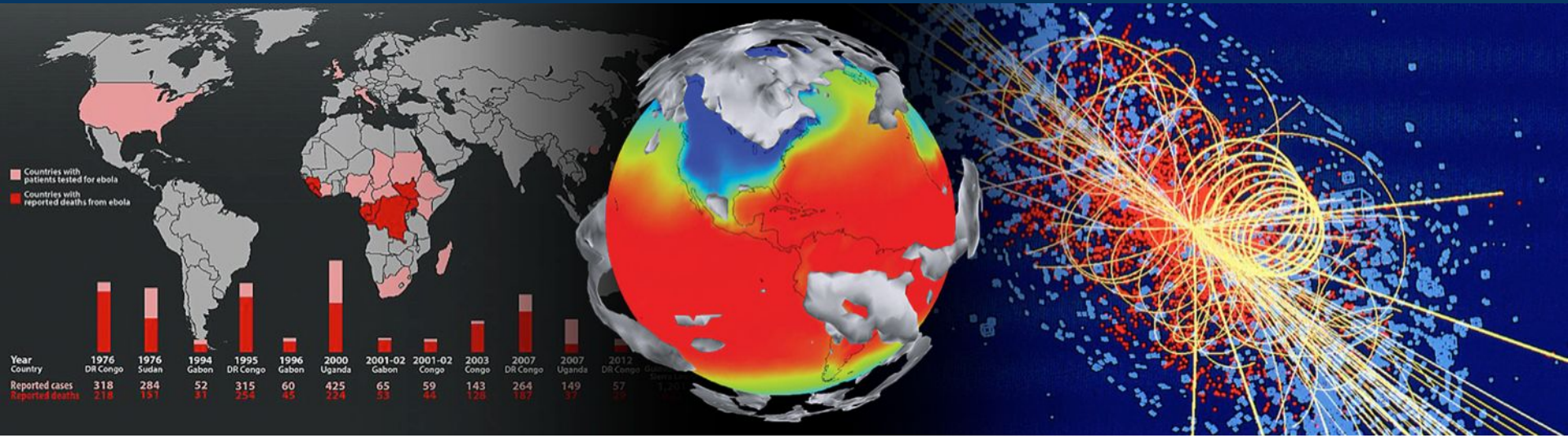
EPSRC and MRC Systems Approaches to Biomedical Science CDT

Introduction to Software Engineering Concepts

Steve Crouch
Software Sustainability Institute
s.crouch@software.ac.uk

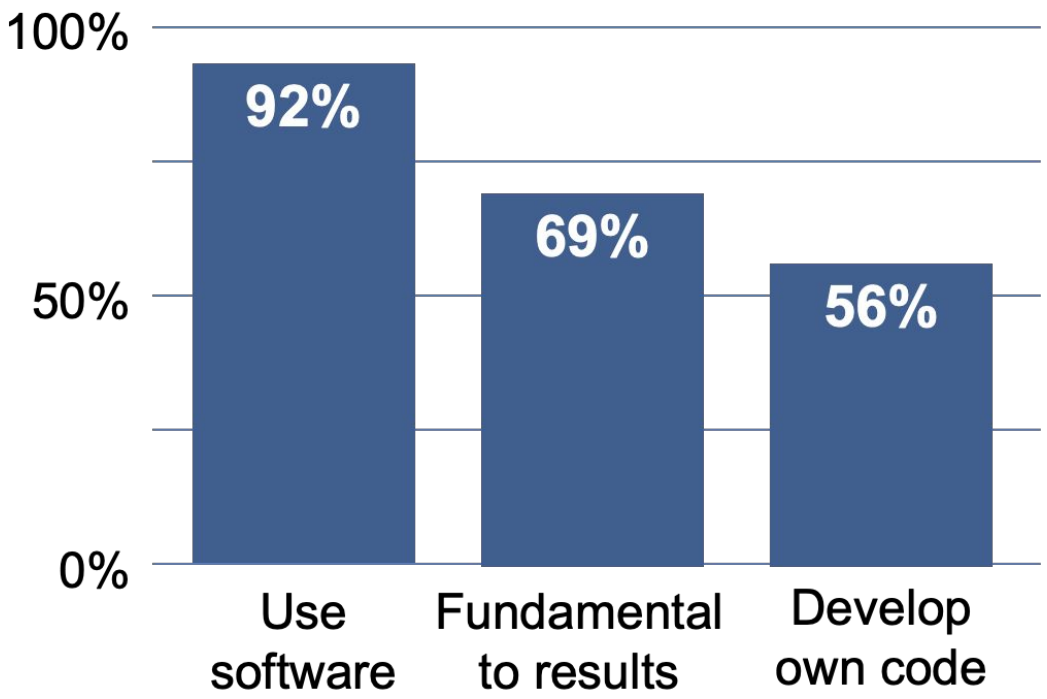
14th October 2019

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?



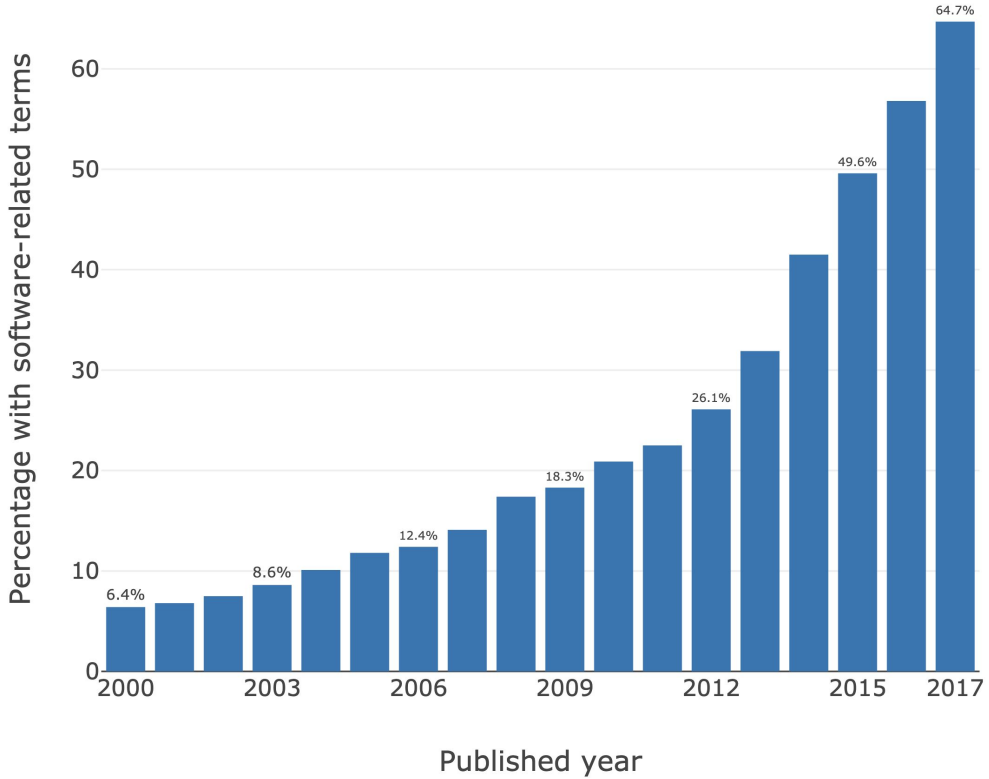
SSI survey of researchers, 2014

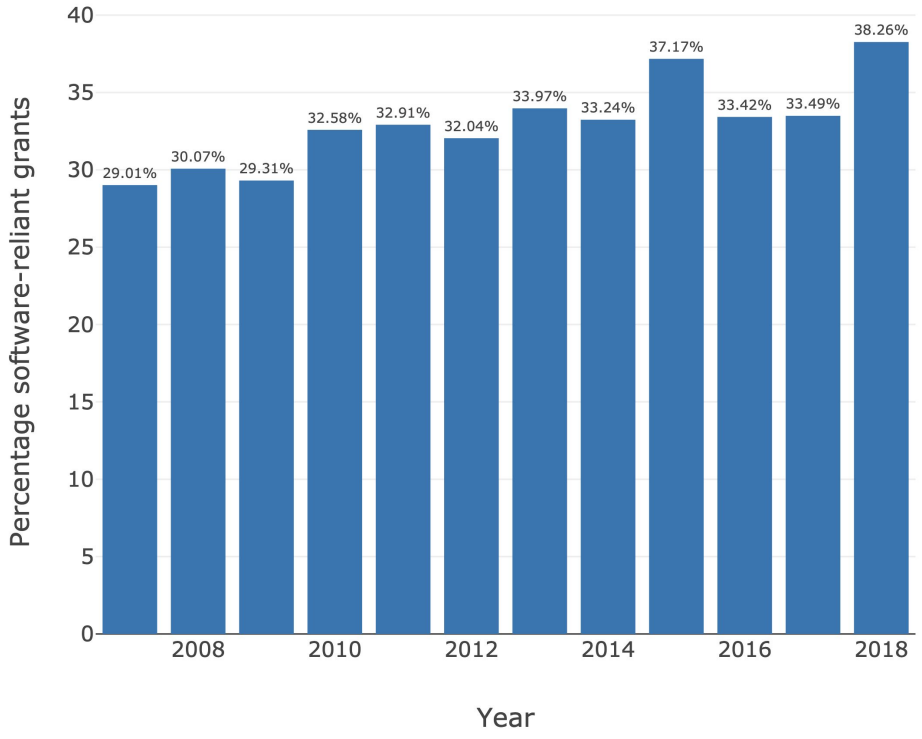
15 Russell Group Universities

Their software use and background

417 respondents

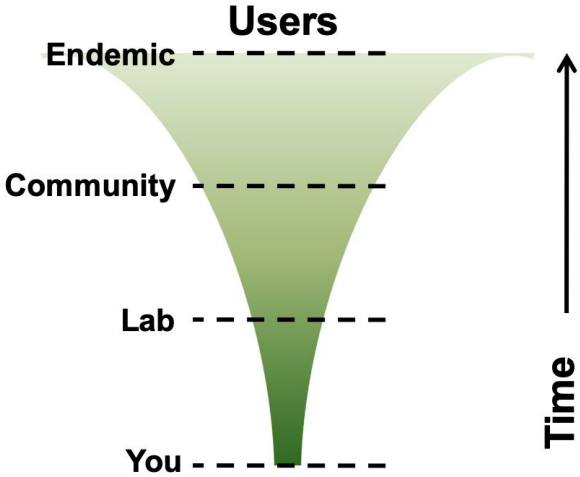
Why should we care about software?





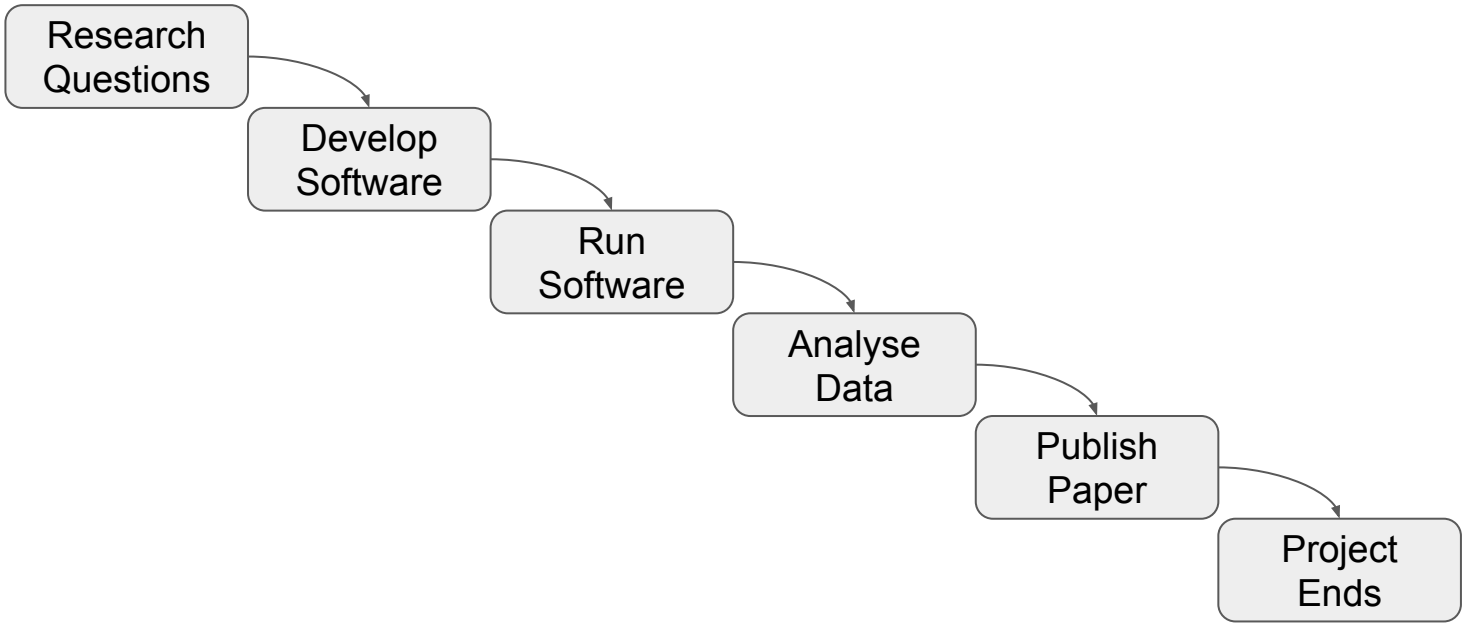
The software you write is important!

- 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!

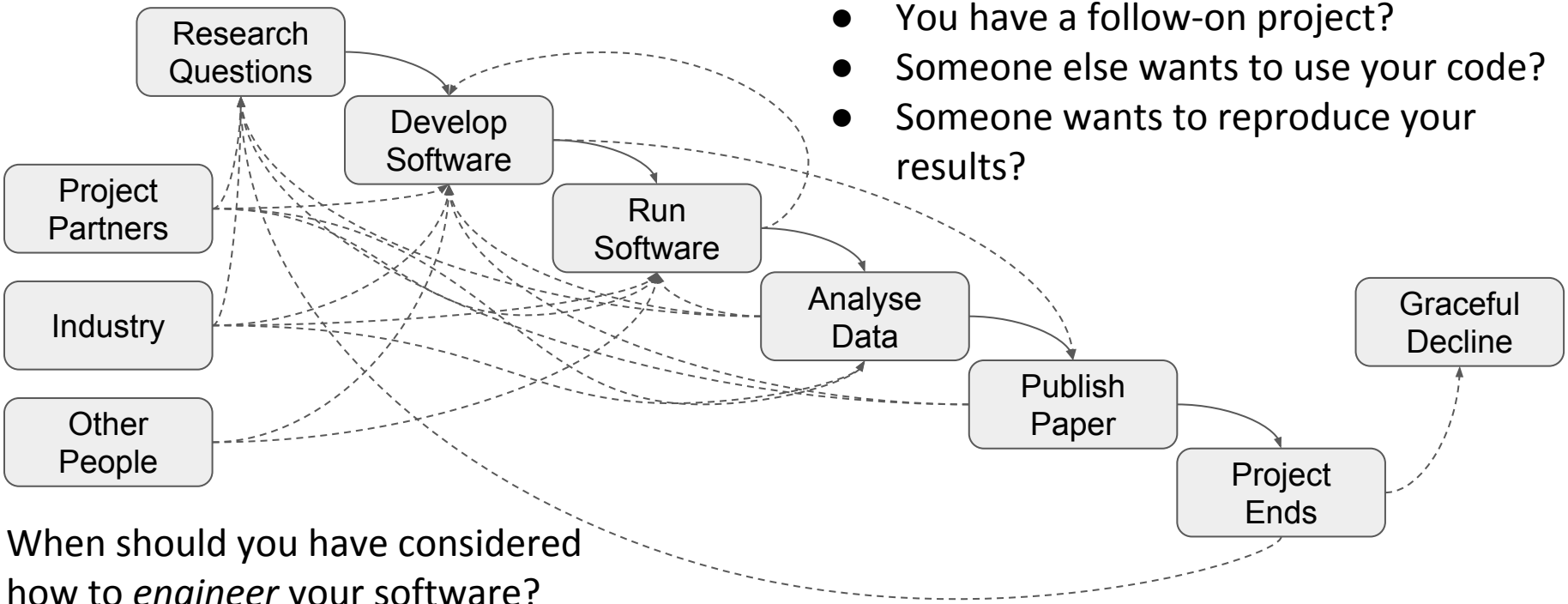


Can it/should it be reusable by others?
...including yourself?

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?

What could go wrong?

- Ariane 5
- $7B
  $500
- Used Ari

EXCEPTION HANDLER DISABLED

BOOM!

de info → **64-bit FP converted to 16-bit signed integer**

Programming vs Engineering

Programming / Coding

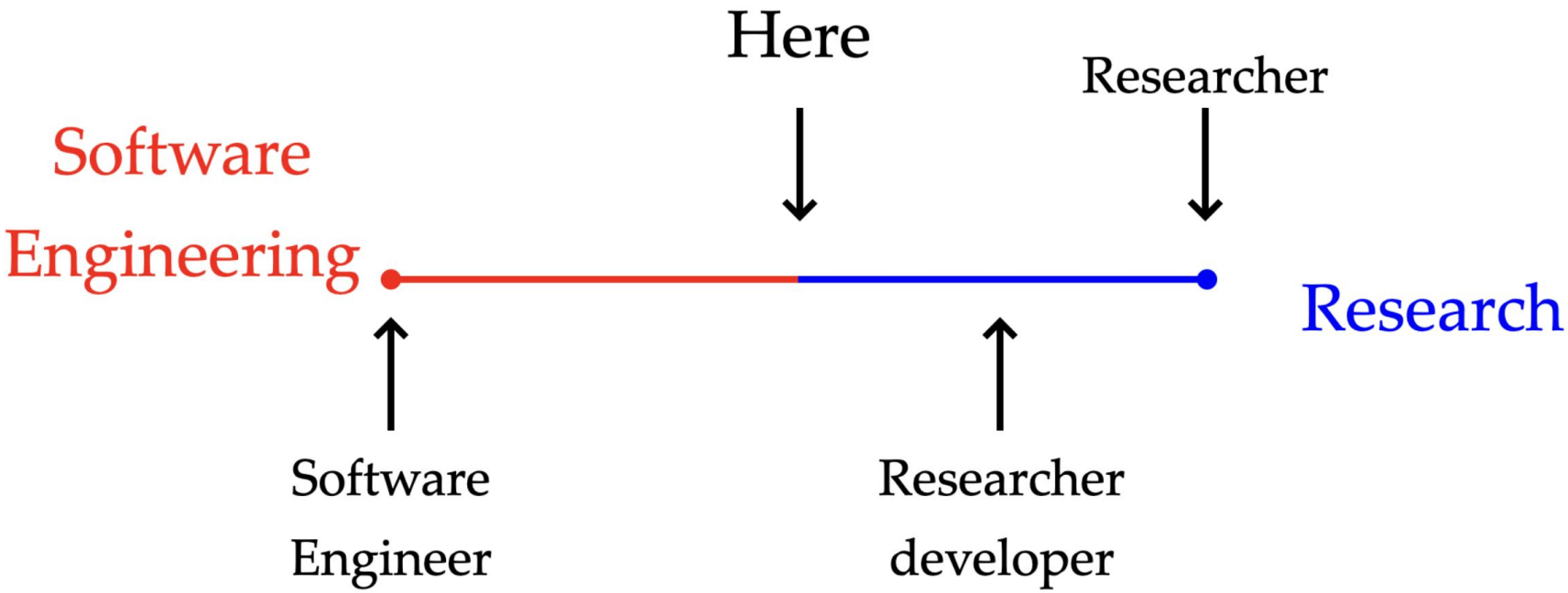
- Focus is on one aspect of software development
- Writes software for themselves
- Mostly an individual activity
- Writes software to fulfil research goals (ideally from a design)

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'

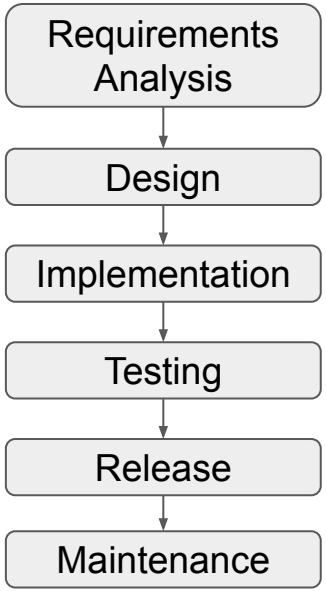
Software is far more than that…

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

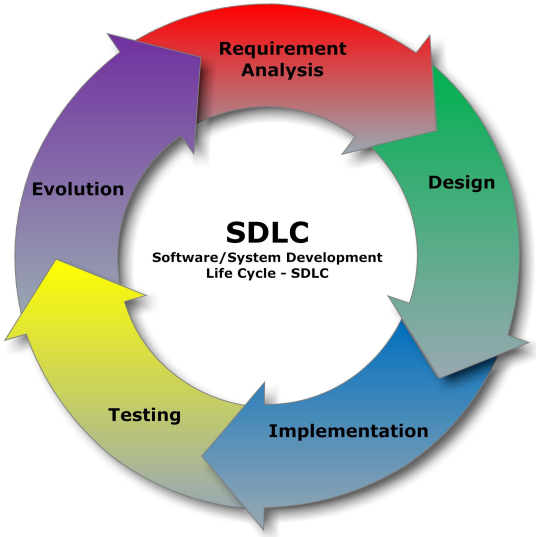
But also...

- Architecture
- Implementation of algorithms
- Data model
- Programming paradigm
- Documentation
- ...

Waterfall Model



Agile Model

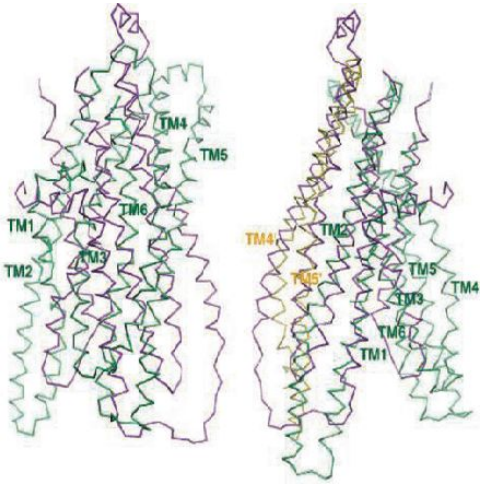


Testing

- Humans are fallible! Our software will contain defects
  - In requirements, design, as well as code

- 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

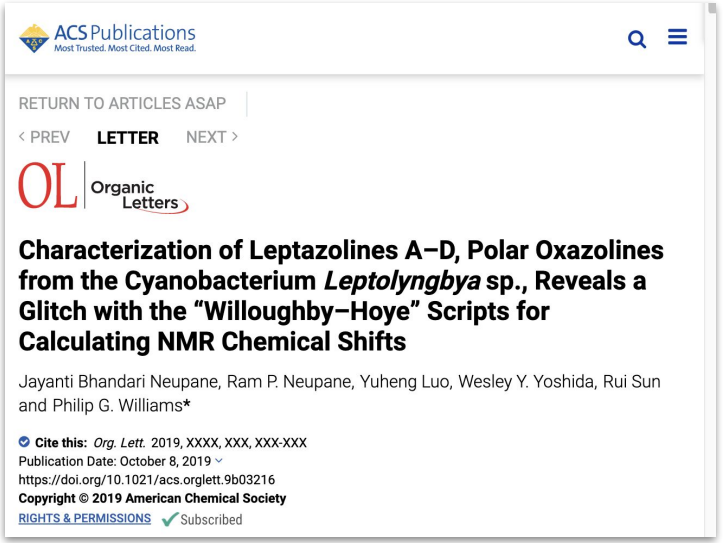


"I didn't question it then. Obviously now I check it all the time."
- Geoffrey Chang[2]

… STOP PRESS …

… 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**.

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



ACS Publications
Most Trusted. Most Cited. Most Read.

RETURN TO ARTICLES ASAP

‹ PREV **LETTER** NEXT ›

OL | Organic Letters

Characterization of Leptazolines A–D, Polar Oxazolines from the Cyanobacterium *Leptolyngbya* sp., Reveals a Glitch with the "Willoughby–Hoye" Scripts for Calculating NMR Chemical Shifts

Jayanti Bhandari Neupane, Ram P. Neupane, Yuheng Luo, Wesley Y. Yoshida, Rui Sun and Philip G. Williams*

Cite this: *Org. Lett.* 2019, XXXX, XXX, XXX-XXX
Publication Date: October 8, 2019
https://doi.org/10.1021/acs.orglett.9b03216
Copyright © 2019 American Chemical Society
RIGHTS & PERMISSIONS ✓Subscribed

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

Optimisation

*"Three orders of magnitude in **machine speed** and three orders of magnitude in **algorithmic speed** add up to six orders of magnitude in solving power. A model that might have taken a year to solve 10 years ago can now solve in less than 30 seconds."*

– Robert Bixby, review of linear programming solvers from 1987-2002

- Faster code, faster results!
- Understanding trade-offs
  - Maintainability, accuracy
- When & where to optimise?
  - 80/20 rule, code profiling

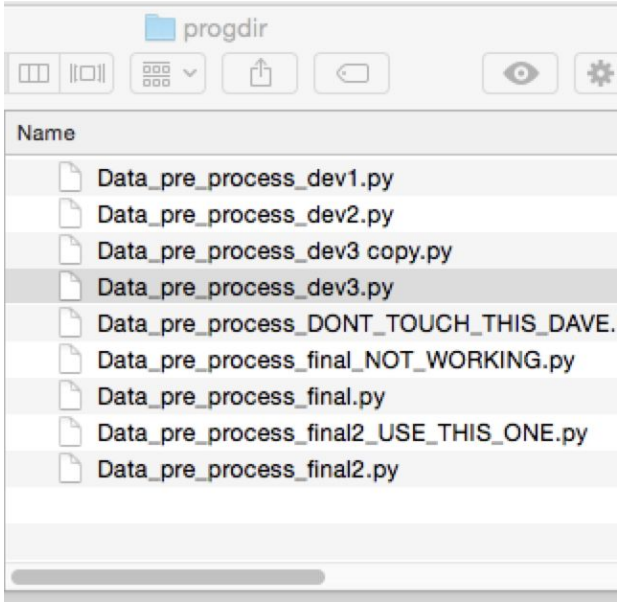
Amdahl's Law:

Time to result = Develop Time (D) + Time to Run (R)

As effort is put into reducing R, overall time required to get new result is dominated by writing, testing, maintaining, installing, configuring software.

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

Group projects

1. Mathematical model to quantify pharmacokinetics & pharmacodynamics [Roche]
    - Existing PK-PD solutions difficult to use - a user-friendly interface is required
    - Design and develop fast ODE solving and robust parameter estimation/inference
    - To promote PK-PD modelling to wider pharma community and its wider application

2. MRI brain segmentation for elderly neurodegenerative disease [GE Healthcare]
    - Need for accurate and robust MRI segmentation tool for problematic brain regions
    - Generalisable methodology to perform well with variance in MRI acquisition parameters
    - Should be available/usable by broad community & comparable in accuracy and computation time to commonly available methods

3. Expansion/improvement of Fragalysis for early stage drug discovery [Diamond]
    - Addition of new Fragalysis algorithms and their integration into HPC/cloud infrastructure
    - Python API needed to allow users to access underlying algorithms in open source fashion
    - Documentation, tutorials, and improved UI design required

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