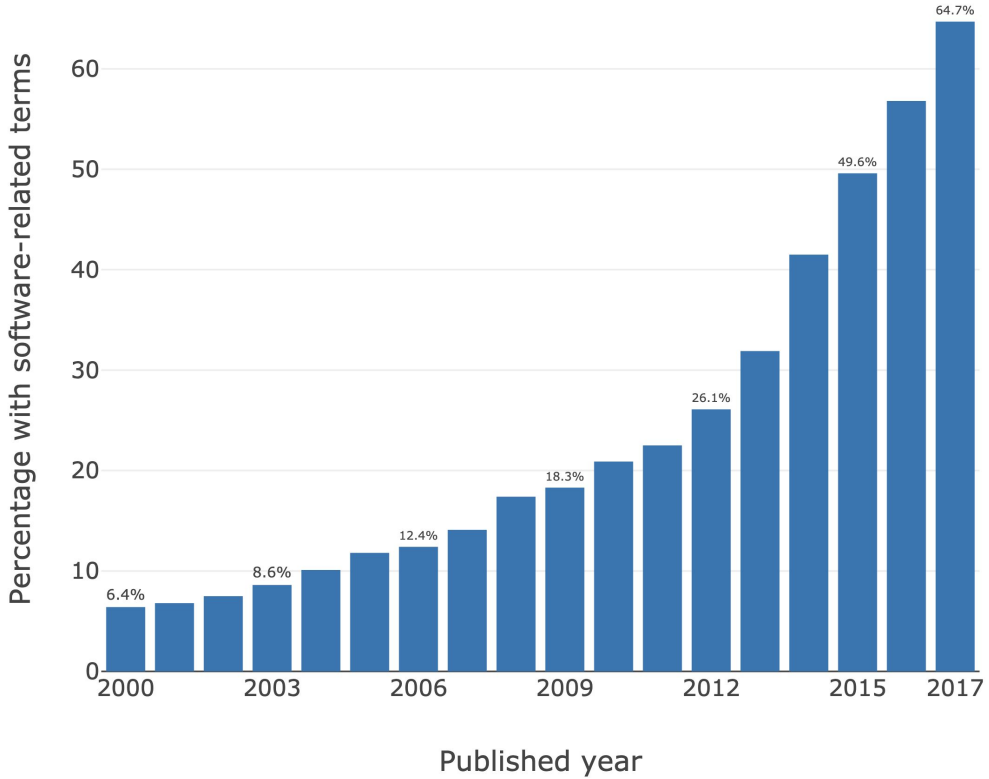


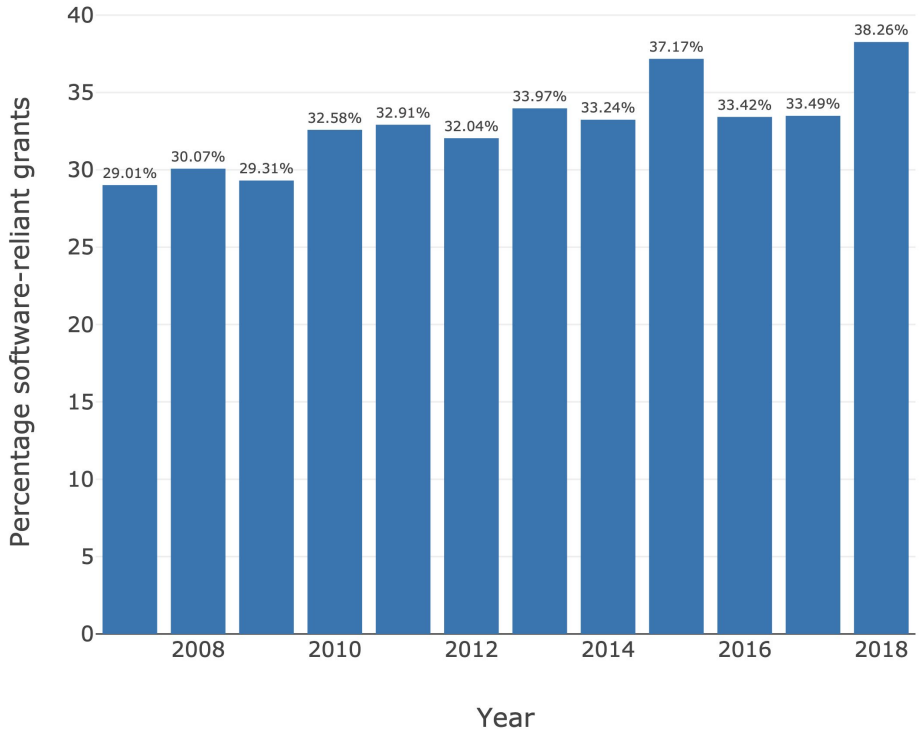
SSI survey of researchers, 2014[1], 417 respondents
15 Russell Group Universities
Their software use and background



- Institutional perspective
- University of Southampton software study, 2019

Why should we care about software?

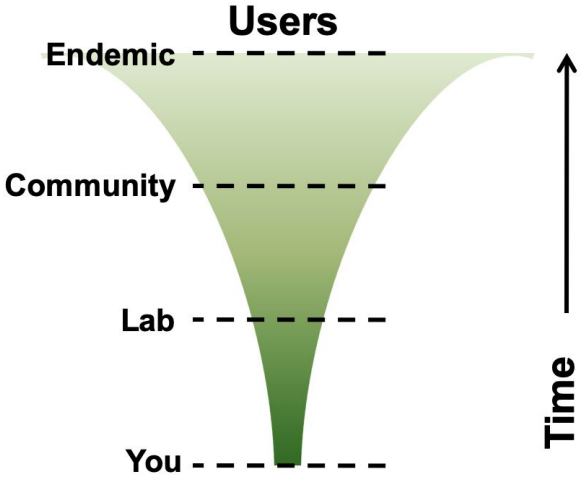




[3]

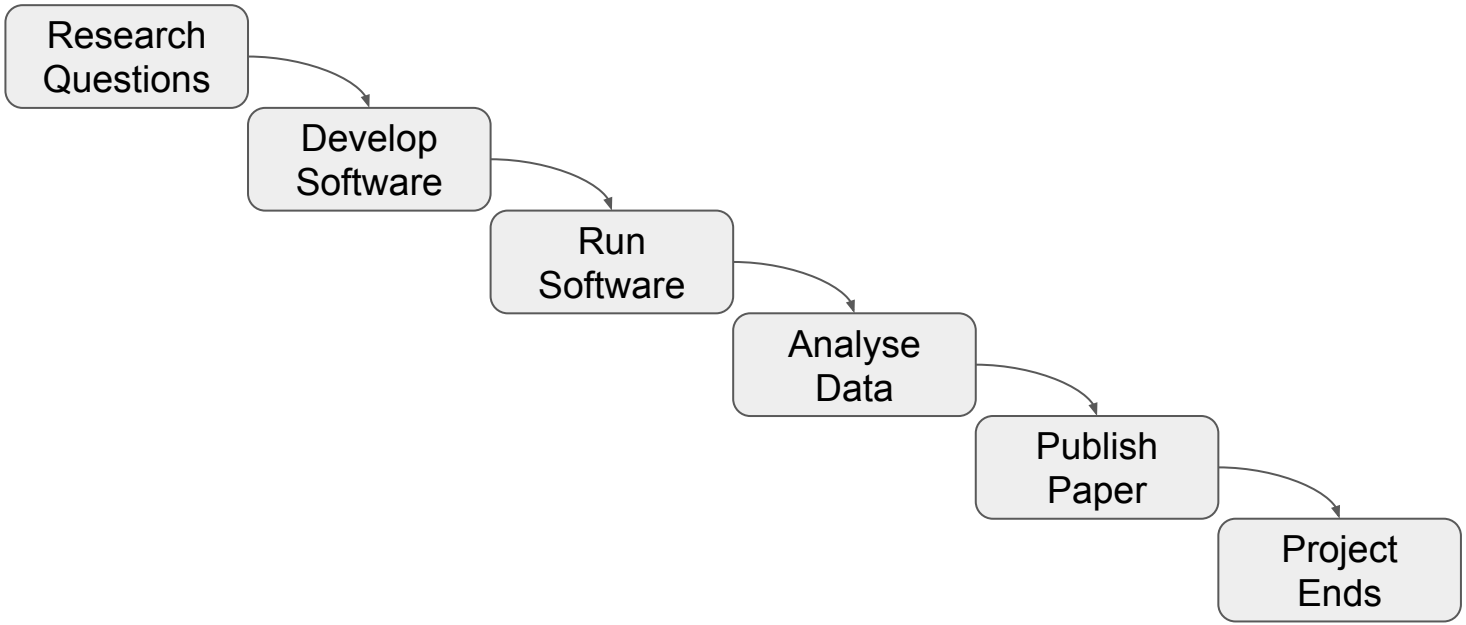
The software you write is important!

- Software inherently contains *value*
  - Produces results, contains lessons learnt, effort
- Difficult to gauge to what extent it might be used in the future
  - By who?
  - Which parts?
  - Which projects?
  - Reproducibility – from publications!

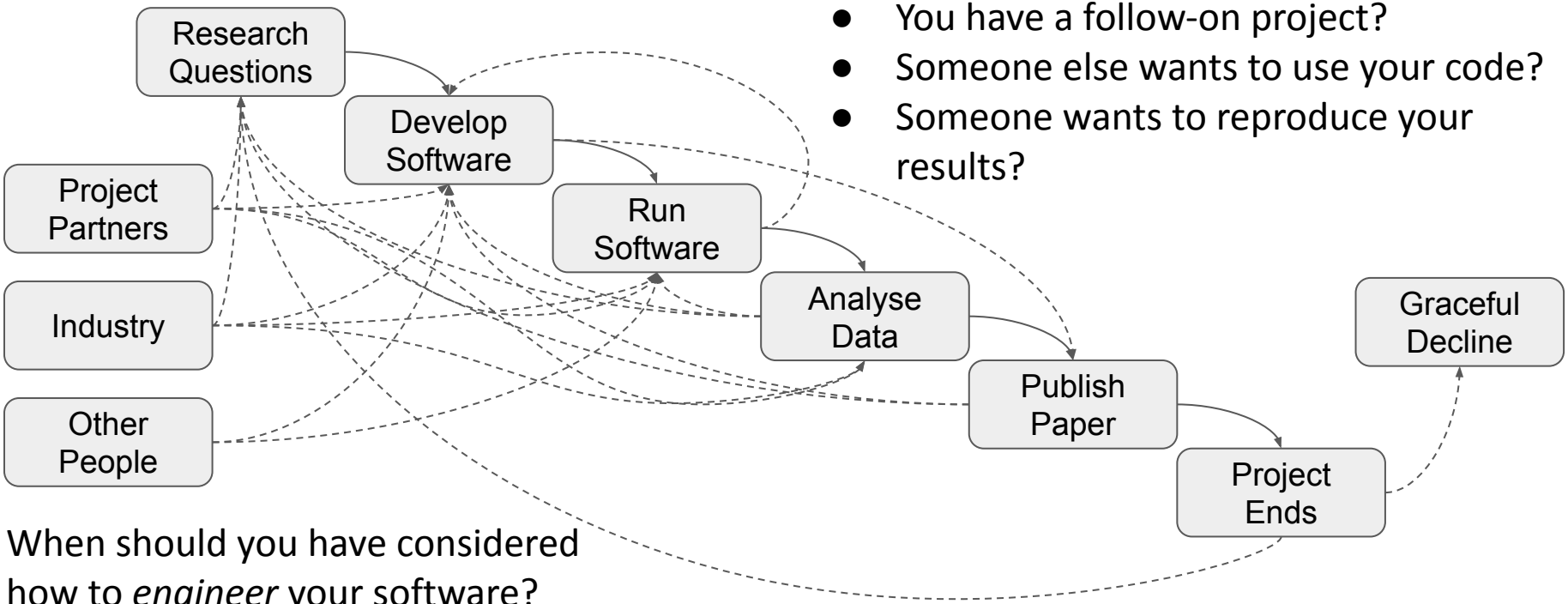


Can it/should it be reusable by others?
...including yourself?

A typical research software lifecycle



In reality...



What happens when…

- You have a follow-on project?
- Someone else wants to use your code?
- Someone wants to reproduce your results?

When should you have considered how to *engineer* your software?

When?

"The best time to plant a tree is 20 years ago.

The second best time is now."

What could go wrong?

- Ariane 5
- $7B d… …nt
  $500 million rocke…
- Used A…

EXCEPTION HANDLER DISABLED

BOOM.

…g…dance
…altitude info

→

64-bit FP converted to 16-bit signed integer

Programming vs Engineering

Programming / Coding

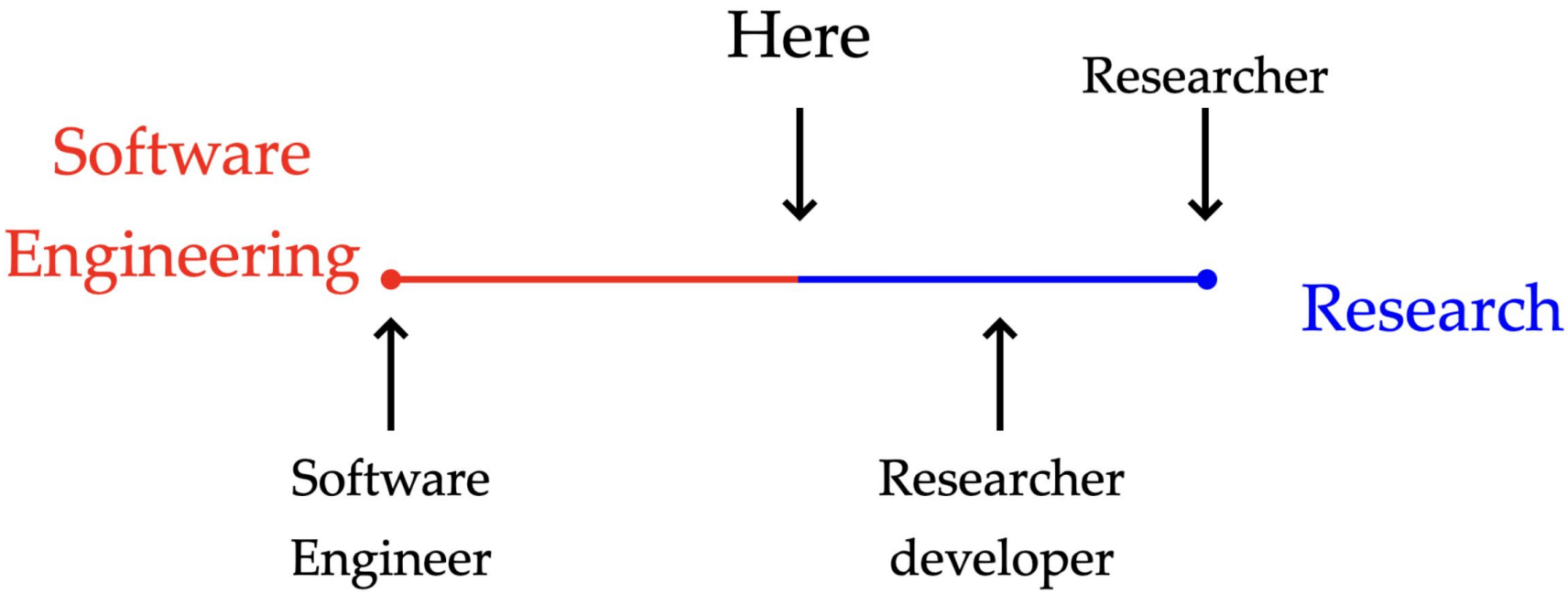
- Focus is on one aspect of software development
- Writes software for themselves
- Mostly an individual activity
- Writes software to fulfil research goals (ideally from a design)

Engineering

- Considers the *lifecycle* of software
- Writes software for *stakeholders*
- Takes *team ethic* into account
- Applies a *process* to understanding, designing, building, releasing, and maintaining software

"Programmers tend to start coding right away. Sometimes this works."
- Eric Larsen, 2018

Where are you?



Beyond building a 'sequence of instructions'

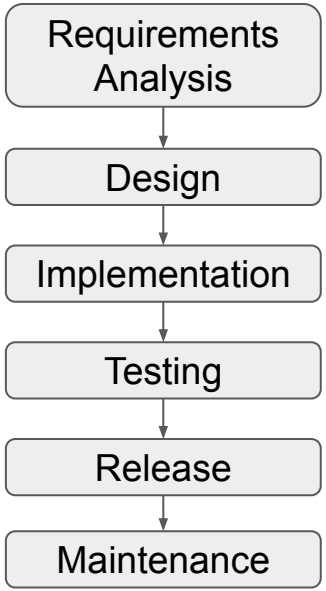
Software is far more than that…

- **Outcome of a *development process***

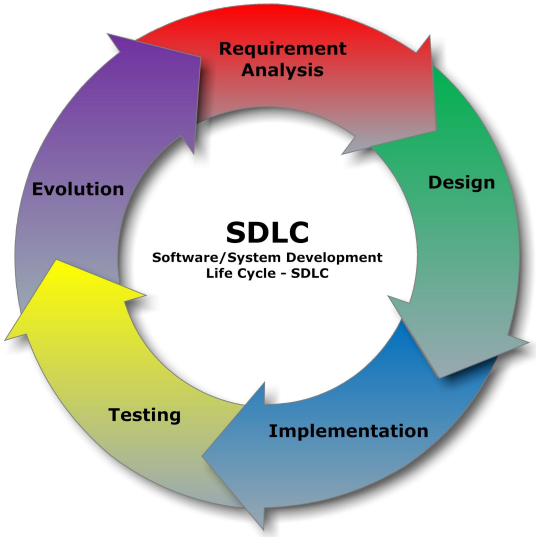
But also...

- Architecture
- Implementation of algorithms
- Data model
- Documentation
- *Best practices* and *conventions ...*

Waterfall Model



Agile Model

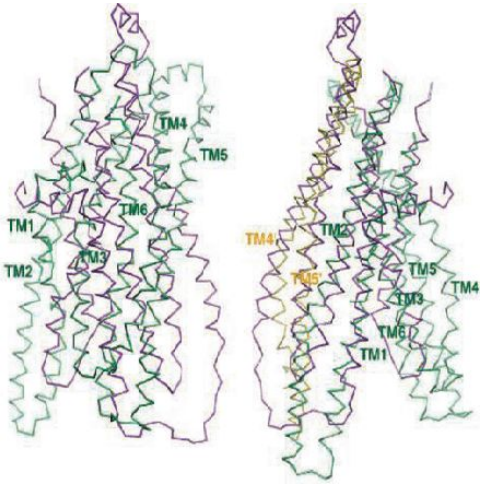


Testing

- Humans are fallible! Our software will contain defects
  - In requirements, design, as well as code
  - 1-10-150 hours to fix in design/development/production

- Validation: are we building the right product?
- Verification: are we building the product right?
  - Manual testing, unit testing, automated testing, code reviews

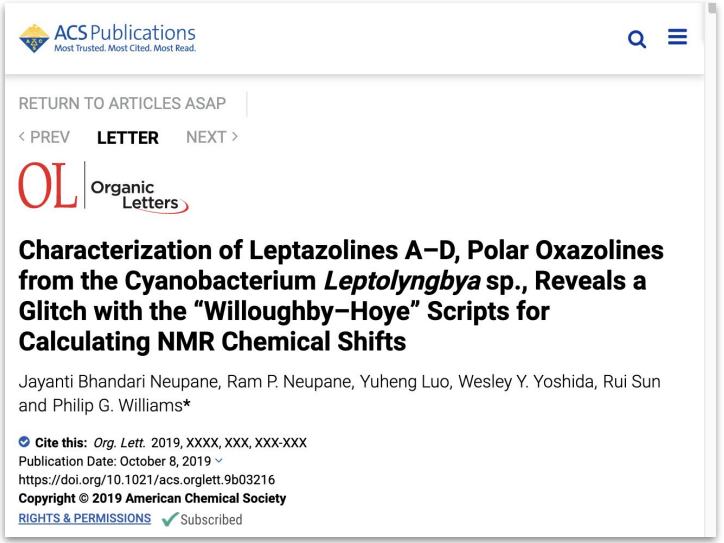
- Highly-cited papers published on multidrug resistance transporters between 2001 - 2010
- Results couldn't be reproduced - 5 retractions
- Caused by error in an *internal software utility*
  - Flipped two columns of data, inverting electron-density map used to derive protein structure



"I didn't question it then. Obviously now I check it all the time."
- Geoffrey Chang[4]

Platform support?

… Density functional theory nuclear magnetic resonance calculations established the relative configurations of 1 and 2 and revealed that **the calculated shifts depended on the operating system when using the "Willoughby–Hoye" Python scripts to streamline the processing of the output files, a previously unrecognized flaw that could lead to incorrect conclusions**.

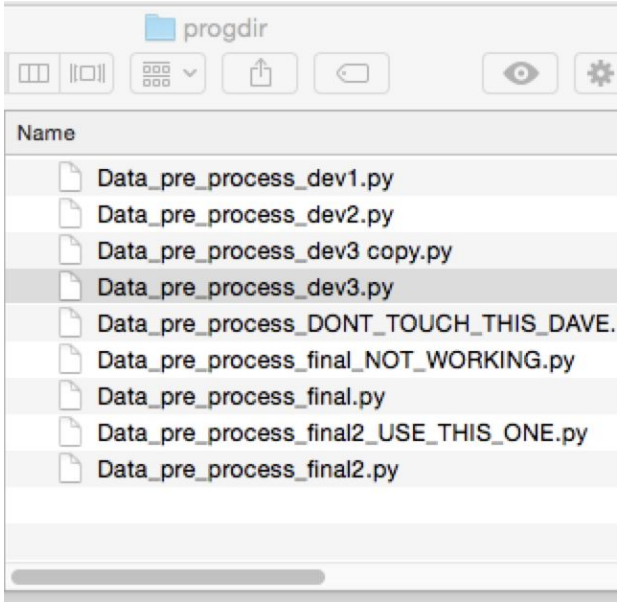


- Due to *different sorting of file names* on different operating systems

Organic Letters, October 8 2019
https://doi.org/10.1021/acs.orglett.9b03216

Code management & collaboration

- *Version control* provides a full history of your project's software and other assets
- Makes for easy:
  - Backups
  - Collaboration
  - Recovering from dead-ends
- What should be in version control?
  - Code, documentation, tests, test data, analysis scripts
  - Reports, papers, etc.
- Packaging and deployment



"If you're not using version control, whatever else you might be doing with a computer, it's not science."

- Greg Wilson, SWC

Other key points

- These skills will **save you time**
- Always assume others will use and develop your software
- Be clear on requirements and assume they will change
- Funders are increasingly expecting software outputs to be sustainable and reusable

More on software engineering

Robert L Glass, Addison-Wesley Professional

Group mini-project

For week 2, in same groups as those for Zoom...
Design and implement Python library to specify & solve a Pharmacokinetic model, which should ideally have the following functionality:

- pip installable
- github repository, with issues + PRs that fully document development process
- unit testing with good test coverage
- fully documented, e.g. README, API documentation, OS license
- continuous integration for automated testing/doc generation
- Ability to specify form of the PK model
- Users can specify protocol independently from the model
- Ability to solve for drug quantity in each compartment over time
- Ability to visualise the solution of a model, compare two different solutions
- Something else? Feel free to suggest alternative features!

Group projects

SABS students

- Theme 1: Computational & Data-Driven Structural Approaches to Drug Discovery
  - Drug Discovery Game [Roche]
- Theme 2: Cellular Microscopy and Image Analysis Underpinning Biomedical Discovery
  - Computer Vision-based Clinical Imaging Quality Control [GE Healthcare]
- Theme 3: Physiological Modelling Underpinning Biomedical Discovery
  - Epidemiological modelling [Roche]

For DTP/NERC students - a Python GUI application

- Tree Modelling with L-Systems
- Calculations for Planetary Reference Models

General daily teaching structure - Monday

09:30-10:00 Introduction / Q&A	***Main room***
10:00-12:30 Self-learning session 1	***Pre-assigned rooms***
12:30-13:30 Lunch	***Advisory (instructors' may be unavailable)***
13:30-14:30 Software engineering projects presentation	
14:00-14:30 Q&A session	***Main room***
14:30-17:00 Self-learning session 2	***Pre-assigned rooms***
17:00 Finish	***Advisory (can keep working if you like)***

Each room will have 'roving' demonstrators, Take breaks as you need!

General daily teaching structure - rest of week

09:30-10:00 Welcome and Q&A	***Main room***
10:00-12:30 Self-learning session 1	***Pre-assigned rooms***
12:30-13:30 Lunch	***Advisory (instructors' may be unavailable)***
13:30-14:00 Q&A session	***Main room***
14:00-17:00 Self-learning session 2	***Pre-assigned rooms***
17:00 Finish	***Advisory (can keep working if you like)***

Each room will have 'roving' demonstrators, Take breaks as you need!

A few infrastructure things...

- Ensure you have your full name set in the *Participants* list
  - *Participants* -> hover over your entry, select *More* then *Rename*
- Please mute when not talking
- Need help?
  - In first instance, ask demonstrators for help by raising hand in Zoom room
    - Particularly if there are a lot of people asking questions - demonstrators can answer them in order
    - Or if quiet, just ask them (or your Zoom buddies!)
  - If demonstrator not in room, ask on Slack
- Move Zoom rooms (i.e. to Common Room) at break times if you like
- Be sure to tick off the exercises you complete in Canvas as you go!

A few last things!

- Please bear with us!
- Remember to tick off exercises in Canvas!
- Please fill in the after-course survey!
- Enjoy yourselves!

- Virtual machine: https://bit.ly/SABSVM22

Say hi to your neighbours!

References

[1] "It's impossible to conduct research without software, say 7 out of 10 UK researchers”, http://www.software.ac.uk/blog/2014-12-04-its-impossible-conduct-research-without-software-say-7-out-10-uk-researchers

[2] "1,500 scientists lift the lid on reproducibility", Nature, 533, pp. 424-454, 2016. DOI: https://doi.org/10.1038/533452a

[3]"An investigation of the funding invested into software-reliant research", https://github.com/softwaresaved/software_in_grants_GTR

[4] "Retractions unsettle structural bio", https://www.the-scientist.com/daily-news/retractions-unsettle-structural-bio-46891