

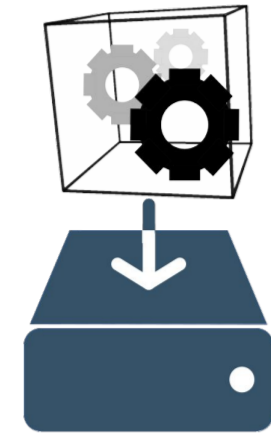
J.P. Almeida de Mendonça<sup>1</sup>, B. Arrondeau<sup>2</sup>, D. Bissuel<sup>3</sup>, J. Daubin<sup>4</sup>, D. Martin-Calle<sup>3</sup>

<sup>1</sup> SIMAP, Université Grenoble Alpes (UGA) - Grenoble INP - CNRS  
<sup>2</sup> GRICAD, Université Grenoble Alpes (UGA) - CNRS

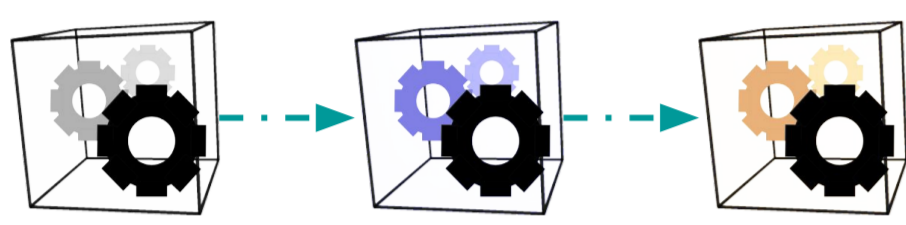
<sup>3</sup> ILM, Université Claude Bernard Lyon 1 - CNRS  
<sup>4</sup> SGLS/LESIM, CEA/DES Saclay

## Objectives

Easier tool **installation**



Easier code **chaining**



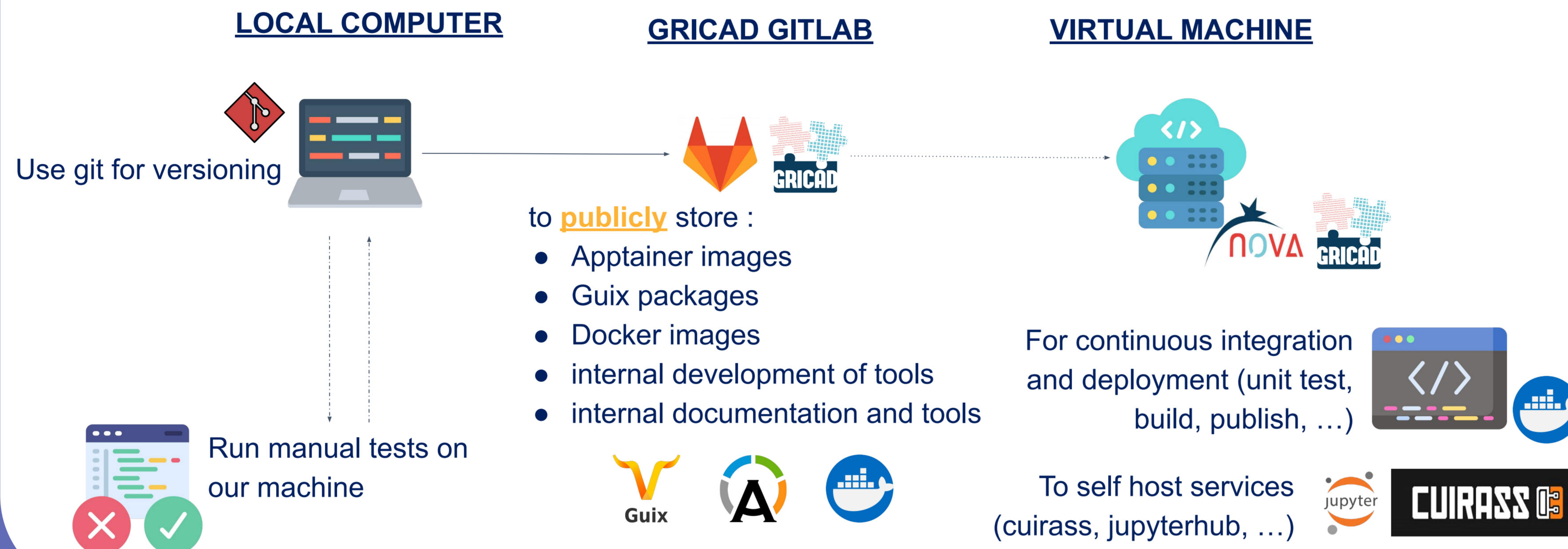
Interface for

- **documentation**
- tool **access**
- user **support**



## Infrastructure

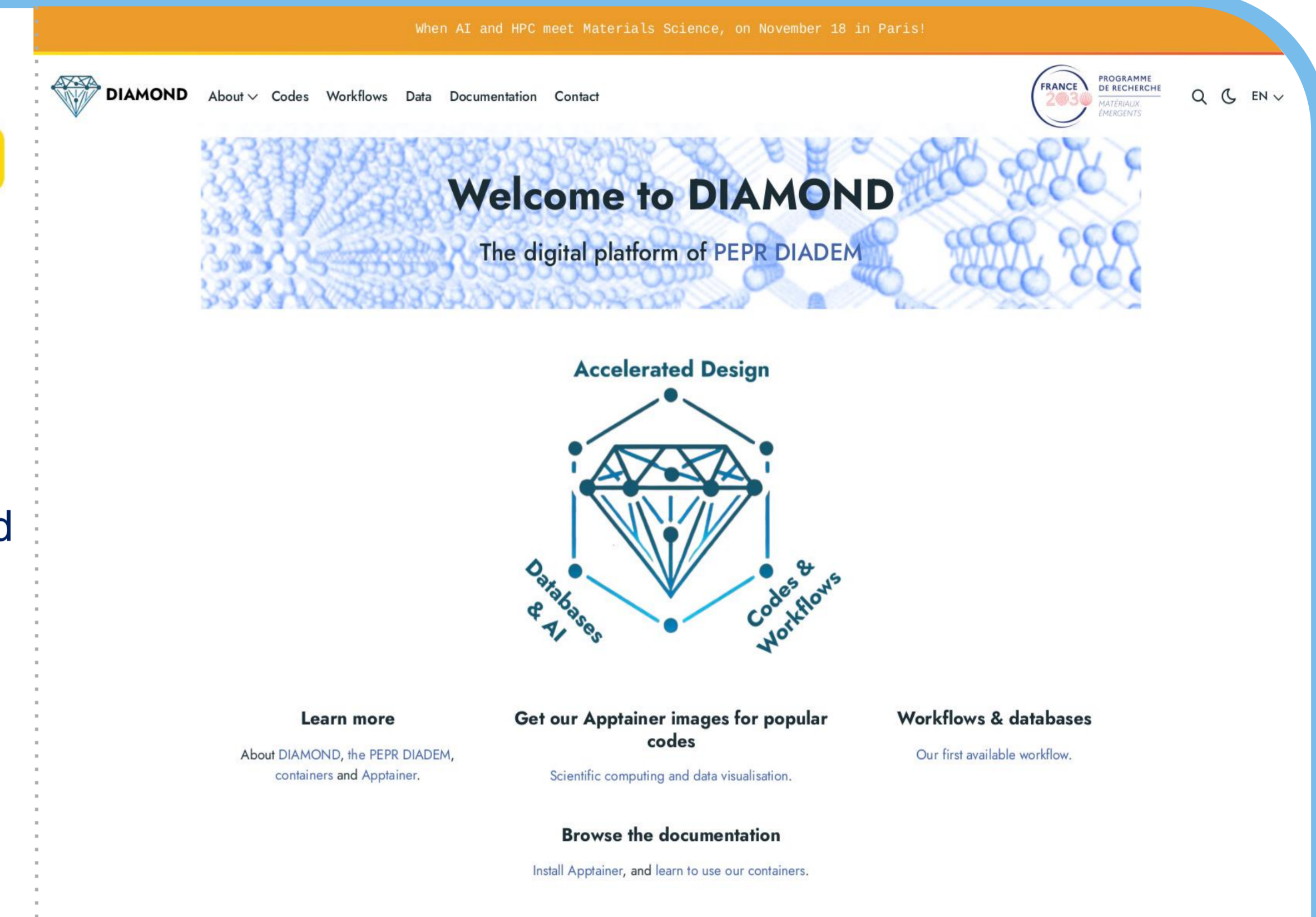
The platform is the **final tool** used by users. It should make everything **accessible** to users, help any user to **contribute** to the project, **report** bugs or **request** for new features. It is also important for the engineer as it makes it easier to **manage** people working on the project and **share resources** between them (for today and tomorrow).



## Website

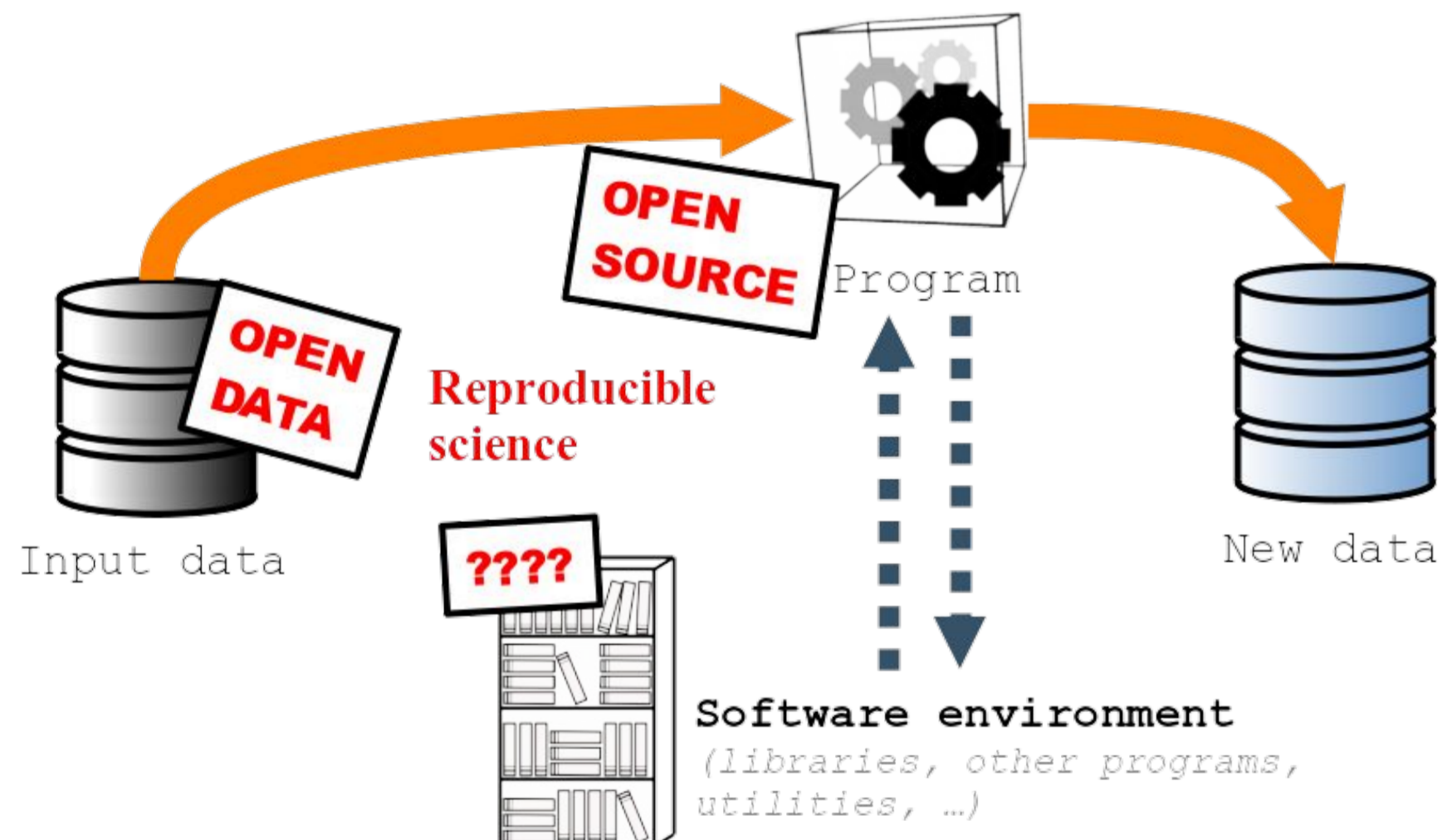
Built with **HUGO**  
Hosted on **GitHub**

- Makes **DIAMOND tools available** for the community.
- Provides **documentation** and **tutorials**.
- Provides **information** and hosts featured **news**.
- All the content is available in both **French** and **English**.
- **Light/dark** mode switch.



See our live demonstration!

## Code containers (and packages)



**Software environment** is important, impacting both **installation** (complex build/deploy processes) and **execution**, but is often forgotten when trying to **replicate results** (on a new machine and in time).

**Better software environment control**

- Install in one line.
- Deploy on any\* machine.
- Long-term\*\* stability.

→ **Freeze the software environment!**

**Packaging**

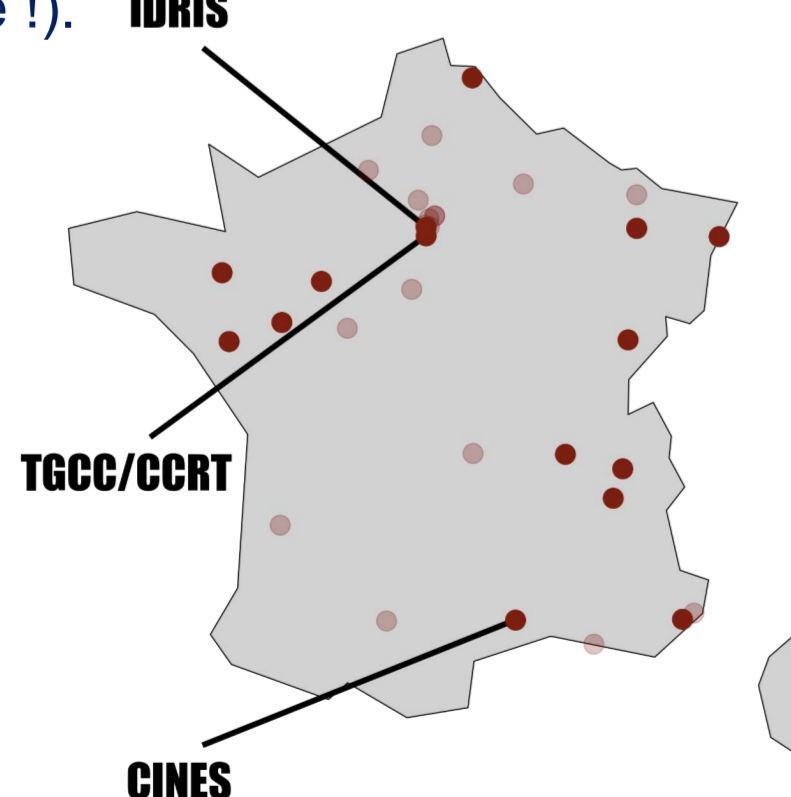
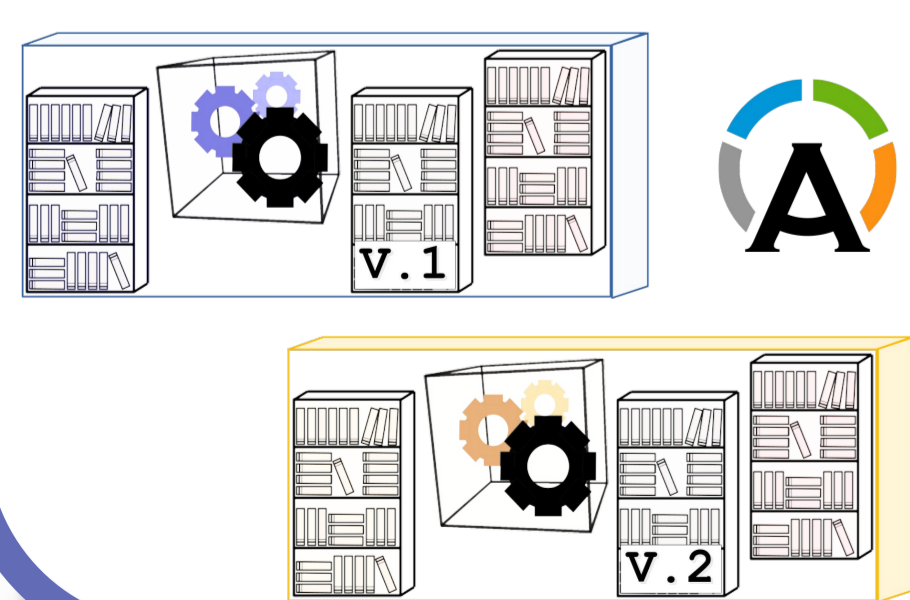
Automate the (un-)install and **update** of softwares and their dependencies with packages (archive files).

**Containerization**

Build immutable lightweight **images** that spawn **containers**, embedding an application and its dependencies (and nothing else!).

**Apptainer (HPC solution)**

```
$ apptainer pull <image>
$ apptainer run <image>
```

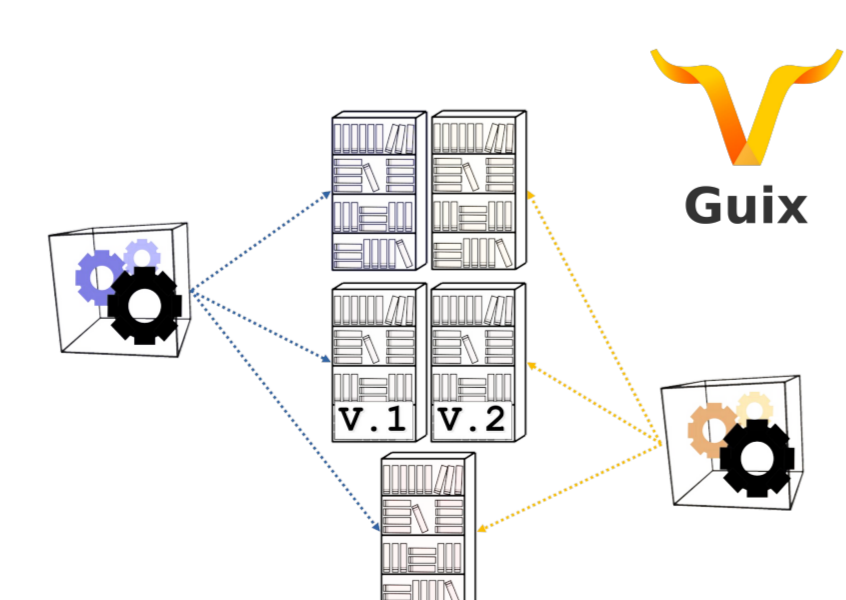


48.5% have a container system

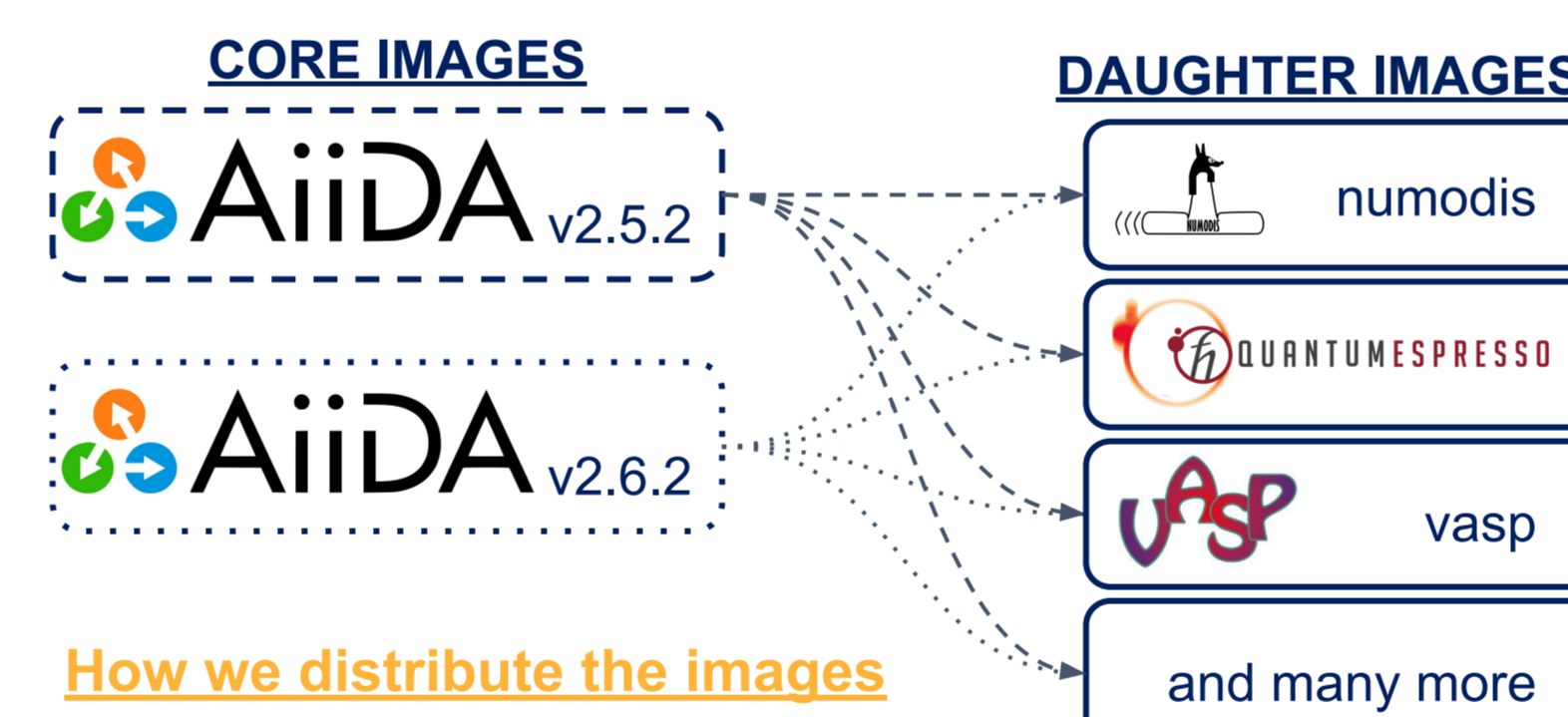
28.1% have guix

**Guix (HPC/repr. science)**

```
$ guix install <package>
$ <executable-name>
```



## Workflows



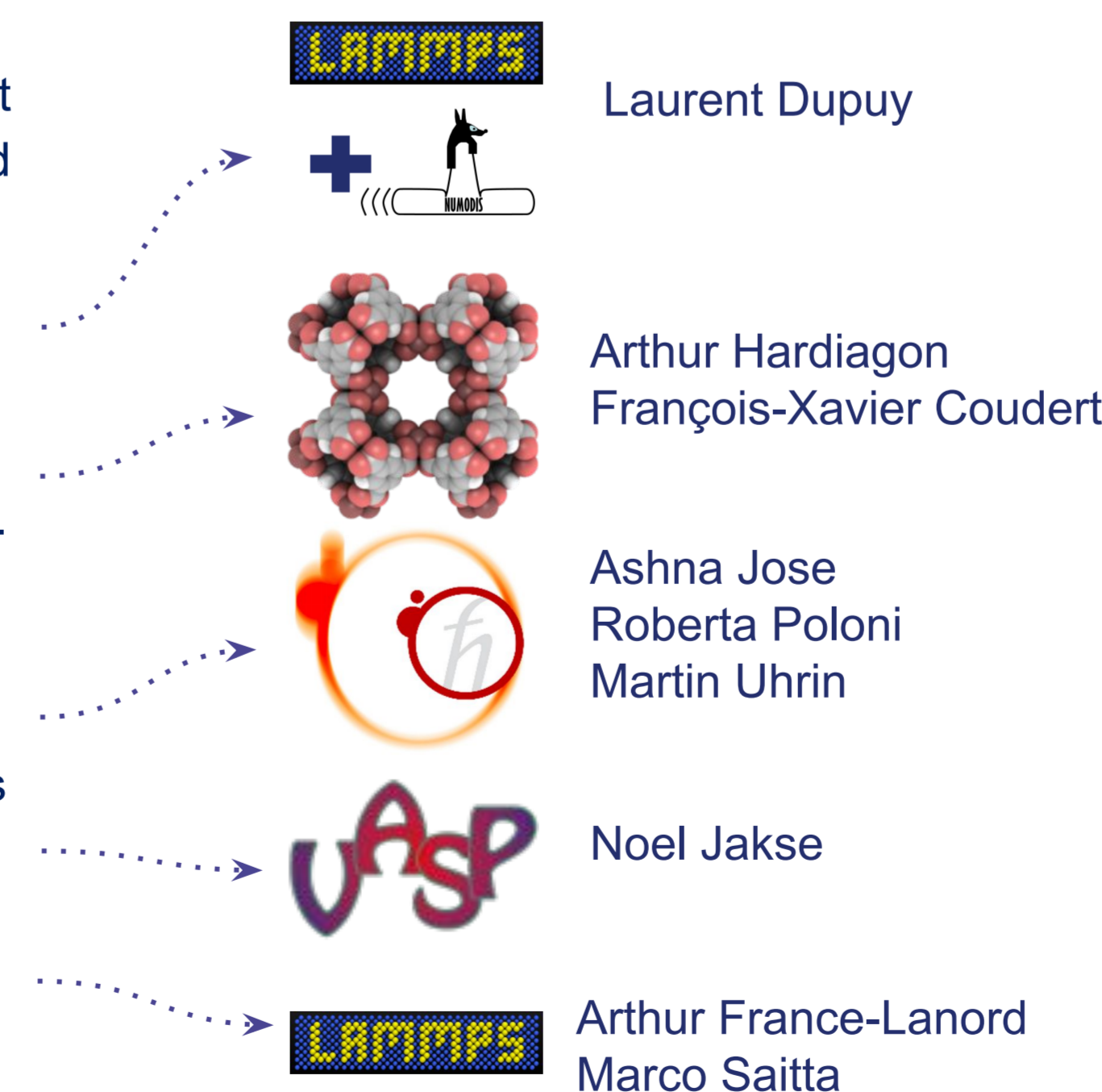
How we distribute the images

Producing high-quality datasets for machine learning models includes **automating the procedures** of data generation to make it **consistent** and **efficient**. For simulation data, WP1 aims to develop a series of **workflows**, using for now **AiiDA** as our engine of choice.

Scientific specialists:

Our engineers are currently involved in the development of a number of workflows, with the help of internal and external scientific specialists:

- **NUMODIS+LAMMPS workflow**, using aiida-numodis and aiida-lammps plugins.
- AiiDA version of **MOFLearning**:
  - already functional for load balancing using aiida-raspa.
  - Works locally and at Jean Zay
- **Quantum Espresso workflow**, for MOF electronic structures.
- **VASP workflow**, for post-processing molecular dynamics using geometry optimisation.
- **MLIP development workflow via n2p2** (by Akshay, in WP3)



## Acknowledgements

- Supervision** Noel Jakse, David Rodney, Pierre-Antoine Bouttier, Nicolas Crouzet
- Technical support** Pierre-Antoine Bouttier
- Connected projects** Akshay Krishna Ammothum Kandy, Arthur Hardiagon, Cinthya Herrera, Imanol Setoain, Irina Piazza
- Infrastructure host** IMAG, GRICAD mesocenter (UGA/Grenoble INP)

This work was supported by a grant from the French government managed by the National Research Agency under the France 2030 program with reference **ANR-22-PEXD-0015**.



Visit the DIAMOND website  
[diamond-diadem.github.io](https://diamond-diadem.github.io)



Our YouTube channel  
[youtube.com/@diamond-diadem](https://youtube.com/@diamond-diadem)



Access our Gitlab projects  
[gricad-gitlab.univ-grenoble-alpes.fr/diamond](https://gricad-gitlab.univ-grenoble-alpes.fr/diamond)

