Assuring Quality Software for Reproducible Research

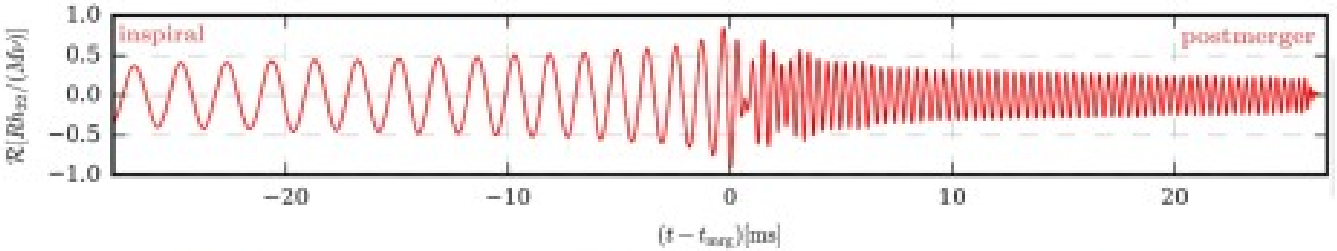
Philip DAVIS
on behalf of the LuTH-Caen group in Virgo :
LPC-Caen, GANIL, LuTH, Observatoire de Strasbourg

In collaboration with : University of California, Fullerton

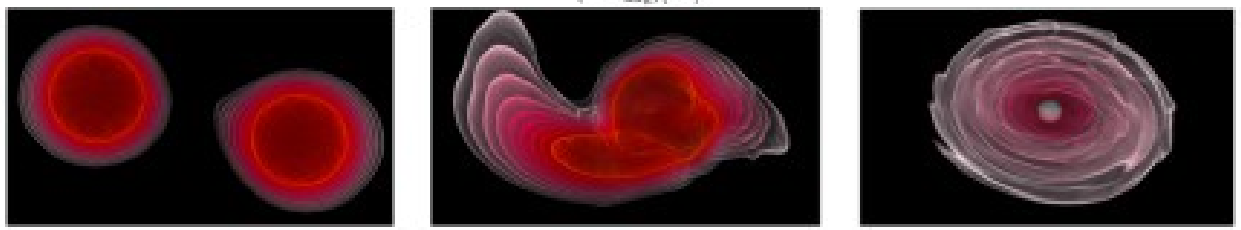
GdR Ondes Gravitationnelles 2024

Background Context

Terrestrial experiments can only probe low-density regimes of the equation of state. For higher densities, require astrophysical constraints, e.g. gravitational waves (GWs) during NS merger events.



Credit : Dietrich et al. 2021



Pre-merger | Merger | Post-merger

Credit : Virgo/ Ligo collaboration

Development of numerical tools for the LIGO-Virgo-Kagra collaboration by members of LuTH-Caen group in Virgo (LPC, LuTH, Strasbourg, GANIL).

The shape of the GW signal (the « waveform ») depends on the property of matter and hence the EoS of the NS.

Comparing observed and simulated waveforms, provides information on the EoS.

Aim of role : raise awareness of good software development practices and data management so that quality numerical tools and data can be used by the scientific community.

Why is this important ?

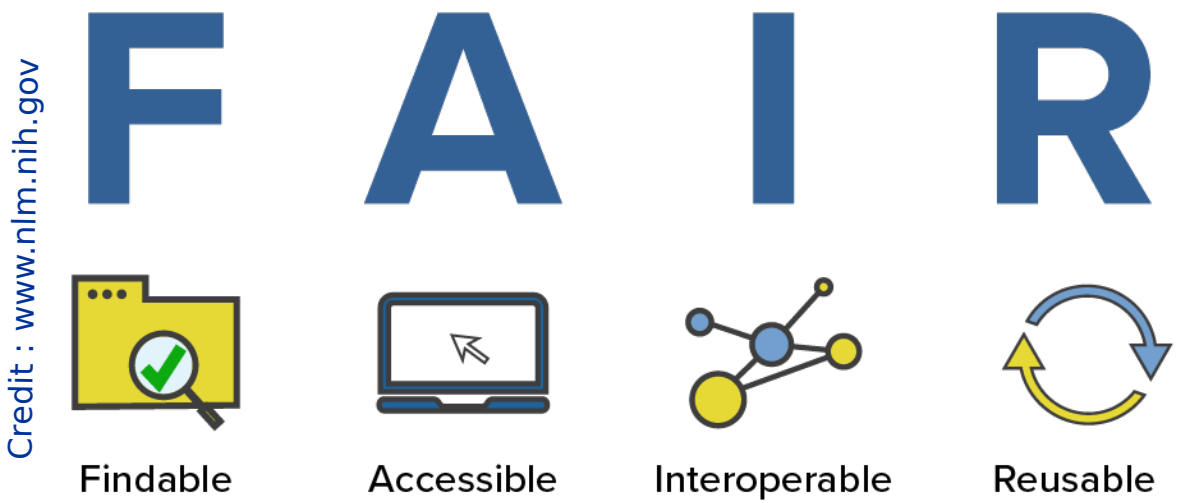
Good software and data practices ensure :

- Robustness and reliabability,
- Transparency,
- Traceability,
- Reproducibility.

These are in turn important for the Open Science initiative, which :

- Improves visibility of research,
- Ensures research can be validated,
- Improves collaborations,
- Reduces duplicated effort.

Code and data should abide by Open Science principles by being...



Credit : www.nlm.nih.gov

Challenges for reproducible science

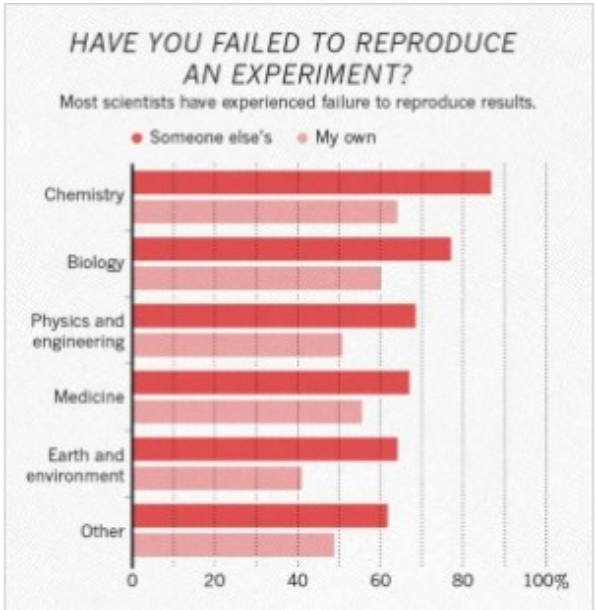
1,500 scientists lift the lid on reproducibility

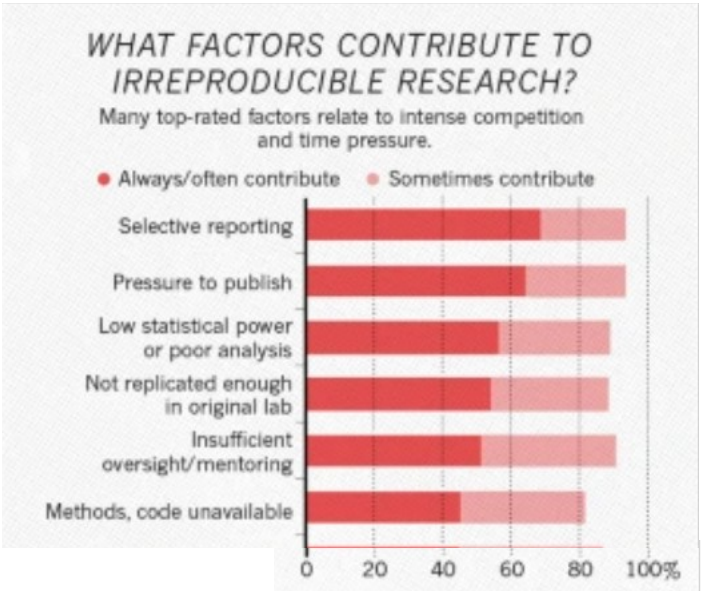
Monya Baker

Nature **533**, 452–454 (2016) | Cite this article

This article has been updated

Survey sheds light on the 'crisis' rocking research.





https://www.nature.com/articles/533452a

Physics/engineering : ~ 70 % of scientists in study have failed to reproduce results,

~ 40 % of respondants said unavailability of codes/ methods always or often contributed.

Also, potential problems with :

- bugs within the code,
- numerical libraries are missing or incompatible with the host machine

By following good coding practices, we can hope to improve our chances of reproducing (numerical) experiments.

Raising awareness of good practices

Created training material covering software development working practices :

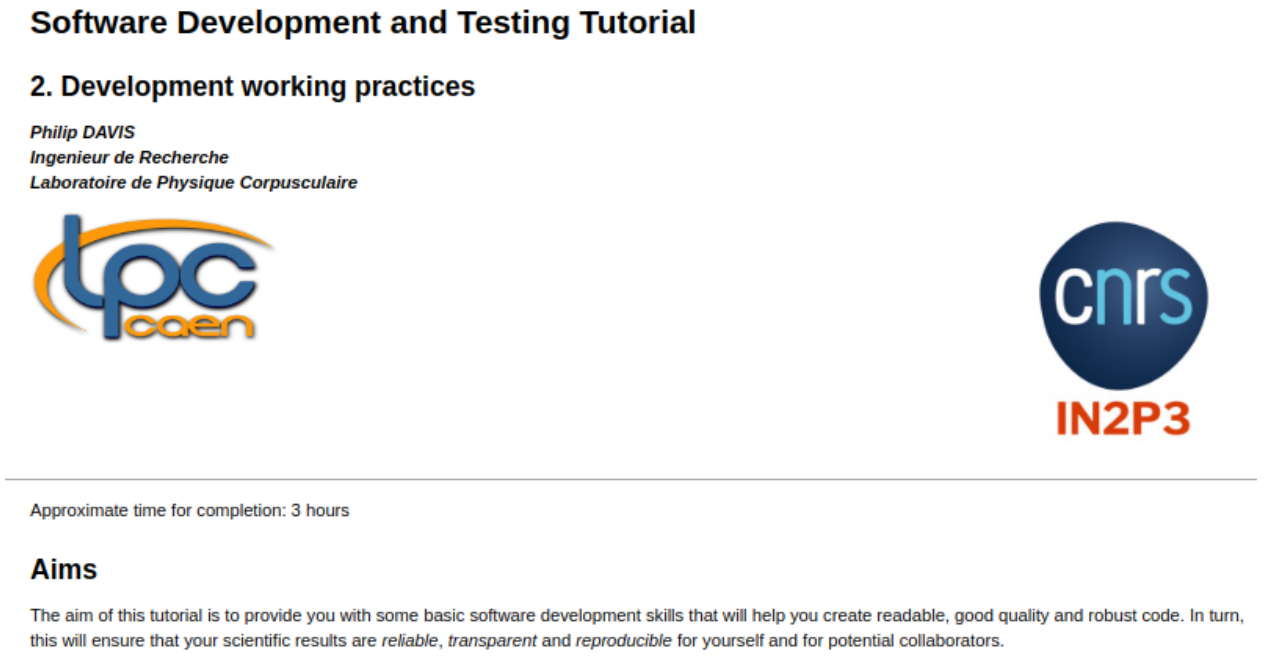
- Version control with git and GitLab,
- Development « workflow » :

Issue → Branch → Commits → Testing → Review → Merge

First course given to LuTH-Caen group members Autumn 2022. Aim to be given yearly.

Next steps :

- Material on publishing code and data,
- Present material at a training Bootcamp at LPC-Caen for PhD students (Nov 2024).



Software Development and Testing Tutorial

2. Development working practices

Philip DAVIS
Ingenieur de Recherche
Laboratoire de Physique Corpusculaire

Approximate time for completion: 3 hours

Aims

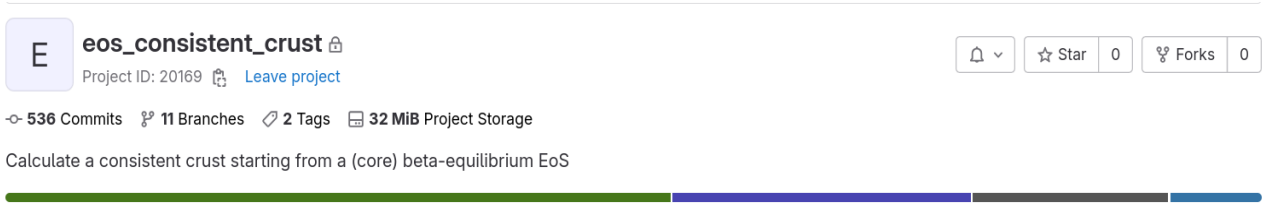
The aim of this tutorial is to provide you with some basic software development skills that will help you create readable, good quality and robust code. In turn, this will ensure that your scientific results are *reliable*, *transparent* and *reproducible* for yourself and for potential collaborators.

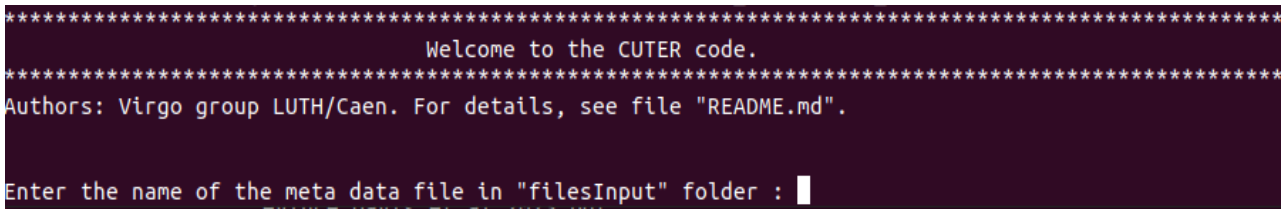
Material located at :
https://gitlab.in2p3.fr/eos-for-virgo/training

CUTER (Crust Unified Tool for Equation-of-State Reconstruction)

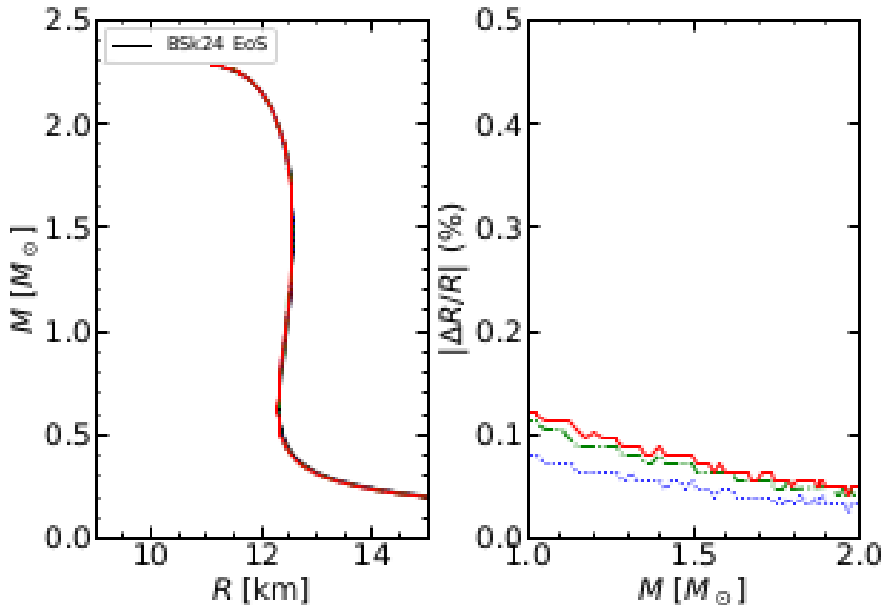
- A NS equation of state is needed to relate different global NS properties, for example mass and radius,

- Inconsistent treatment of NS crust (« non-unified ») can introduce biases.





Davis et al. 2024



Numerical tool, CUTER, developed for the LIGO-Virgo-Kagra collaboration :

- Attach a thermodynamically consistent crust to an equation of state describing the core of a NS,

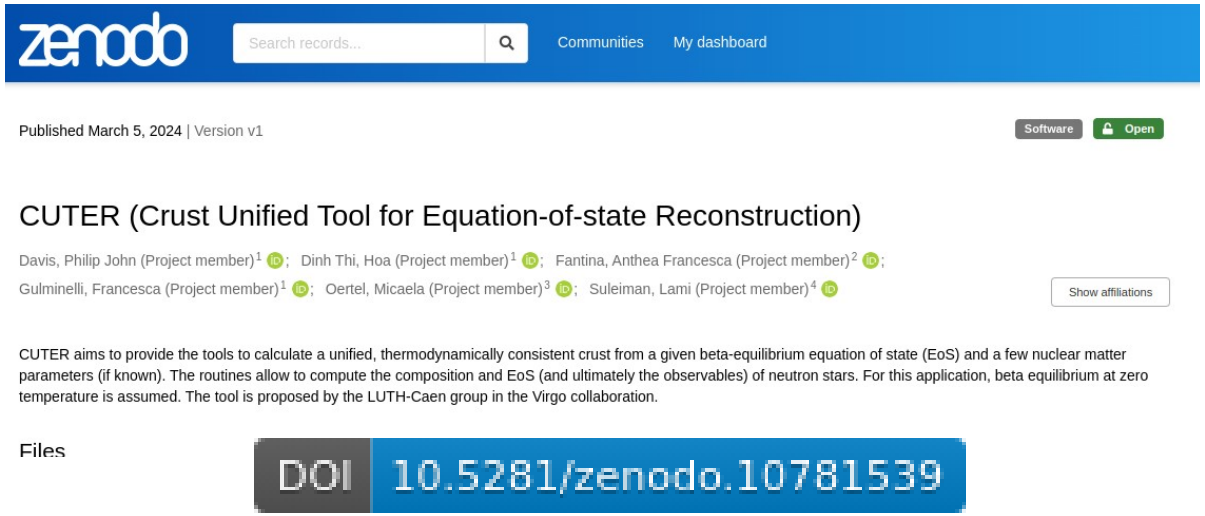
- Aim : reduce errors of inferred global properties of NS. Important for the next generation of gravitational wave detectors (e.g. Einstein Telescope).

CUTER (cont.)

Working practices followed :

- Software development « workflow »
- Hosted on IN2P3 and LIGO GitLab sites,
- Documentation (e.g. README),
- Addition of a License (protect rights of both the users and developers),
- Sign-off by external reviewer,
- `Conda` to manage software environment,
- `Pytest` for automated testing.

`CUTER` was opened to the LIGO-Virgo-Kagra collaboration May 2023. Paper describing the code published in A&A (Davis et al. 2024).
https://doi.org/10.1051/0004-6361/202348402



Since then :

- `CUTER V2` released August 2024 (outer crust reconstruction),
- `CUTER V3` under development (Bayes tools) (forseen spring-summer 2025)

Future plans

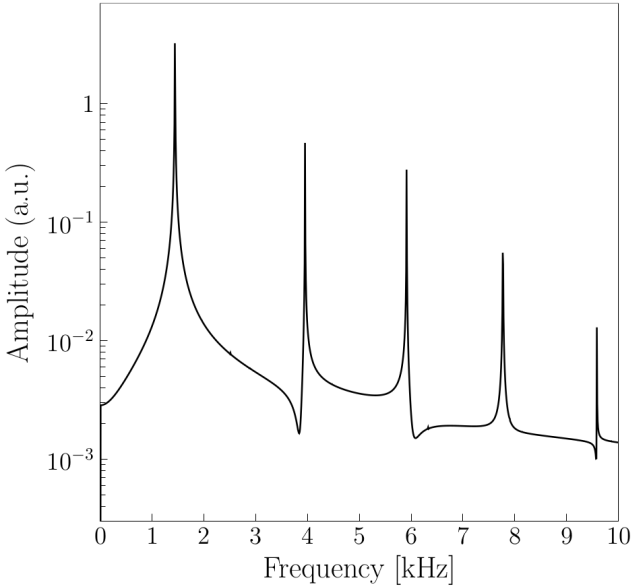
Medium term (3-4 years)

- Parametric study of NSs with a large set of microphysical inputs, simulating possible GW signals, from a post-merger of NS+NS binary,
- In collaboration with researchers from the Observatoire de Strasbourg, in the framework of the *ANR GW-HNS (2023-2025) project,*
- Development of hydro code, ROXAS, to model oscillating NSs and analytical representations of EoS underway.

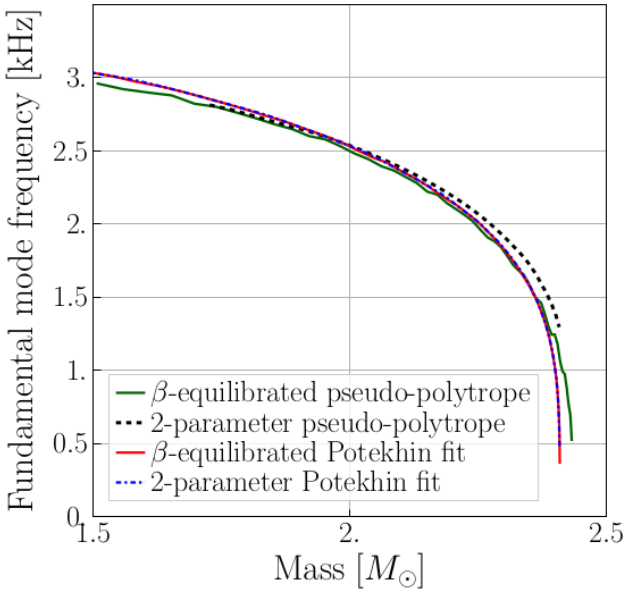
Long term (> 5 years)

- Provide data (e.g. GW waveforms) for the LIGO-Virgo-Kagra analysis pipelines and other collaborators,

Servignat et al. 2023, Class. Quantum Grav. DOI : 10.1088/1361-6382/acc828



Servignat (+Davis) et al. 2023, Phys. Rev. D (DOI: https://doi.org/10.1103/PhysRevD.109.103022

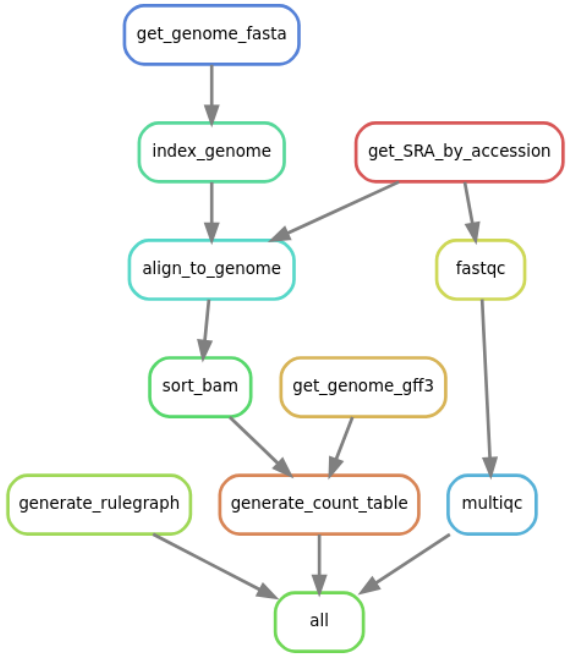


Associated challenges

- Storing, sharing and publication of large datasets,
- Transparency regarding the provenance of data sets (e.g. processing performed, code versions) → meta data ?
- Computationally intensive simulations,
- Managing software environments for multiple langages (`Python, C/C++, Fortran`)
- Managing and automating complex task « workflows ».

Make use of publicly available tools, e.g.

- `Datalad`, `Git/Gitlab` : management of code and data,
- `Docker, Conda` : management of software environments,
- `Snakemake` : automating task workflows.



Credit : nbis-reproducible-research.readthedocs.io

Thanks for your attention
Questions ?

Normandie Université