FAIR_bioinfo : Open Science and FAIR principles in a bioinformatics project

How to make a bioinformatics project more reproducible

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General information

Practical information:

- Dates: June 28th - 30th
- Location: Institut des Systèmes Complexes, 113 rue Nationale, 75013-Paris
- Courses: 9:00 to 17:30
- Meal: 12:30-14:00
- Pauses: 10:30-11:00 + 15:30-16:00
- 2 days of courses + 1 day of course building

Round table:

- Teachers
- Learners

Ressources:

-
- GitLab
- LaTeX

Training schedule

Day 1:

- Introduction to reproducibility
- History management (3 Practical Sessions, git, GitHub)
- Control your development environment (1 PS, CONDA)
- Encapsulation (2 PS, docker)

Day 2:

- Workflow (2 PS, SNAKEMAKE)
- Traceability with notebooks (2 PS, jupyter,)
- IFB resources (2 PS, slurm,)
- Sharing and disseminating (GitHub, zenodo)
- Conclusion

Day 3:

- Empowerment and improvement of resources

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9. 3rd Day

Conclusion

Current schedule

Day 1:

- Introduction to FAIR_bioinfo
- History management (git, GitHub)
- Environment management (CONDA, docker)

Day 2:

- Workflow (SNAKEMAKE)
- Traceability with notebooks (jupyter, markdown)
- IFB resources (S, slurm)
- Sharing and disseminating (GitHub, zenodo)

Let's take a step back.

FAIR_bioinfo

Findable

Easy to find protocols (GitHub, GitHub Pages) with DOI (zenodo)

Accessible

Open source (GitHub, docker, CONDA, ...)

Interoperable

Think "workflow" (SNAKEMAKE + docker / CONDA) locally or on servers (S, slurm)

Reusable

Replayable protocols (jupyter, markdown) in virtual environments (docker / CONDA)

A virtuous cycle

FAIR raw data

+

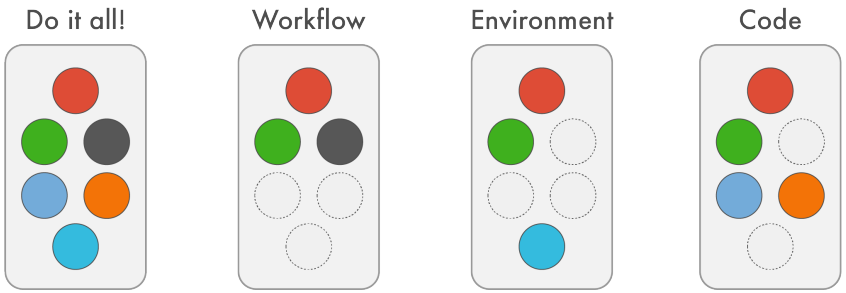
FAIR_bioinfo scripts/protocols

=

FAIR processed data

Swedish similar tutorial

From the NBIS – National Bioinformatics Infrastructure Sweden



nbis-reproducible-research.readthedocs.io/en/latest

Reproducibility checklist[2]

- Code avoid workflows based on point-and-click interfaces (eg. Excel), enshrine computations and data manipulation in code
- Document how code works, define parameters and computational environment required: comments, notebooks and README
- Record key parameters (eg. the 'seed' values of a random-number generator)
- Test functions using positive and negative control data sets, run those tests throughout development
- Guide with master script (eg. 'run.sh') that downloads data sets and executes workflow
- Archive with long-term stability services such as Zenodo, Figshare and Software Heritage (GitHub is impermanent online repository)

[2] Nature

Reproducibility checklist[3]

- Track the project's history with a version-control tools (eg. Git). Note (tag) which version you used to create each result
- Package with ready-to-use computational environments using containerization tools (eg. Docker, Singularity), web services (Code Ocean, Gigantum, Binder) or virtual-environment managers (Conda)
- Simplify and avoid niche or hard-to-install third-party code libraries
- Verify your code's portability by running it in a range of computing environments
- Automate the test of your code with continuous-integration services (eg. Travis CI)

[3] Nature

Adding Tests

Unit test: test a part of the code

```
## module 1
sum <- function(x, y){
    return (x+y)
}

# Unit test
sum(2,2) == 4
```

```
## module 2
power <- function(x, y){
    return (x**y)
}

# Unit test
power(2,2) == 4
```

Functional test: test all the code

```
# Functional test
power(sum(2,2),2) == 16
```

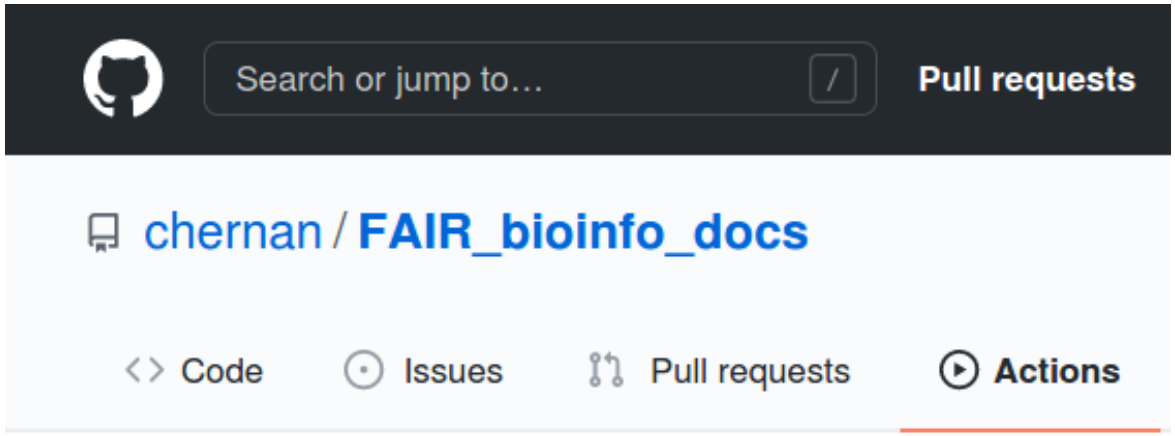
Continuous integration

Automated verification each time the source code is modified that the modifications do not produce:

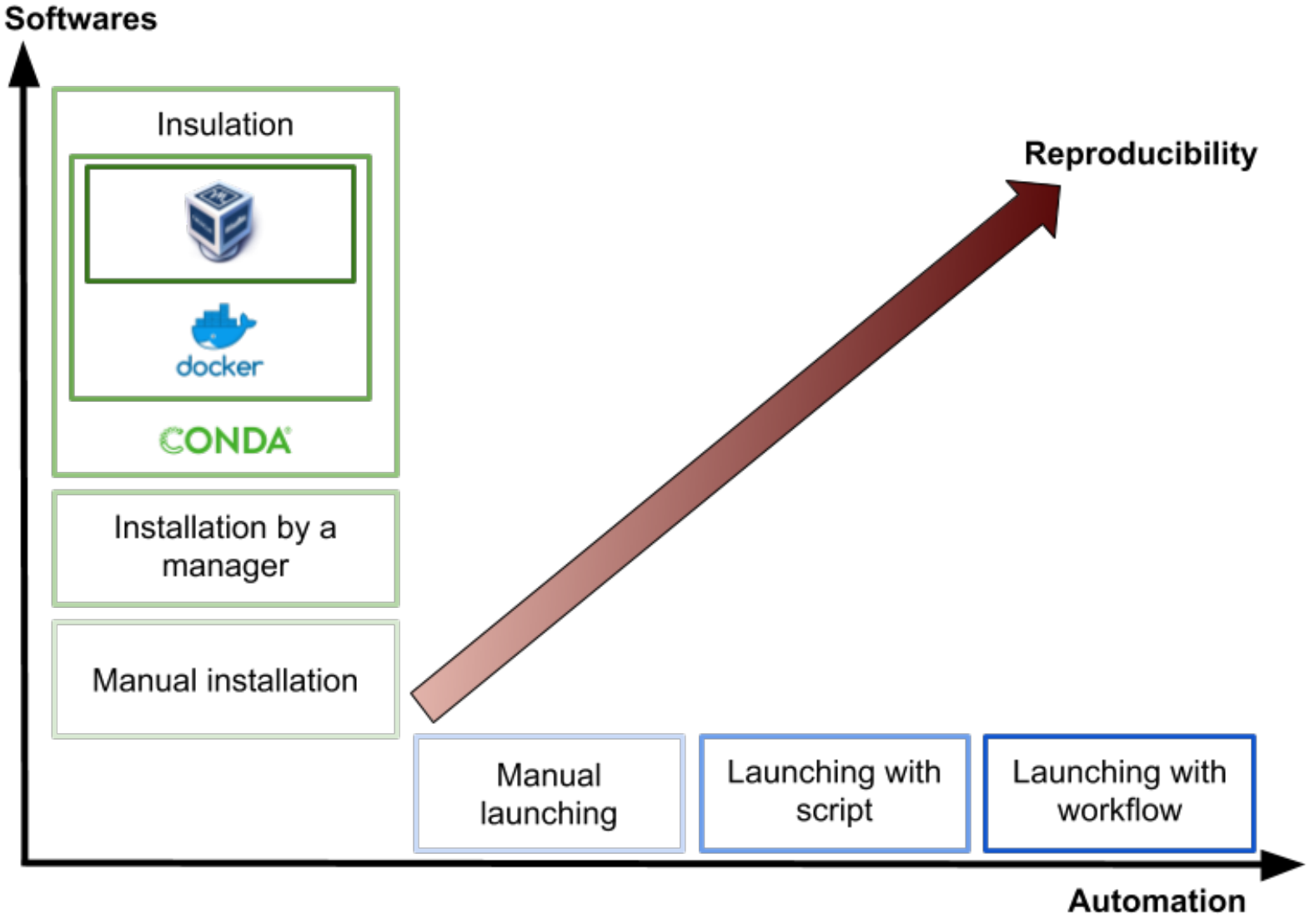
- any regression in the developed application
- any change in the results obtained

Travis CI

circleci



Reproducibility: a multidimensional and multi-level process



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Automation

Manual command lines

↓

Write a shell script

↓

Use a workflow manager

↓

Tests and continuous integration (*)

User analysis (trial-and-error)

Offer a GUI (eg. with R-Shiny) (*)

↓

Save and re-import choices (*)

Softwares

Local installation

↓

Package manager

↓

Conda environment

↓

Image / container

↓

Virtual machine (*)

(*) not carried out in the course

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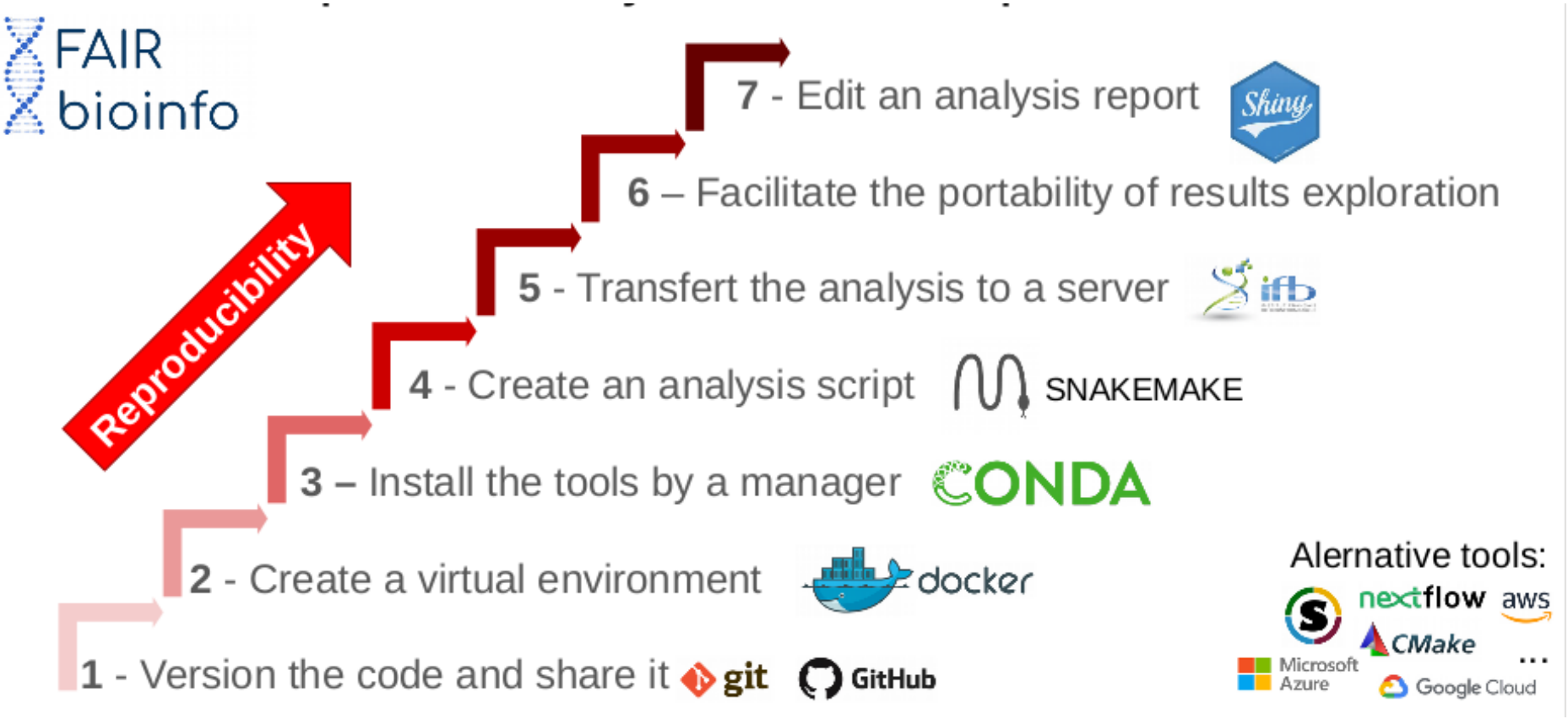

Reproducibility - how far?

Reproducibility to the exact bit?

✗ container uses some resources of the support machine

✓ version control of the env. (Nix, Guix)

HPC and parallelization?

✗ loss of computanional order, multi-threading, identical hardware?

✓ ...?

Thanks

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