



Summary

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Better Scientific Software tutorial @ ISC 2022

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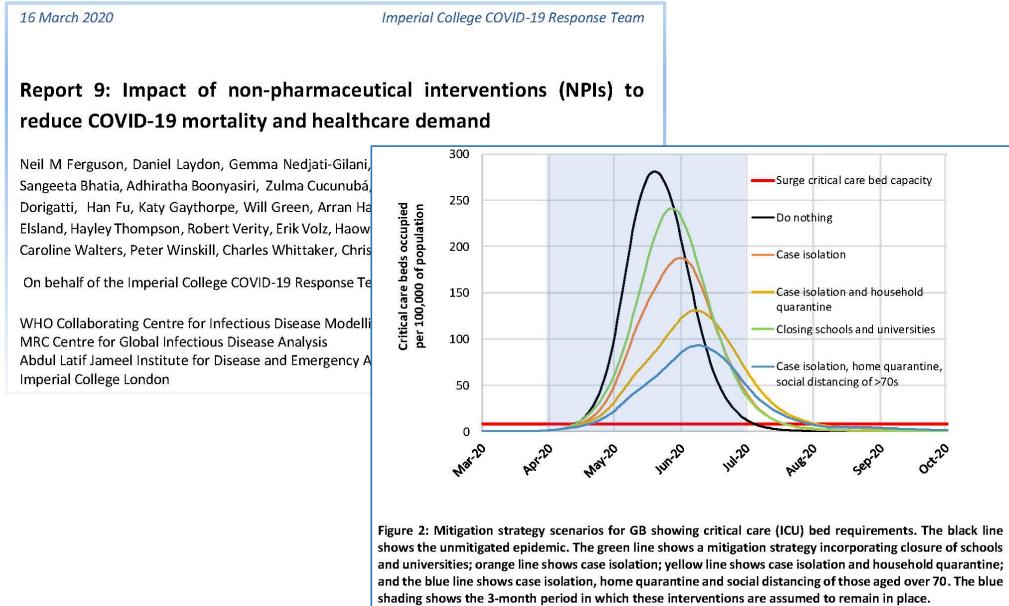
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- **The requested citation the overall tutorial is: Anshu Dubey and Gregory R. Watson, Better Scientific Software Tutorial, in ISC High Performance, 2022, Hamburg Germany. DOI: 10.6084/m9.figshare.19781752**
- Individual modules may be cited as *Speaker, Module Title*, in Better Scientific Software tutorial, ISC, 2022 ...

Acknowledgements

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Software Under the Microscope

- Mar. 16 2020: Neil Ferguson (Imperial College) briefed UK Parliament on epidemiological modeling of COVID-19 pandemic
 - Epidemiological models like this helped prompt government action, but have lots of assumptions
- April 1 2020: Nicholas Lewis (independent climate science researcher in UK) can't easily see where some of the assumptions come from
 - publishes a blog article
 - “Moreover, the computer code... is old, unverified, and documented inadequately, if at all...”



Imperial College UK COVID-19 numbers don't seem to add up

Introduction and summary

A study published two weeks ago by the COVID-19 Response Team from Imperial College (“Ferguson20”) appears to be largely responsible for driving UK government policy actions. The study is not peer reviewed; indeed, it seems not to have been externally reviewed at all. Moreover, the computer code used to produce the estimates in the study – which on Ferguson’s own admission is old, unverified and documented inadequately, if at all – has still not been published. That, in my view, shows a worrying approach to a matter of vital public concern.

<https://doi.org/10.25561/77482>
<https://www.nicholaslewis.org/imperial-college-uk-covid-19-numbers-dont-seem-to-add-up/>
<https://www.nature.com/articles/d41586-020-01003-6>



The Press Picks Up the Story

Headline and quotes from the Fox News article

"In our commercial reality, we would fire anyone for developing code like this and any business that relied on it to produce software for sale would likely go bust," David Richards, co-founder of British data technology company WANDisco, told the Daily Telegraph.

"Models must be capable of passing the basic scientific test of producing the same results given the same initial set of parameters...otherwise, there is simply no way of knowing whether they will be reliable," said Michael Bonsall, Professor of Mathematical Biology at Oxford University.

CORONAVIRUS · Published May 16

Imperial College model Britain used to justify lockdown a 'buggy mess', 'totally unreliable', experts claim

Scientists from the University of Edinburgh have further claimed that it is impossible to reproduce the same results from the same data using the model. The team got different results when they used different machines, and even different results from the same machines.

"There appears to be a bug in either the creation or re-use of the network file. If we attempt two completely identical runs, only varying in that the second should use the network file produced by the first, the results are quite different," the Edinburgh researchers wrote on the Github file. A fix was provided, but it was the first of many bugs found within the program.

<https://www.foxnews.com/world/imperial-college-britain-coronavirus-lockdown-buggy-mess-unreliable>
<https://www.telegraph.co.uk/technology/2020/05/16/coding-led-lockdown-totally-unreliable-buggy-mess-say-experts/>



What you May Not Have Heard

- April 22 2020: Imperial collaborates with Microsoft to refactor and clean up the code, which is released on GitHub
- May 10 2020: Phil Bull rebuts criticisms of the Imperial code
 - Which spurs further discussions within some groups focused on scientific software
- May 29 2020: CODECHECK independently reproduces results of Imperial's Report 9

<https://github.com/mrc-ide/covid-sim/>
[https://philbull.wordpress.com/2020/05/10/why-you-can-ignore-reviews-of-scientific-code-by-commercial-software-developers/amp/](https://philbull.wordpress.com/2020/05/10/why-you-can-ignore-reviews-of-scientific-code-by-commercial-software-developers/)
<http://doi.org/10.5281/zenodo.3865491>

tl;dr: Many scientists write code that is crappy stylistically, but which is nevertheless scientifically correct (following rigorous checking/validation of outputs etc). Professional commercial software developers are well-qualified to review code style, but most don't have a clue about checking scientific validity or what counts as good scientific practice. Criticisms of the Imperial Covid-Sim model from some of the latter are overstated at best.

CODECHECK certificate 2020-010
<https://doi.org/10.5281/zenodo.3865491>



Item	Value
Title	Report 9: Impact of non-pharmaceutical interventions (NPIs) to reduce COVID-19 mortality and healthcare demand. March 16, 2020.
Authors Reference	Neil Ferguson, COVID-19 Response Team Imperial College Preprint https://doi.org/10.25561/77482



Some Observations

- Your code is likely to live longer than you expect, and may be used in ways you don't expect by people you don't know – plan for it!
- Increasingly, consequential decisions are made based on computational results
 - The codes generating those results may (justifiably) be subject to greater scrutiny
- The scientific credibility of software is strongly connected to good software engineering practices
 - Documentation
 - Testing, verification, and (where possible) validation
 - Code readability and quality metrics

Question: Should we excuse scientific software for being “crappy stylistically”?

Hint: crappy code can hide bugs



Science through computing is,
at best,
as credible as the software that produces it!

Today, We Covered Many Topics...

- Project management
- Collaboration around software development
- Designing software for flexibility and extensibility
- Testing strategies for complex software systems
- Systematic refactoring of large, complex software systems
- Reproducibility

And there are Many More We Didn't Have Time For

- Documentation
- Licensing
- Continuous integration testing
- Packaging and distribution
- Issue tracking
- Configuration and build
- Debugging strategies
- Building and sustaining communities around software
- Software publication and citation
- Requirements gathering
- Understanding and debugging floating-point math
- Performance and performance portability
- ...
- **Also important topics, but...**
- Less distinction between research software and other software
- More informational resources available
- Next-level concerns for starting researchers
- There's only so much time in the day!

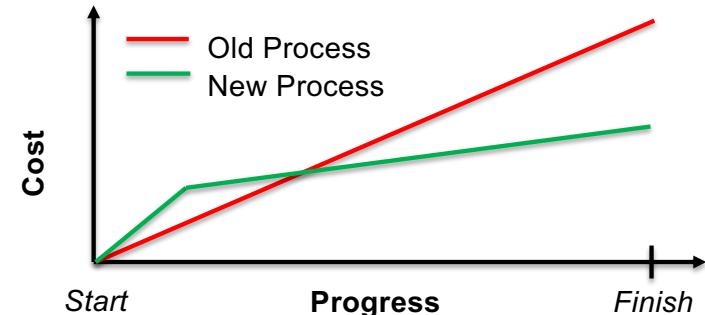


But you're a researcher.
You can't afford to spend
“all” of your time on
software engineering.

A Final Recommendation: Continual, Incremental Software Process Improvement

Target: your project should include “just enough” software engineering so that you can meet your short-term and longer-term scientific goals effectively

1. Identify your team’s “pain points” in your software development processes
 - Help: RateYourProject assessment tool:
<https://rateyourproject.org/>
2. Set a goal for something to improve
 - Target processes and behaviors, not just tasks
 - Pick something that you can address in a few months that will give you a noticeable benefit
3. Agree on a plan to address it, identify markers of progress and what is “done”
 - Write them down
 - Help: Progress tracking card examples:
<https://bssw-psip.github.io/ptc-catalog/catalog>
4. Work your plan, track your progress
5. When you are done, celebrate...
11 ...then pick a new pain point to address



The new process costs something to implement, but it pays off over time

Productivity and Sustainability Improvement Planning
<https://bssw.io/psip>



A goal of [BSSw.io](https://bssw.io) is to provide resources for improving your software processes. If you find useful resources that aren't on BSSw.io, consider contributing. Its easy and quick.

IDEAS
productivity

ECP
EXASCALE
COMPUTING
PROJECT

Thanks, and Keep in Touch!

- Email comments and questions to bssw-tutorial@lists.mcs.anl.gov
- We'll provide feedback on pull requests in the hands-on repository
- See the tutorial web site for an archive of all the materials from this tutorial
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 - RSS feed: <https://bssw.io/items.rss>

