



ITB Tech Talks

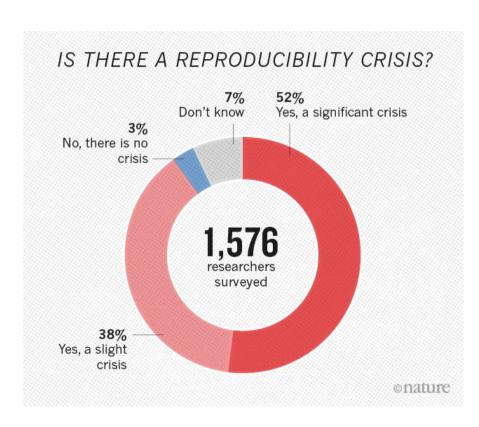
- Motivation: Improve Reproducibility, Reusability, Open Science & Quality of Computational Biology
- Content: Technologies for Computational & Theoretical Biology
- Format: Short talks 10 minutes, life demo required
- Core technologies
 - git
 - jupyter notebooks/lab
 - virtual environments & pip
 - docker
- Core libraries (python/R)
 - data science (pandas, numpy, tensorflow, scikit learn)
 - visualization (matplotlib, plotly)
 - reports (knitr)







Reproducibility/Reusability Crisis



"Really Reproducible Research" (1992) inspired by Stanford Professor Jon Claerbout:

"The idea is: An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete ... set of instructions [and data] which generated the figures."

David Donoho, 1998

How long would it take you to reproduce your results from your last (computational) paper?

Versioning Crisis

"FINAL".doc



FINAL. doc!



FINAL_rev.2.doc



FINAL_rev.6.COMMENTS.doc





FINAL_rev.8.comments5. CORRECTIONS. doc



JORGE CHAM @ 2012

FINAL_rev.18.comments7. corrections 9. MORE. 30. doc corrections. 10. #@\$ %WHYDID



FINAL_rev.22.comments49. ICOMETOGRADSCHOOL????.doc



WWW. PHDCOMICS. COM

git to the rescue

- Git is a free and open source distributed version control system.
 - tiny footprint
 - lightning fast performance
 - works for everything from small to very large projects
- GitHub is a code hosting platform for version control and collaboration.
 - social coding
 - alternatives: GitLab, BitBucket, SourceForge



What can git do for you?

- Work anywhere & offline
- Decentralized backups
- Version control & track changes
 - diffs & branches
- Revert & experiment
 - revisions & branches
- Collaborative editing/work
 - Pull requests
- Reproducible research
- Releases & snapshots
 - citable code
- Issue tracker
- Continuous integration
 - unit tests
 - commit hooks

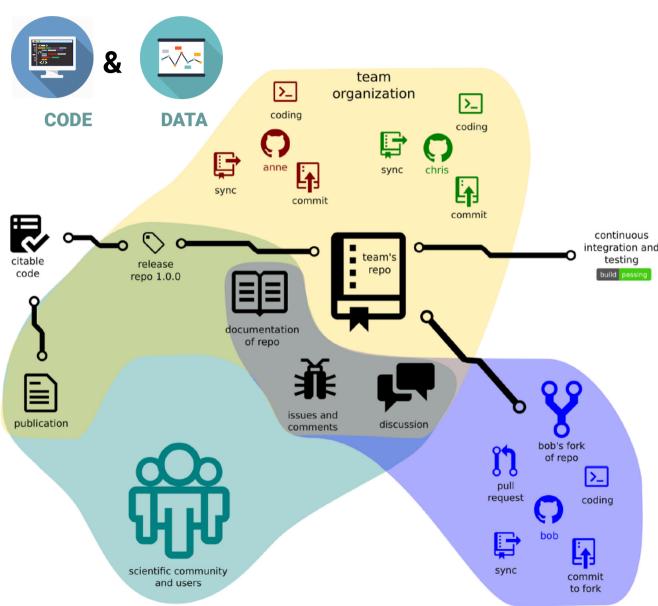
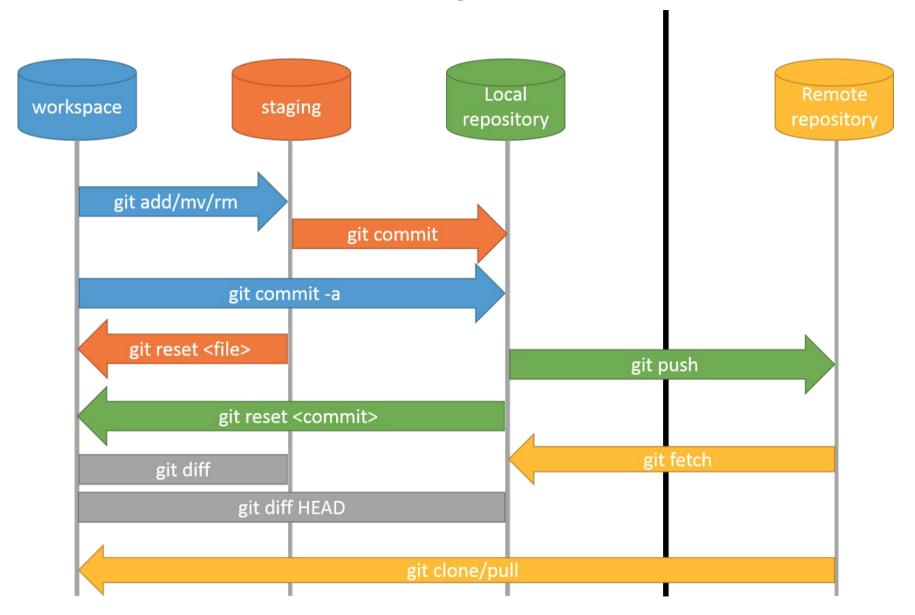


Fig 1. The structure of a GitHub-based project illustrating project structure and interactions with the community.

Perez.Riverol2016

How does git work?



References

 Perez-Riverol, Y.; Gatto, L.; Wang, R.; Sachsenberg, T.; Uszkoreit, J.; Leprevost, F. d. V.; Fufezan, C.; Ternent, T.; Eglen, S. J.; Katz, D. S.; Pollard, T. J.; Konovalov, A.; Flight, R. M.; Blin, K. & Vizcaíno, J. A.

Ten Simple Rules for Taking Advantage of Git and GitHub. PLoS computational biology, 2016, 12, e1004947

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 PLoS computational biology, 2016, 12, e1004668
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 Git can facilitate greater reproducibility and increased transparency in science.
 Source code for biology and medicine, 2013, 8, 7
- Tutorials
 https://try.github.io/levels/1/challenges/1
- Information/Books

https://git-scm.com/ https://git-scm.com/book/en/v2