

Best Practices for Scientific Computing

Sunniva Indrehus

A lavterskel talk

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UiO : **University of Oslo**

► Credit

- The software engineer team of the Community Terrestrial Systems Model (CTSM)-group at the National Center for Atmospheric Research (NCAR) for discussions and [ideas](#)
- The [Nordic-RSE](#) (Research Software Engineer) community
- Consultants and engineers in Cognite and BearingPoint

Outline

Good scientific software

Best practices for scientific computing

How to get "good" scientific software?

Conclusion

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What is good scientific software?

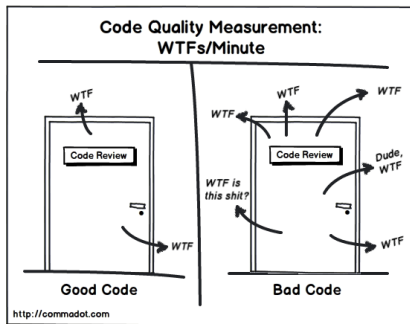
[1], [2], [3], [4], [5]

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- [1] Greg Wilson et al. “Best practices for scientific computing”. In: PLoS Biol 12.1 (2014), e1001745
 - [2] Ask HN: Why aren't more programmers in academia? <https://news.ycombinator.com/item?id=19475588>. Retrieved 09:01, April 21, 2021.
 - [3] Programming In Academia Vs Industry. <https://medium.com/@rdaszy/programming-in-academia-vs-industry-5fb52852ea39>. Retrieved 09:04, April 21, 2021.
 - [4] On the quality of academic software. <https://lemire.me/blog/2012/06/18/on-the-quality-of-academic-software/>. Retrieved 09:07, April 21, 2021.
 - [5] THE LOW QUALITY OF SCIENTIFIC CODE. <https://techblog.bozho.net/the-astonishingly-low-quality-of-scientific-code/>. Retrieved 09:27, April 21, 2021.

Good scientific software

► My answer

- Something that works
- Standardized
- Understandable
- Reproducible [6]
- Maintainable [**]



[6] Neural Information Processing Systems: The Machine Learning Reproducibility Checklist. <https://www.cs.mcgill.ca/~jpineau/ReproducibilityChecklist.pdf>. Retrieved 08:57, April 21, 2021.

[**] Common estimate: spending 20% of the developing time for maintenance work

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Best practices for scientific computing

► My point of view

Learning from success stories [8], [9]:

- Version control
- Workflow optimization
- Documentation
- Containerization
- (Modern) editor

[8] Greg Wilson et al. “Best practices for scientific computing”. In: PLoS Biol 12.1 (2014), e1001745

[9] Big Tech. https://en.wikipedia.org/wiki/Big_Tech. Retrieved 16:03, April 20, 2021.

Best practices for scientific computing

► My point of view

- Version control
- Workflow optimization
- Documentation
- Containerization
- (Modern) editor



Best practices for scientific computing

► My point of view

- Version control
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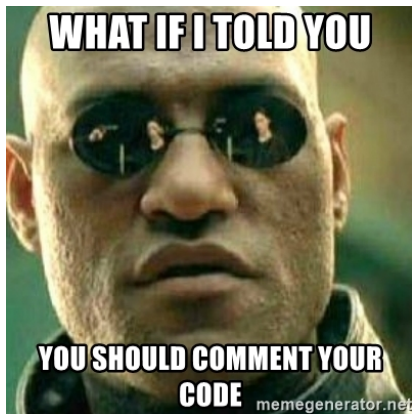
Credit: <https://www.i-programmer.info/programming/theory/1332-goto-spaghetti-and-velociraptor.html>

What happens when using spaghetti code

Best practices for scientific computing

► My point of view

- Version control
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Best practices for scientific computing

► My point of view

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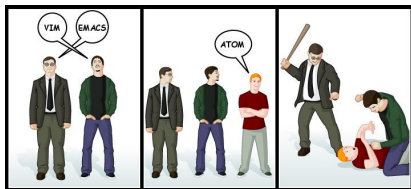


Credit: <https://www.pinterest.co.uk/pin/536209899356890025/>

Best practices for scientific computing

► My point of view

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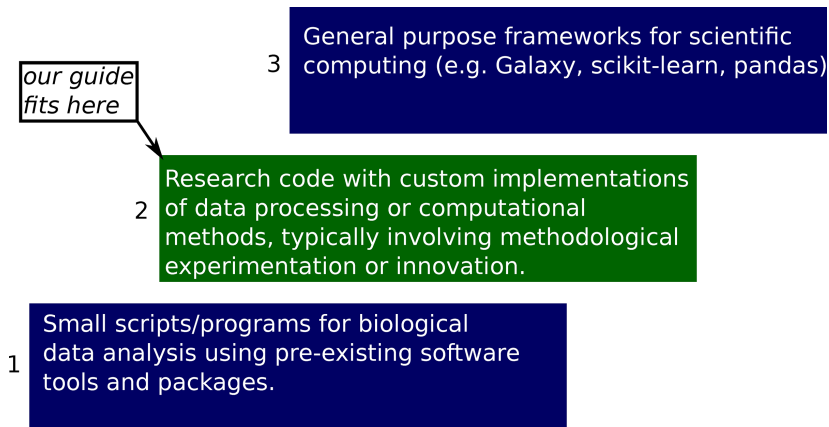


Credit : <https://i.redd.it/798mjzkwmiiz.jpg>

The fight of the editors

Best practices for scientific computing

► A typical project



Credit: <https://doi.org/10.1371/journal.pcbi.1008549.g001>

Typical computational projects

Outline

Good scientific software

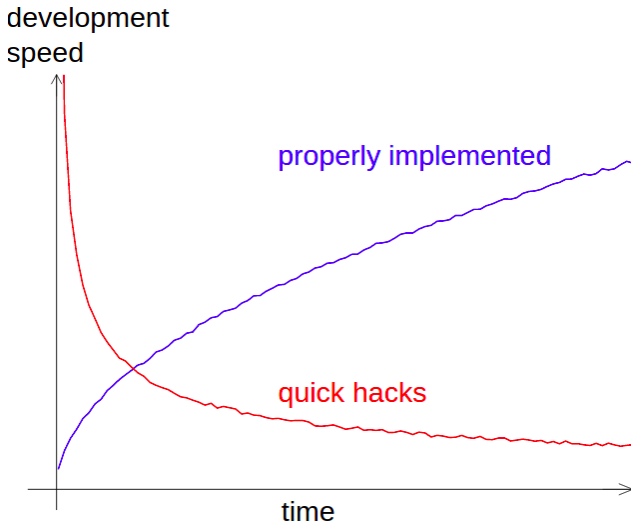
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How to get "good" scientific software?

► Clarification of expectations



Credit: Radovan Bast, adapted from "Simple Made Easy" by Rich Hickey

How to get "good" scientific software?

► Establish a common mindset

This user will “tack-on” code or assets, without working through how it fits in the whole picture. Or, won’t have team-members or staff helping them improve the code.

Result: shanty town or slowly degrading/regressing code/infrastructure



This user will have a team of peers, who all care about each other’s work, and will be open working through review with the team/staff, because they see the whole mission, and feel valued.

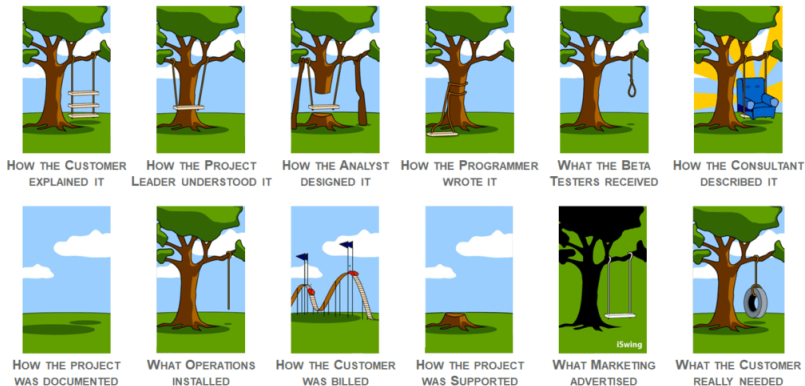


Credit: Ryan Knox

Extreams of community mindsets

How to get "good" scientific software?

- Choose 'good enough' practices



Credit: <https://www.action-engineering.com/blog/agile-acceptance-criteria/>

Unwanted stages of software development [10]

How to get "good" scientific software?

- ▶ Some practical tips to achieve goals in a team
- ▶ Common onboarding of team in the beginning of the project
- ▶ Identification of community goals and prioritizations
- ▶ Decide on a platform for collaboration
- ▶ Pair programming and sprints

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► Question

Why should we care about 'good enough' software engineering practices?

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► Answer

The quality of the software results will at best be
as good as the software itself