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Summary of Key Points

Hammitzsch, Johnston, Kuzak, Kraft, Leinweber

TIB, 13. July 2018 Recording: doi.org/10.5446/37828
FAIR Data & Software (Carpentries-based workshop) **#TIBFDS**

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Summaries

1. **FAIR principles**
2. General remarks
3. Additional references, recommended resources, etc.
4. Survey

On the FAIR principles

- **Open consultation on FAIR data action plan** of the European Open Science Cloud expert group (deadline 5 Aug 2018):
  GitHub.com/FAIR-Data-EG/Action-Plan - feel free to voice your opinion!

- FAIR does not mean open (data)

- There are different degrees of FAIRness, as research disciplines, resource types (e.g. data and software) and their requirements are strongly varied - but the shared goal is quality & good scientific practice

- FAIR (in its origins) focuses first and foremost on machine to machine interactions, only secondary on human to machine (or human to human) interactions

- DMPs/SMPs and a licence help to keep data/software FAIR

- Depending on the discipline, the researchers background and legal aspects: "Partly FAIR may be FAIR enough"

- REMEMBER: 'As open as possible, as closed as necessary'

THE CARPENTRIES

merged in 2017

software carpentry

DATA CARPENTRY

up & coming

library carpentry

∀uthorCarpentry

High-Performance Computing

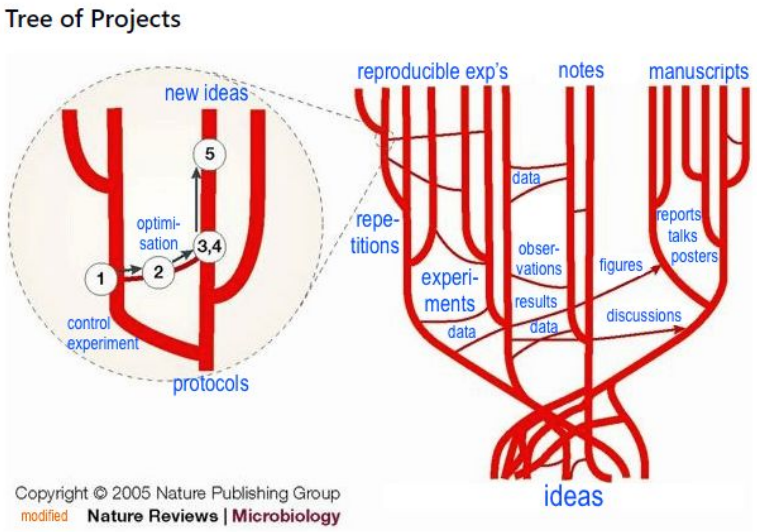
- teach computing & data skills to scientists
  - things that “work too well to be worth teaching” doi.org/10.12688/f1000research.3-62
  - youtu.be/1e26rp6qPbA?t=35s
- collaborative, community-developed lessons: bio- & genomics, geospatial, social, ...
- evidence-based pedagogical methods (sources)
  - instructor training & mentoring
  - learning-by-doing & live coding

Interested in setting up a local group?

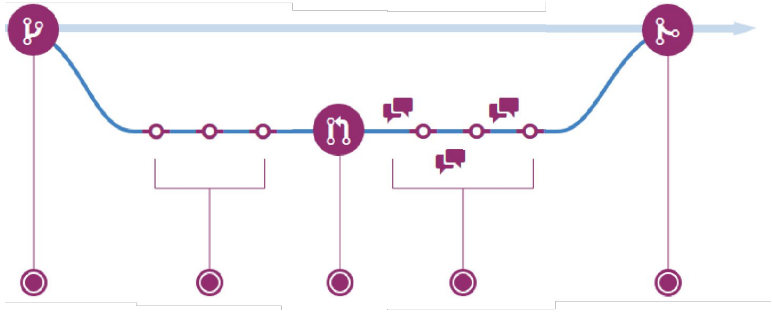
Please contact Carpentries@TIB.eu!

Accessible projects through public Git repos

1. **VC** because **self-documenting/-explaining** a project's evolution
2. easier **publication** & opportunity for **collaborations**
   a. Pull/Merge Requests = workflow for 21st century => fearless change, smooth review workflow, automation potential
   b. **issue tracker, website hosting, project management, etc.**
3. GitHub + Zenodo.org = DOI

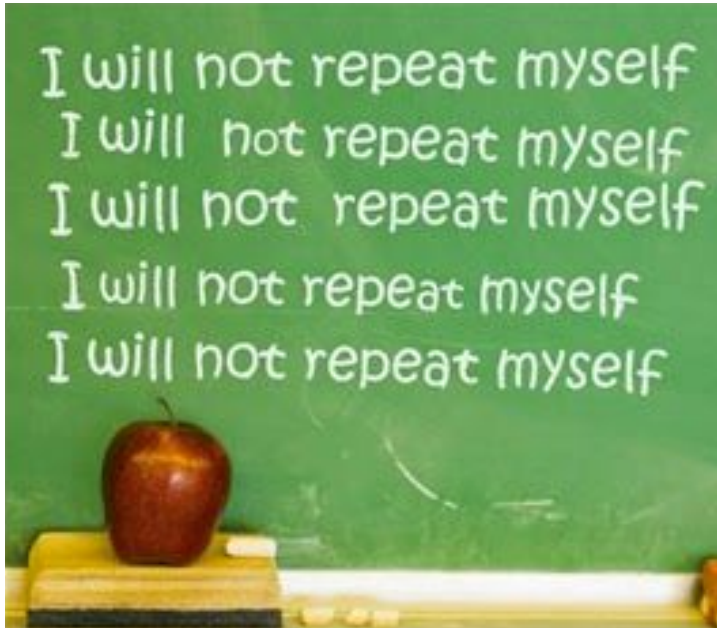


Git repo can be single source of truth & communication channel



guides.GitHub.com/introduction/flow

Accessible, interoperable & reusable code through functions



- scripts without code duplication may not need functions
- but instead of copy-pasting: stay DRY, not WET
  en.Wikipedia.org/?curid=3291957
- code is a liability / technical debt

"Programs are meant to be read by humans and only incidentally for computers to execute."

Donald Knuth (inventor of TeX)
flickr.com/vonguard (cropped; CC-BY-SA-2.0)

- concise function names are the beginning of good documentation
- individual & automatic "unit testing"
- more comprehensive approach: packaging!

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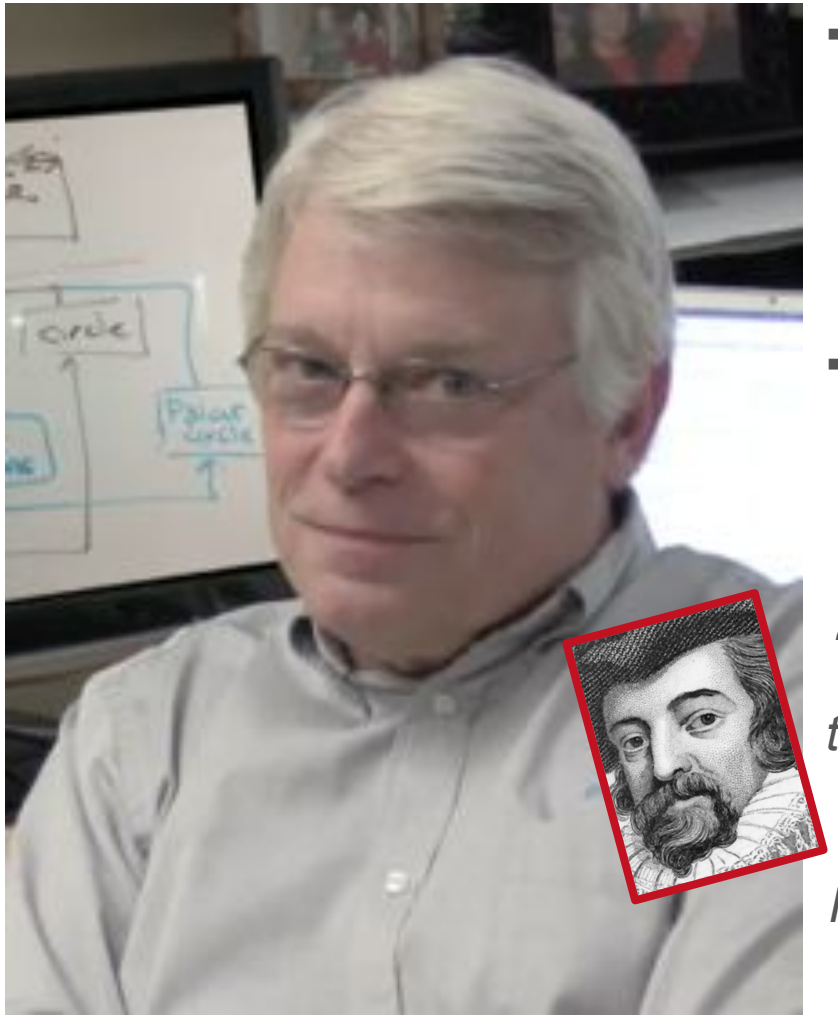
Refactoring (software hygiene)



by Tim-bezhashvyly (CC BY-SA 4.0)

- changing code internally, without changing its behaviour
  - renaming functions, variables, etc.
  - extracting duplicate code into new functions
  - re-organising code, files, etc.

- tests remove the fear from this process
  - automation & quick feedback make this fun
  - exercism.io/languages/r & /python

"You don't go fast by rushing [but by] taking your time, studying the problem, thinking carefully, cleaning up." -- Robert C. Martin

*First make it work, **then make it right**, and, finally, make it fast.*

-- Stephen C. Johnson and Brian W. Kernighan

“... finally, make it fast”. If it’s *really* necessary:

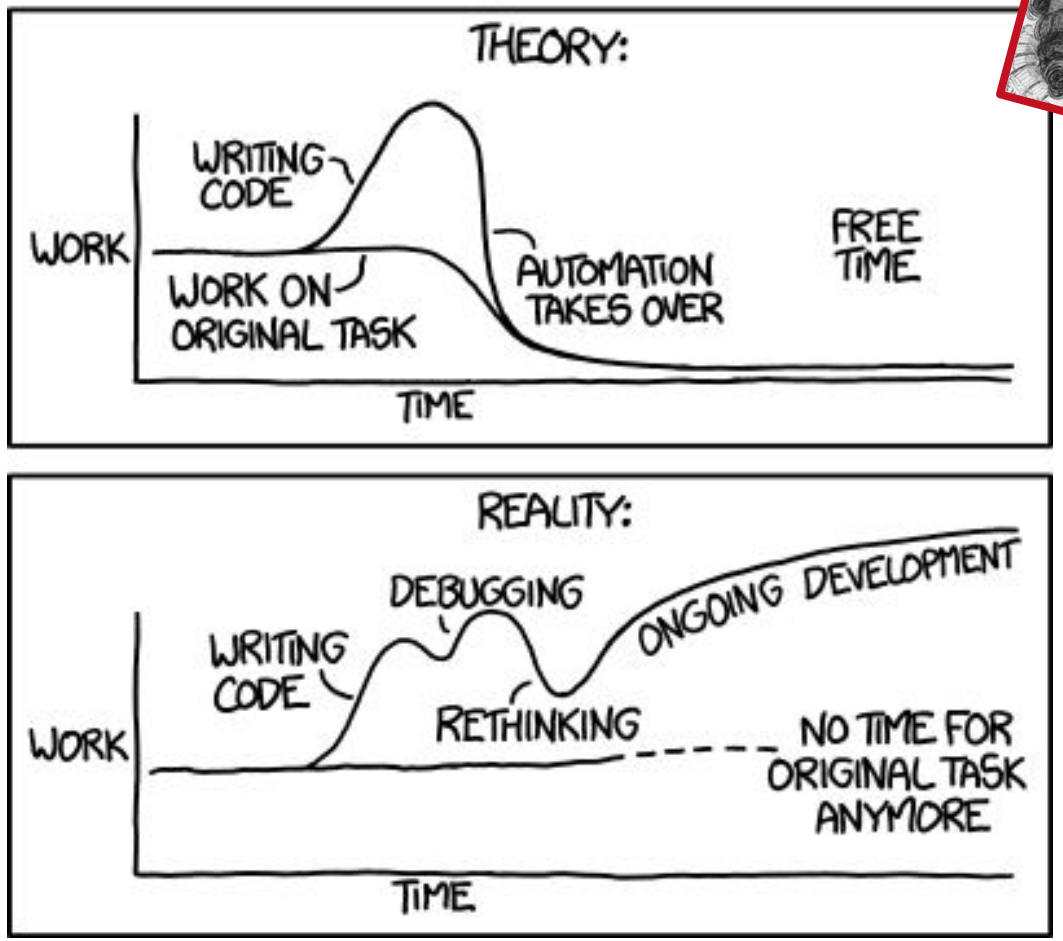
1. **Profile / benchmark**
2. **Identify bottleneck (under your control?)**
3. **(If yes) Remove**
4. **Profile / benchmark again**
5. **Identify next bottleneck**
6. **...**

wiki.python.org/moin/PythonSpeed

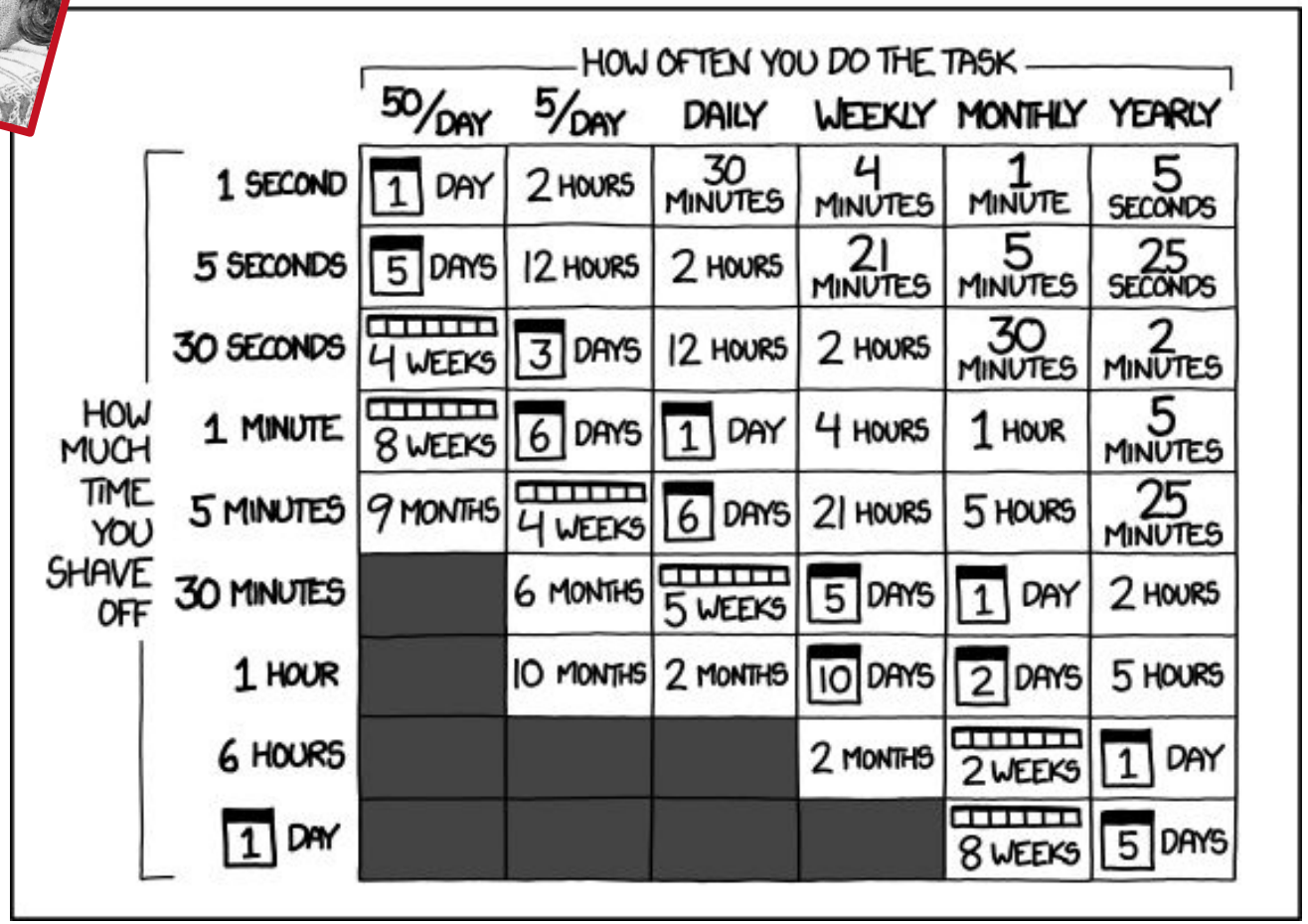
TGMStat.WordPress.com/2013/09, RStudio.GitHub.io/profvis & Adv-R.had.co.nz/Profiling.html

- for measuring individual functions: CRAN.R-project.org/package=microbenchmark

“... finally, make it fast”. A word of warning...



xkcd.com/1319

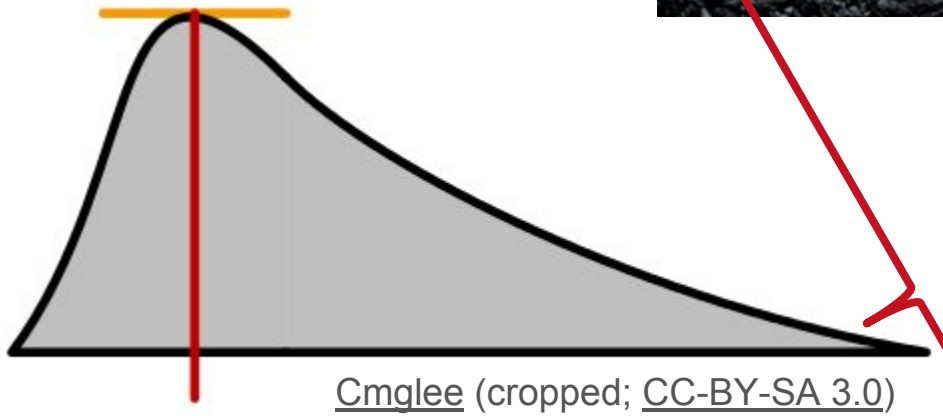


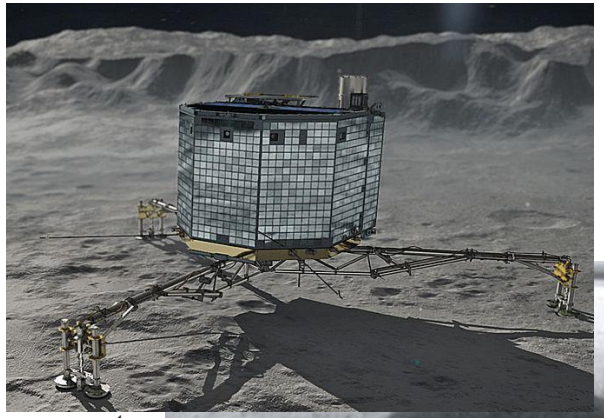
xkcd.com/1205

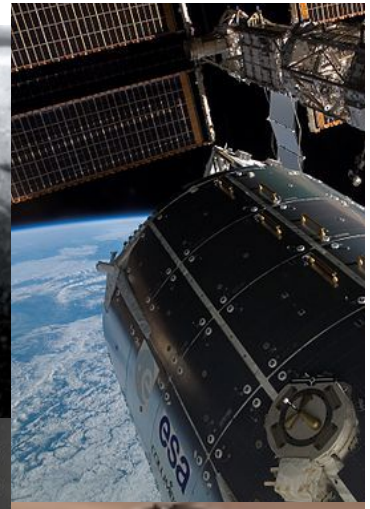
One more thing about “best practices”...

- By the time any “practice” becomes widely recognised as “best”, it’s average
- more = harder to choose
  - “best practices in scientific computing” doi:10.1371/journal.pbio.1001745
  - “good enough practices” doi:10.1371/journal.pcbi.1005510
  - “4 simple recommendations” doi:10.12688/f1000research.11407.1
  - “10 recommendations” doi:10.1186/2047-217X-3-31
  - etc....

Pick one, follow it and evaluate next level at next project start.







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Resources that help you find licences & info about them

a certain *type* of licence

ifrOSS .org (German)

news about court cases

Just tell me one...

ChooseAlicence.com (GitHub)

UFAL.GitHub.io/public-licence-selector/

`summary(licences)`

tldrLegal.com

I want to read more...

opensource.guide/legal

scholar.Google.com/scholar?q=Stodden

Morin et al. (2012) ... licencing for the Scientist-Programmer. doi.org/0.1371/journal.pcbi.1002598

doi.org/10.1371/journal.pcbi.1005510

Most important: pick one! For software, "MIT, BSD, or Apache [are] good enough"

Additional references, recommended resources, etc.

- General: guide.eScienceCenter.nl & OpenSource.guide
- Conference videos! But beware of “hype-driven development”...
  - R-project.org/conferences.html, RStudio.com/conference & RStudio.com/resources/webinars
    - GitHub.com/RStudio/webinars
  - conference.SciPy.org & YouTube.com/user/EnthoughtMedia/playlists
  - YouTube.com/user/GotoConferences/playlists (IT development & management)
- Blogs
  - blog.GitHub.com/category/education
  - about.GitLab.com/blog/categories/open-source & /releases
  - suistainable software.ac.uk/blog
- GitHub.com/awesomedata/awesome-public-datasets
- on technical debt & software sustainability
  - ivory.idyll.org/blog/2017-pof-software-archivability.html & ivory.idyll.org/blog/2018-oss-framework-cpr.html
  - Gael-Varoquaux.info/programming/software-for-reproducible-science-lets-not-have-a-misunderstanding.html
  - nadiaeghbal.com/tragedy-of-the-commons
- UNIX philosophy of software development: catb.org/~esr/writings/taoup/html/ch01s06.html
- building larger software systems: laputan.org
- practice more: programminghistorian.org, Software & Data Carpentry lessons
  - bio-informatics problems: rosalind.info

Additional references, recommended resources, etc.

- textbooks
  - Effective Computation in Physics (physics.codes)
  - Advanced R, R for Data Science, R packages & more: hadley.nz
  - teaching: Carpentries.GitHub.io/instructor-training/reference.html#books
- courses: OpenScienceMOOC.GitHub.io
- about automatic software tests and TDD: WatirMelon.blog/testing-pyramids, blog.cleancoder.com,
  - TDD in many languages: exercism.io

- try.GitHub.io,
- reading: Think-like-a-git.net,

- our R lesson: TIBHannover.GitHub.io/FAIR-R
- package source & guides: ROpenSci.org & CRAN.R-project.org
- naming R packages: njtierney.com/post/2018/06/20/naming-things/ & GitHub.com/ROpenSciLabs/available
- packaging & reproducible reports: GitHub.com/BenMarwick/rrtools

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Thanks to Konrad Förstner, Luke Johnson, Mateusz Kuzak and Martin Hammitzsch!

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Farewell!

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