

FAIR Bioinfo 2024 - Strasbourg



FAIR Bioinfo 2024 Conclusion

INRAC

CNIS

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Cea



BiGEst



- Introduction to FAIR & Open Science
- Notebooks with Jupyter
- Getting started with conda
- Getting started with Git and Github
- Distributing your pipeline with Docker and Apptainer
- Creating a Snakemake workflow
- IFB calculation cluster (SLURM)
- GitHub Pages and Zenodo



How to make a computational research project reproducible using several different tools





https://nbis-reproducible-research.readthedocs.io/en/course 2104/introduction/









FAIR4RS Principles - Findable



F1. Software is assigned a globally unique and persistent identifier.

F1.1. Components of the software representing levels of granularity are assigned distinct identifiers.

F1.2. Different versions of the software are assigned distinct identifiers.

F2. Software is described with rich metadata.

F3. Metadata clearly and explicitly include the identifier of the software they describe.

F4. Metadata are FAIR, searchable and indexable.

Barker, M., Chue Hong, N.P., Katz, D.S. et al. Introducing the FAIR Principles for research software. Sci Data 9, 622 (2022). <u>https://doi.org/10.1038/s41597-022-01710-x</u>



FAIR4RS Principles - Accessible

A: Software, and its metadata, is retrievable via standardised protocols.

A1. Software is retrievable by its identifier using a standardised communications protocol.

A1.1. The protocol is open, free, and universally implementable.

A1.2. The protocol allows for an authentication and authorization procedure, where necessary.

A2. Metadata are accessible, even when the software is no longer available.

Barker, M., Chue Hong, N.P., Katz, D.S. et al. Introducing the FAIR Principles for research software. Sci Data 9, 622 (2022). <u>https://doi.org/10.1038/s41597-022-01710-x</u>



I: Software interoperates with other software by exchanging data and/or metadata, and/or through interaction via application programming interfaces (APIs), described through standards.

I1. Software reads, writes and exchanges data in a way that meets domain-relevant community standards.

I2. Software includes qualified references to other objects.





R: Software is both usable (can be executed) and reusable (can be understood, modified, built upon, or incorporated into other software). R1. Software is described with a plurality of accurate and relevant attributes. R1.1. Software is given a clear and accessible license. R1.2. Software is associated with detailed provenance. R2. Software includes gualified references to other software.

Barker, M., Chue Hong, N.P., Katz, D.S. et al. Introducing the FAIR Principles for research software. Sci Data 9, 622 (2022). <u>https://doi.org/10.1038/s41597-022-01710-x</u>







R3. Software meets domain-relevant community standards.







Automation



Interactive user analysis





Data

- What if the data is not 100% FAIR?
- How do you manage large volumes of data?
- How do you manage data and metadata updates?



Code

- How can we be sure that the code will always be accessible?
- Is it acceptable if adaptations have to be made? At what point?
- Should all the code be provided (for value enhancement, creation of a start-up, etc.)?





Competence and sensitivity

- Willingness but technical inability to do so
- "Why do it, there's no point".
- Too time-consuming

Coverage

- Should everything be reproducible?
- When should it be done?
- At the beginning? But what if it doesn't work?
- At the end?







Reproducibility to the exact bit?

Container uses some resources of the support machine

 \Rightarrow version control of the env : Nix, Guix

HPC and parallelization?

Loss of computational order,

multithreading, identical hardware?

















IFB training courses on FAIR

- 1. FAIR principles for the management of research data in the life sciences (FAIRdata)
- 2. FAIR principles in a Bioinformatics project (FAIRbioinfo)



https://moodle.france-bioinformatique.fr/





https://www.france-bioinformatique.fr/formations





Our helpers

Alix and Laurent

IFB Core Cluster taskforce

Julien, Gildas, and all those who provide in the shadows

Organisations BiGEst, IGBMC, IBMP, IFB

