La reproductibilité des calculs en Python

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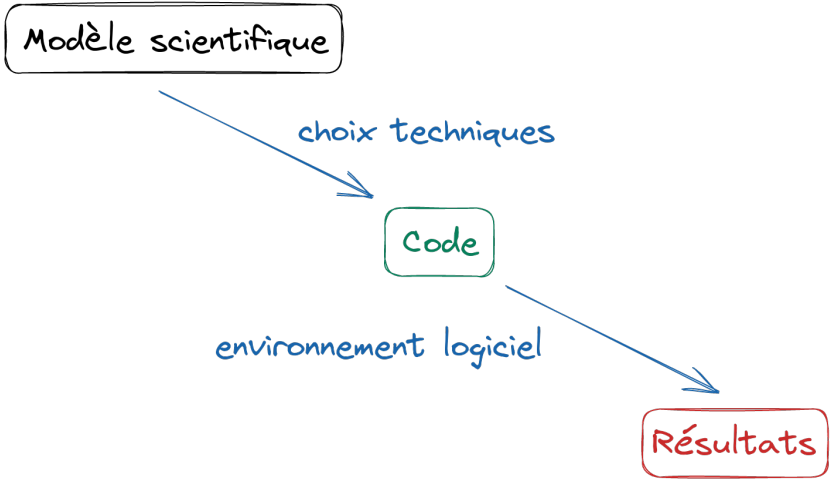
Plan

1. Principes de la reproductibilité computationnelle
2. Application à l'univers Python
3. Conseils pratiques

Schéma du calcul scientifique



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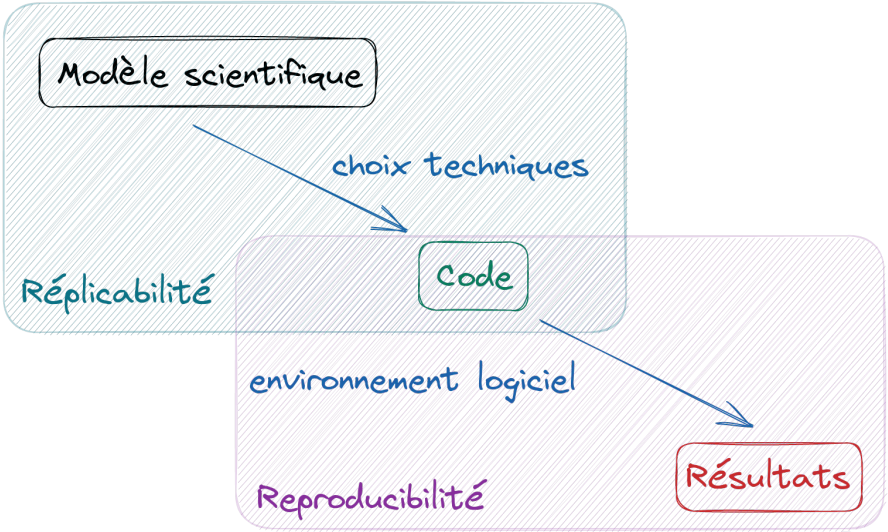

Re. . .bilité(s)

Reproductibilité

Obtenir des résultats **identiques** (octet par octet)
sur une **autre** machine,
avec le **même** code et les **mêmes** données

Documentation du calcul : code, données, environnement logiciel

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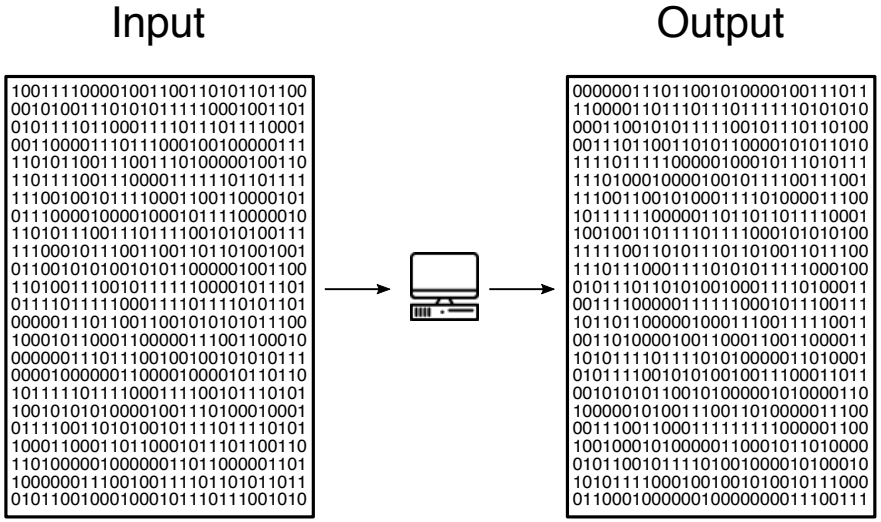
Réplicabilité

Obtenir des résultats **équivalents**
avec une **autre** implémentation
du **même** modèle scientifique

Documentation du modèle scientifique
Validation des choix techniques

What's a computation ?



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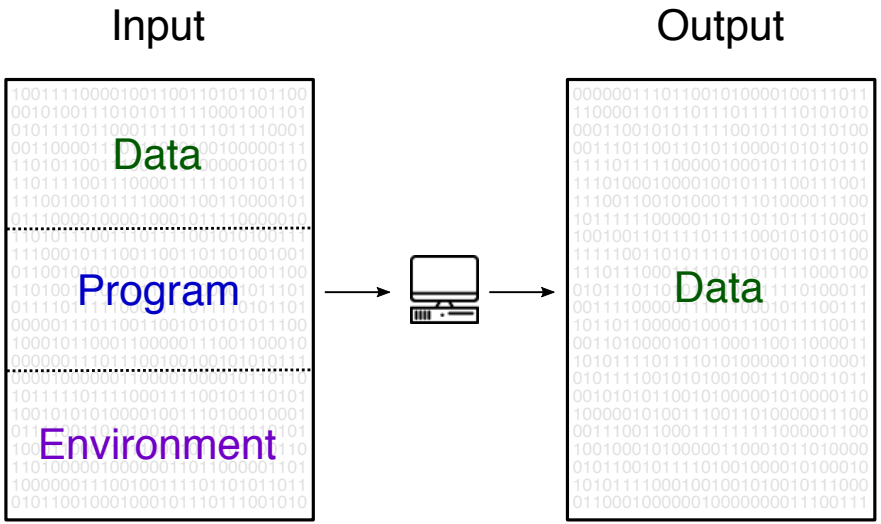
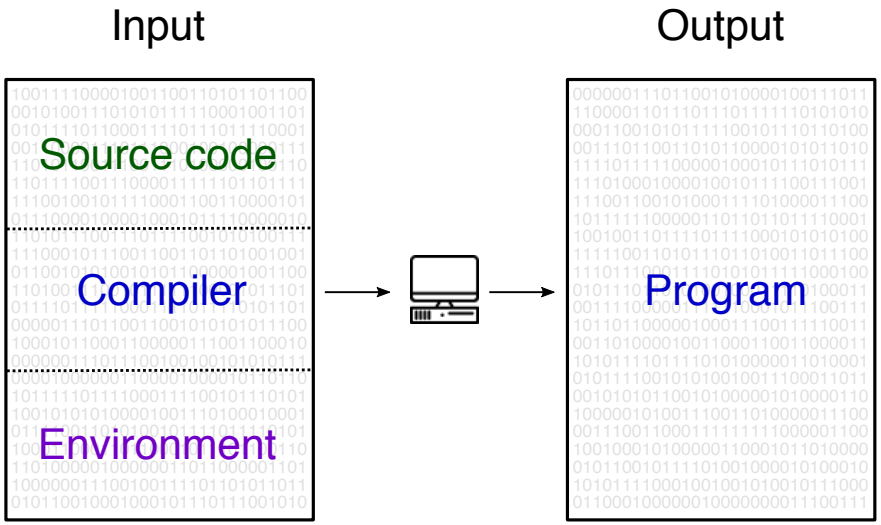


Computer by Creative Stall from the Noun Project

Compilation is computation



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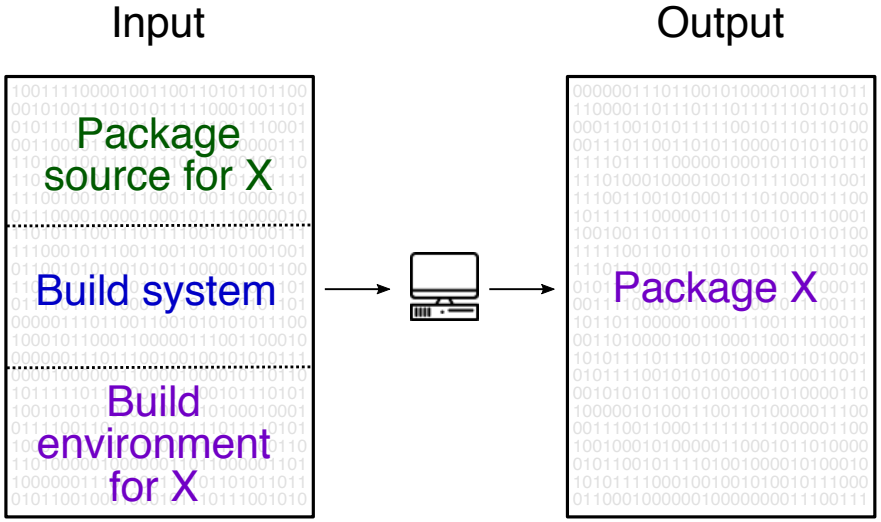
Package building is computation



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Reproducibility

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- **Irreproducible output $\longrightarrow$ something has changed !**
- Most often it's the environment.

Deployment vs. archiving

Deployment

- **Goal** : facilitate the use of software tools
- Prepare for distribution
- Install
- Update
- *Newer is better*

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Archiving

- **Goal** : preserve a precise software stack for reproducibility
- Make a complete snapshot
- Re-deploy a snapshot
- *Newer is different*

Package managers

Designed for deployment, not archiving

`apt`, `rpm`, `homebrew`, `pip`, ...

all but two : **Guix** and **Nix**

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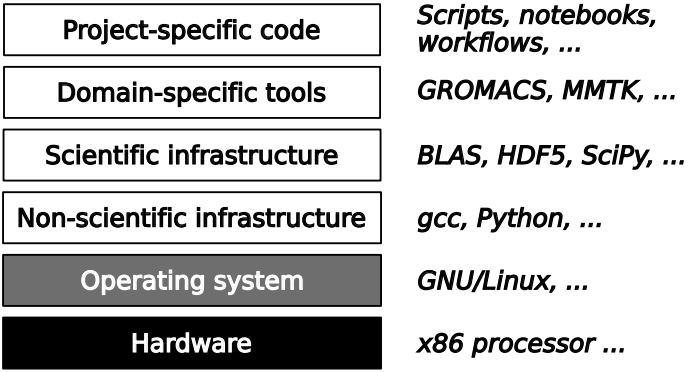
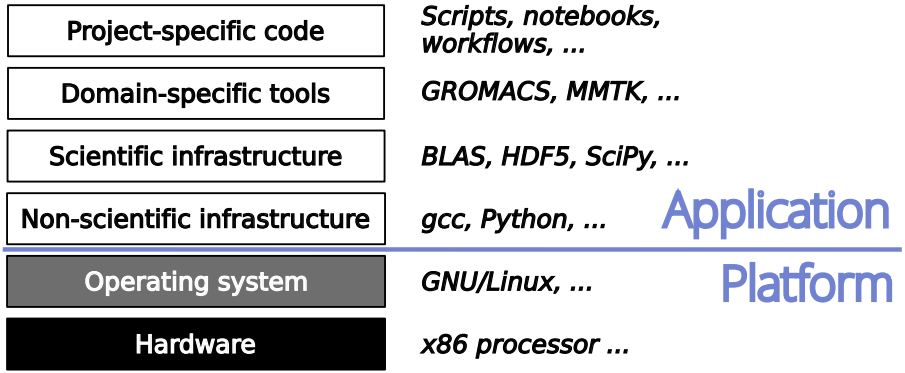
- Compatibility checks by version number and $\geq$ relations
- The build environment is not recorded...
- ... and is thus not reproducible ...
- ... meaning packages are not reproducible either !

A typical scientific software stack



Foundation : the platform



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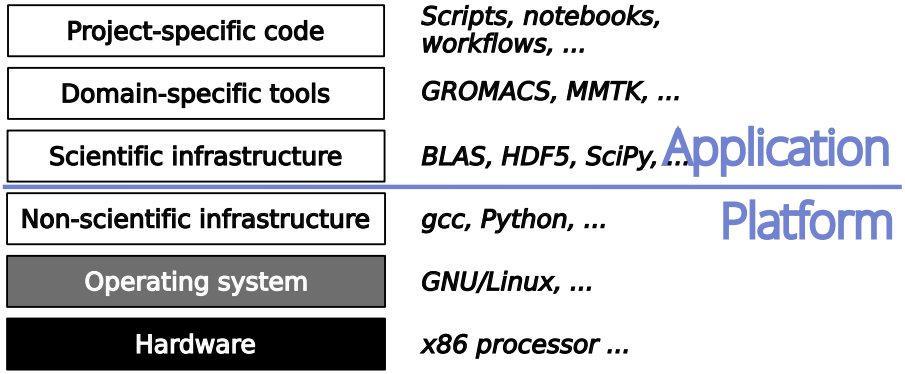

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The only OS that supports
reproducibility is **Linux** !

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Scripts, notebooks, workflows :

- Run in Guix/Nix containers
- Stored in a version-controlled repository
- Repository can also contain pure Python dependencies as source code

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- one environment level
- packages *not* reproducible

Guix

- Linux only
- recursive environments
- packages reproducible

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A Conda environment *without hashes* is cross-platform but not reproducible (and may fail).

Containers

Designed for deployment, not archiving

- Large binary files (“images”)
- In general not reproducible
- Not inspectable
- Not modifiable

Useful complement for an environment definition, but not a substitute !

Don’ts

- **Don’t confuse reproducibility with deployment for reuse**
- Don’t use Python-only package managers
- Don’t use packages that you cannot build yourself from source
- Don’t refer to “current” or “latest” versions
- Don’t use container images without a build recipe (`Dockerfile`)