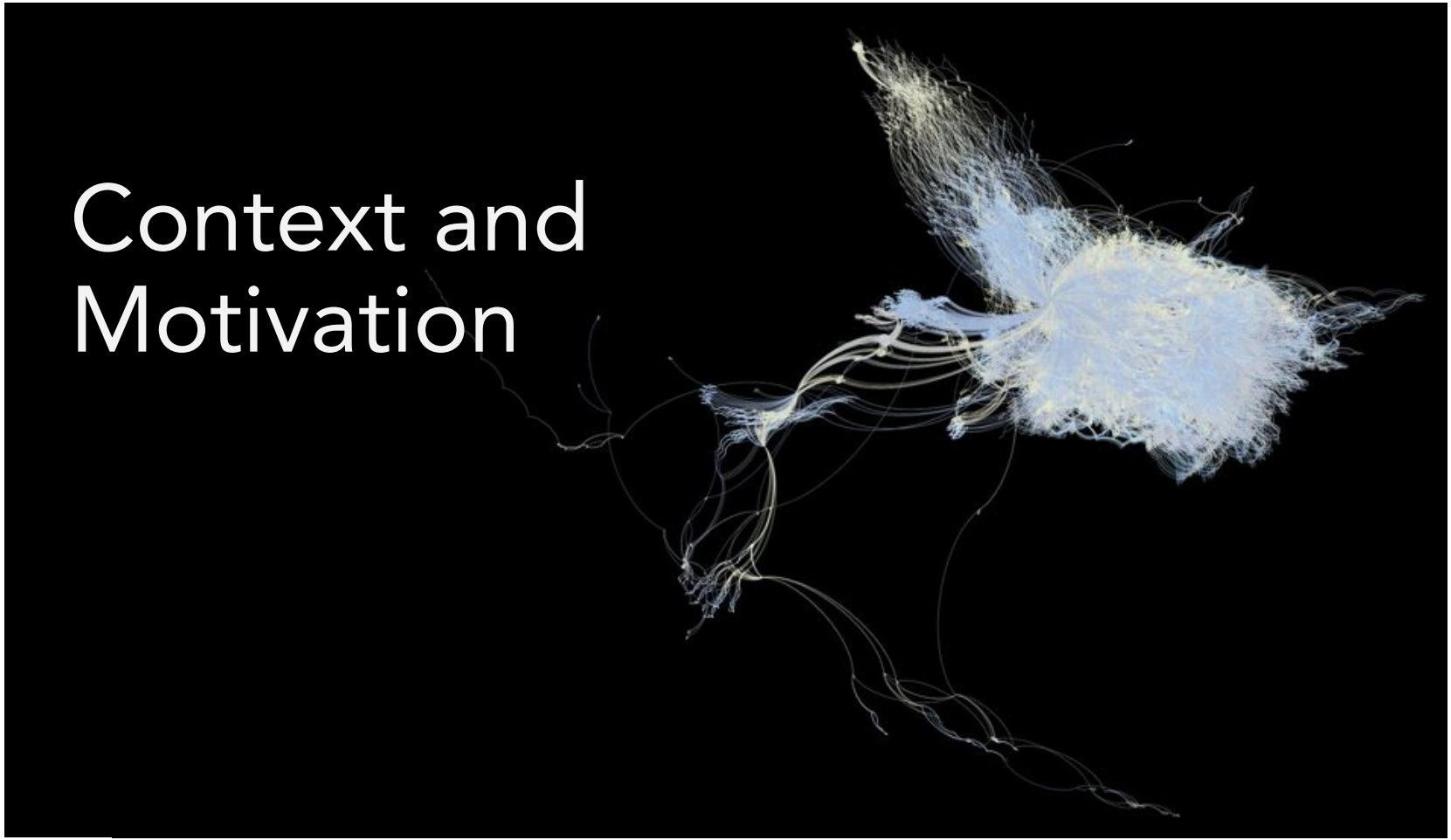
Introduction to AiiDA

Francisco Ramirez

MARVEL NATIONAL CENTRE OF COMPETENCE IN RESEARCH · MaX DRIVING THE EXASCALE TRANSITION · swissuniversities · FNSNF Swiss National Science Foundation · INTERSECT · MarketPlace · EPFL

Context and Motivation



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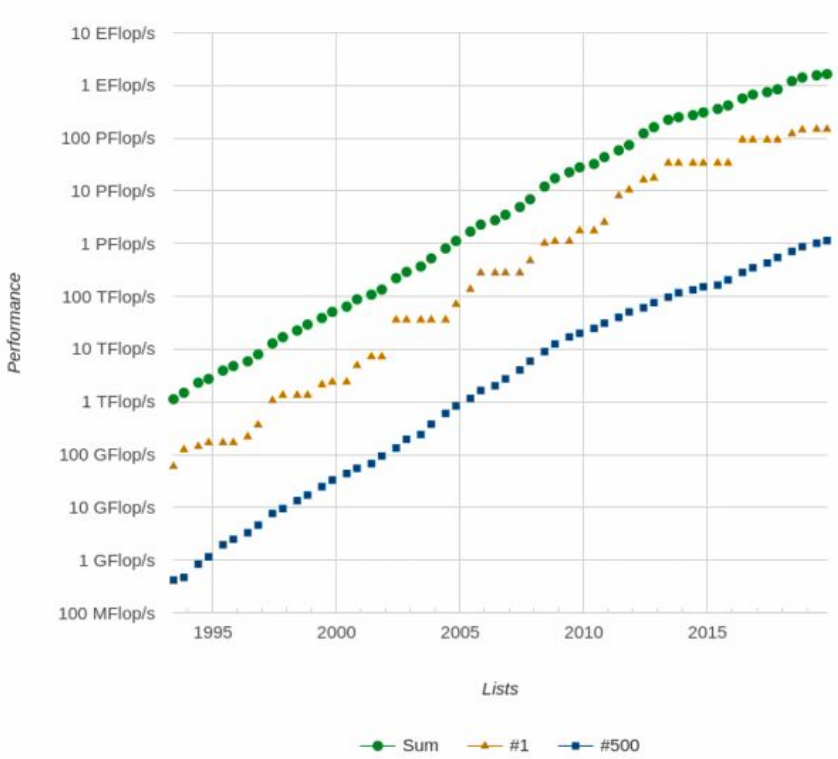
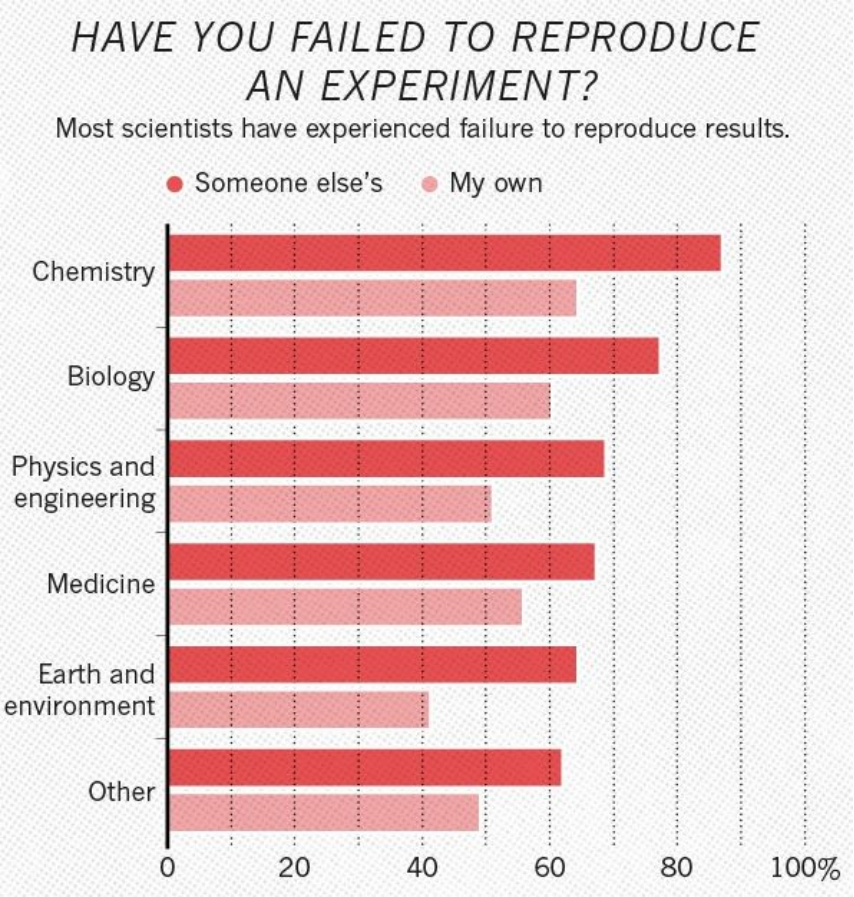
The rise of HTC and HPC

- Computational resources keep becoming more powerful: new tools needed to efficiently utilize them.
- This allows to push the boundaries of research:
  - more complex and precise calculations (HPC)
  - more extensive studies of larger samples (HTC)
- Community of material sciences: one of the most invested in this endeavor.



[1] https://www.top500.org/

A Crisis of Reproducibility



- Reproducibility: key property of the scientific method.
- Computational sciences: best equipped to address this problem (high levels of control over variables VS real life experiments).
- Even so, reproducibility is also difficult to achieve for them: why is that?

Nature 533, 452–454 (26 May 2016) doi:10.1038/533452a

The Provenance Model

- In order to see how this two elements interact, we need first to understand the complexity of scientific research.
- We need to model the procedures involved in research work...

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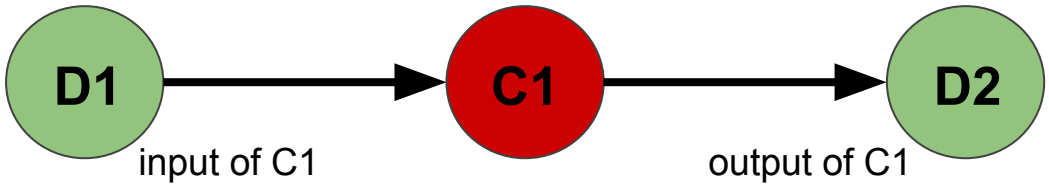

Information not only on the nodes but also on the links!

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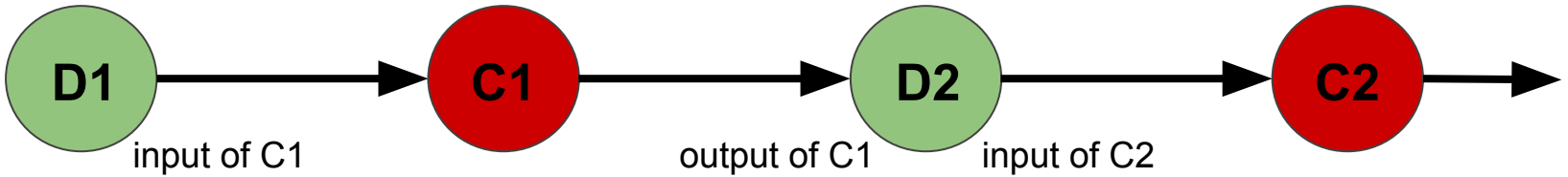

Organizing Information

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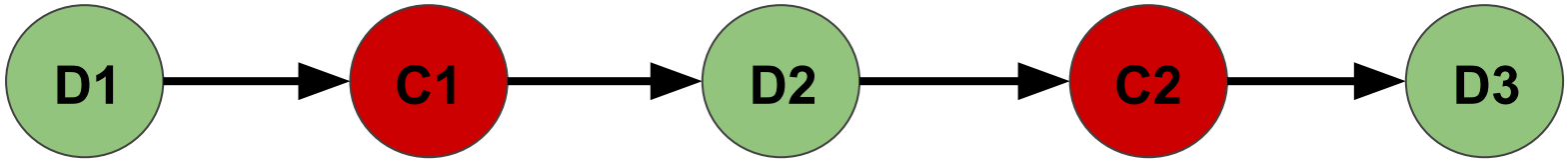
- Typical organizational system: folder structure (not well suited to represent these workflows).



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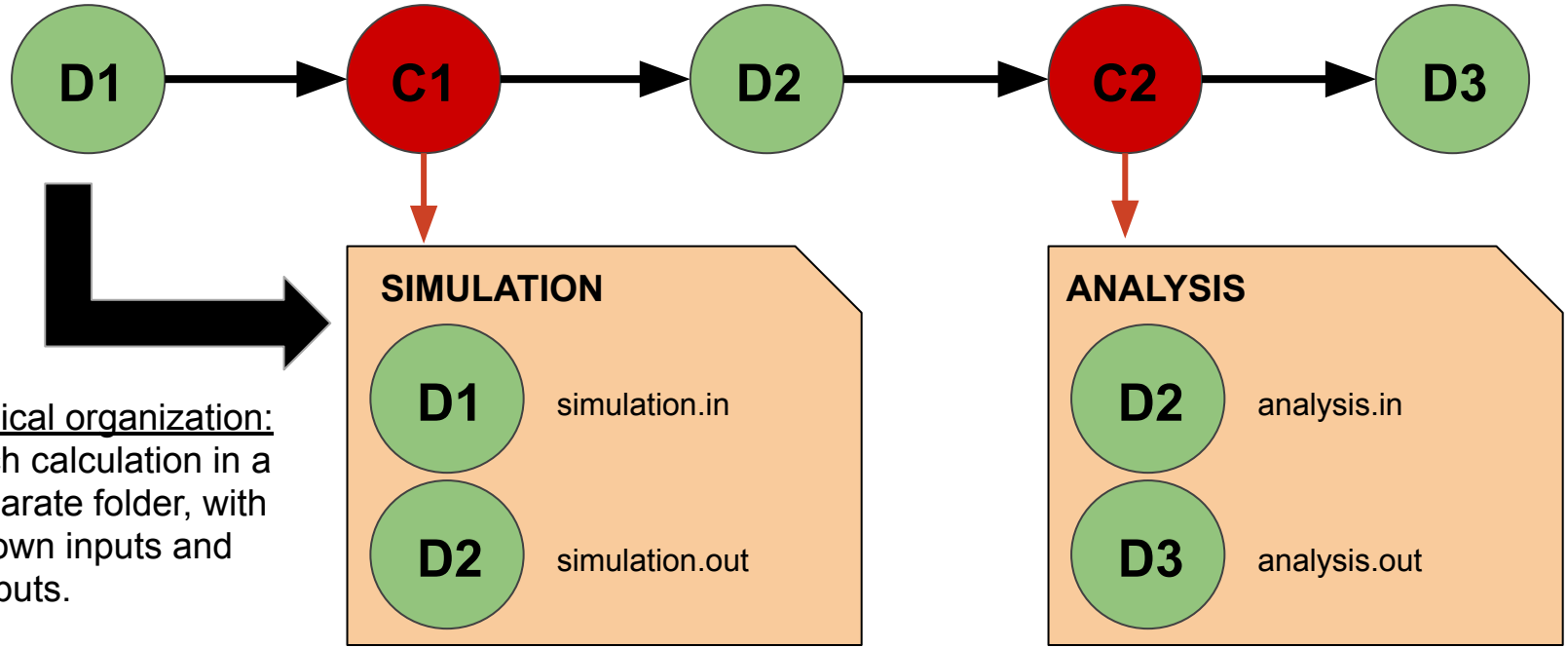

Typical organization: each calculation in a separate folder, with its own inputs and outputs.

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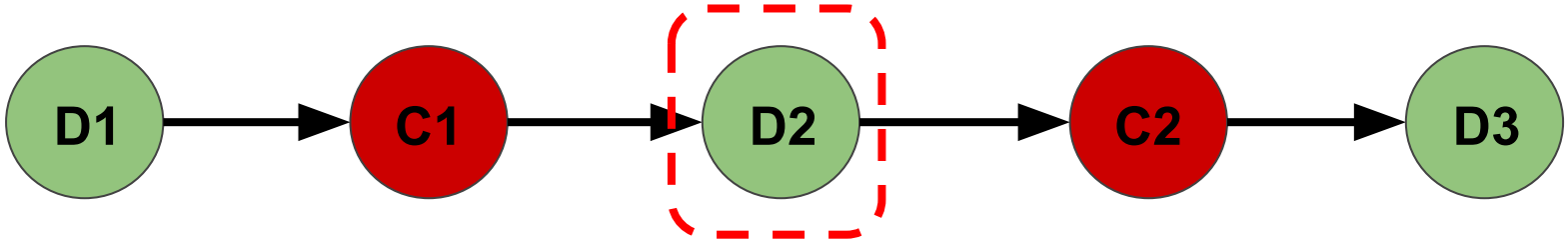
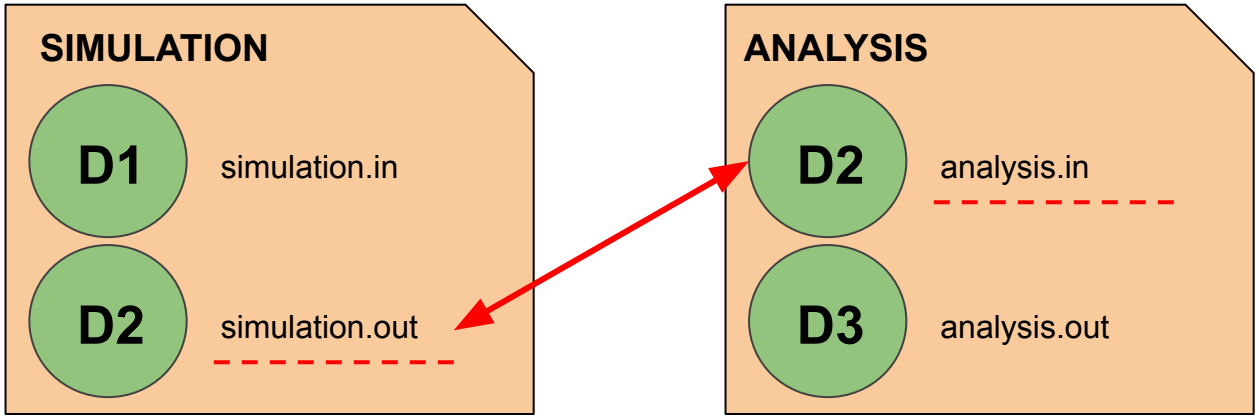


Problem:
The connections between pieces of information gets lost.
Other approaches possible: you always sever links.



The Complexity of Research

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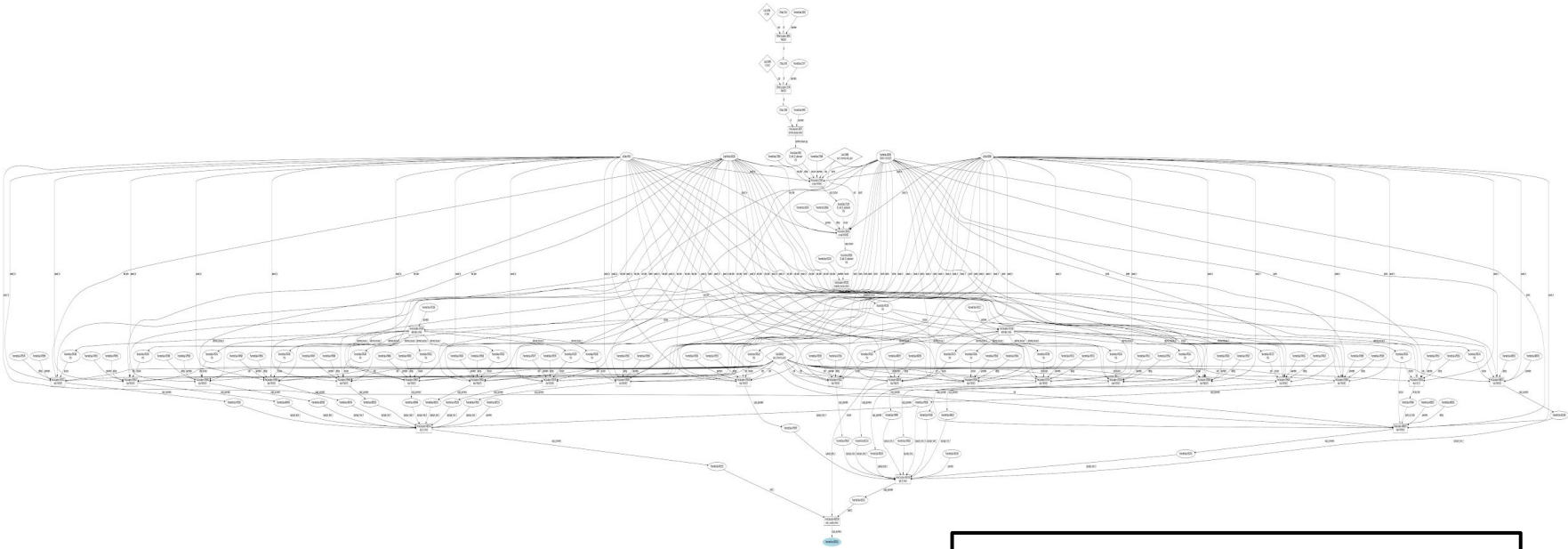
- Real scientific workflows can be much more complex…



Calculation of the elastic constant for 1 material

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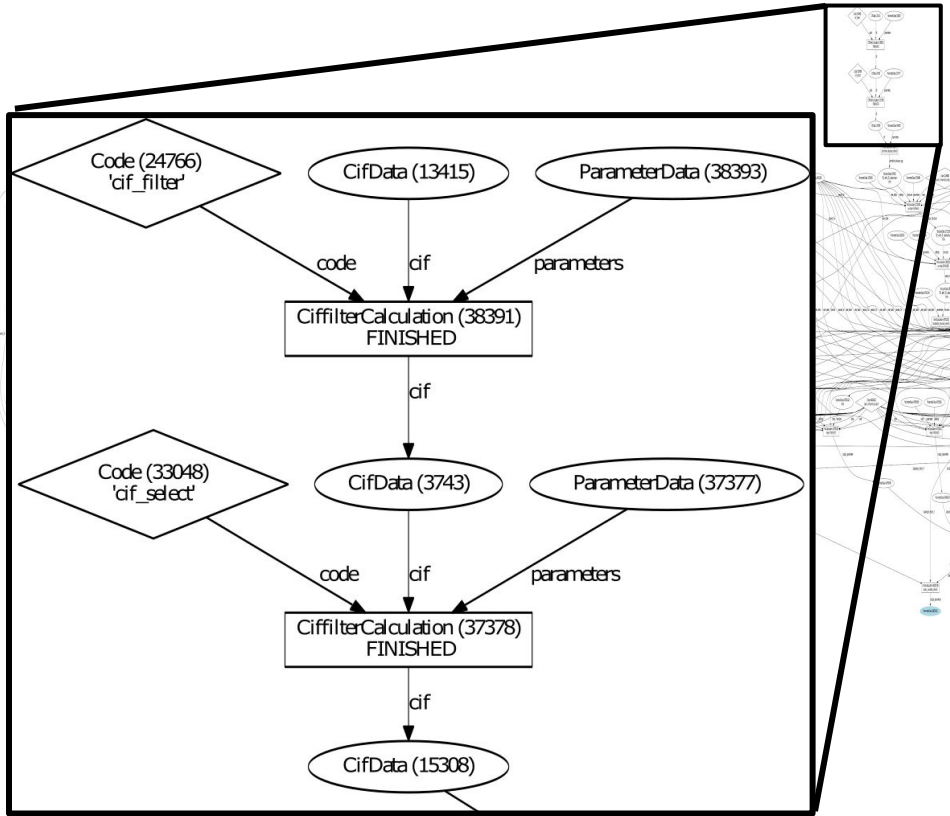

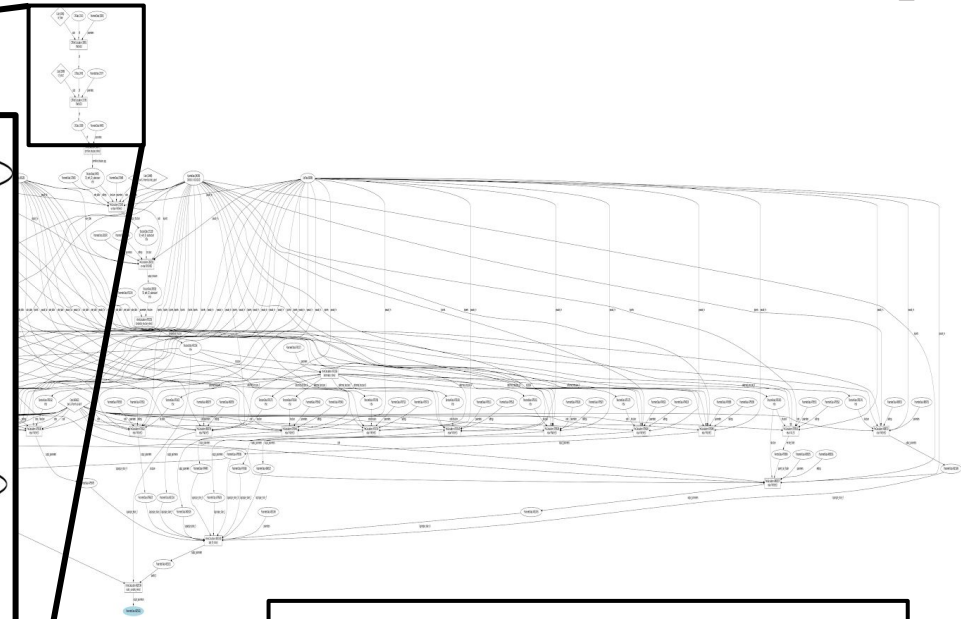

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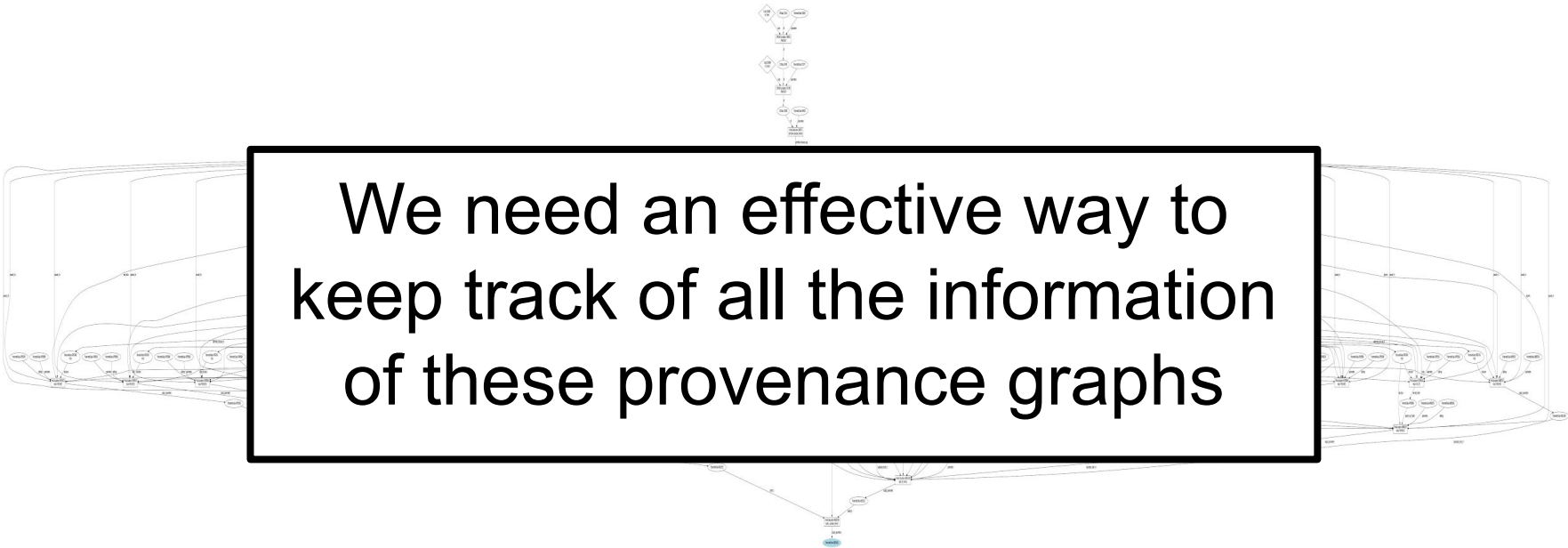

We need an effective way to keep track of all the information of these provenance graphs

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The Platform

AiiDA

General Overview

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What AiiDA is...

- Python Library (pip-installable)
- ORM for scripting
- Command line interface

What AiiDA does...

- Controls remote resources and manages calculation jobs
- Tracks the provenance and organizes the data.

General Overview

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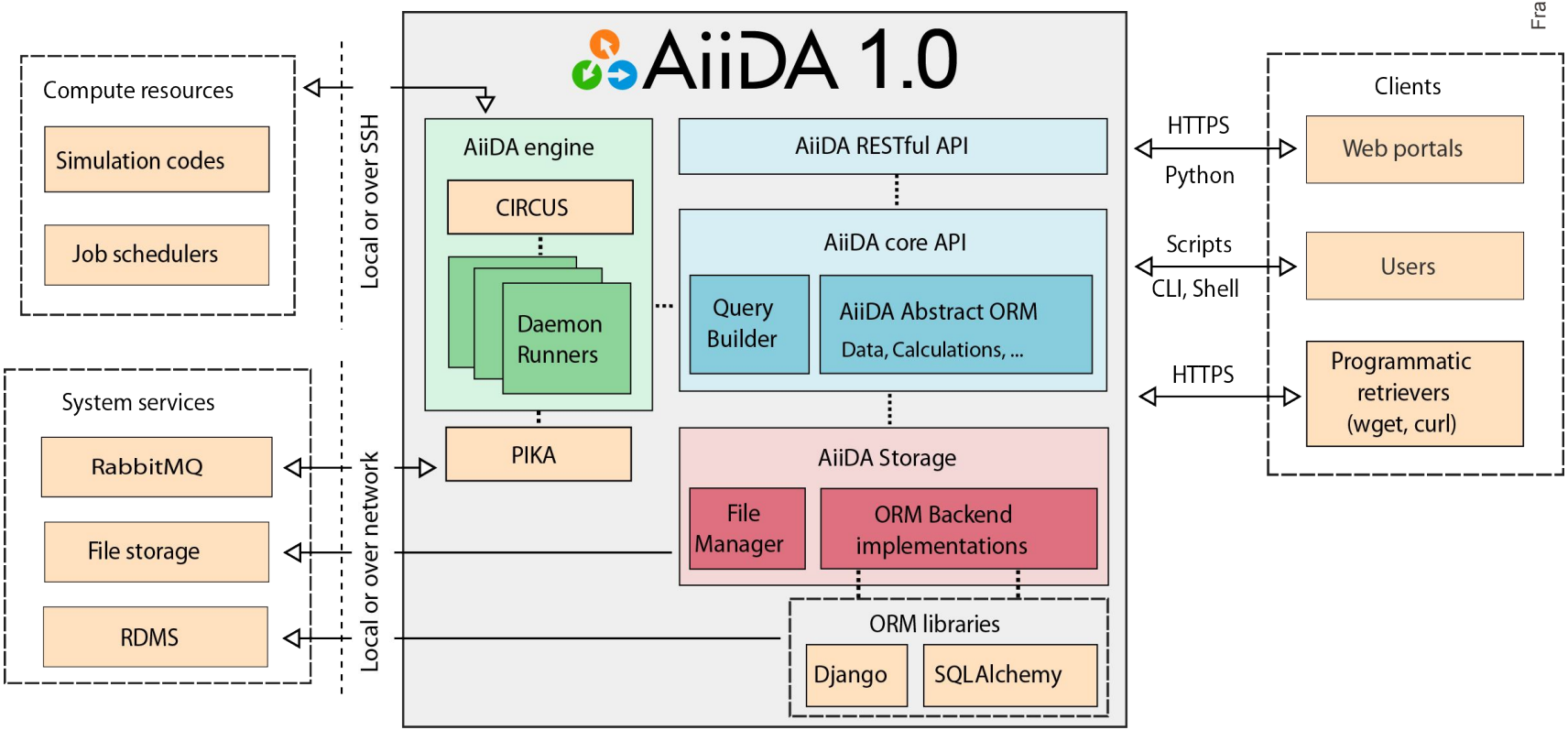

How it works

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```
cmd$
```

procedure_tracked.py

```
def times2( number ):
    return 2 * number


def plus1( number ):
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data0 = 10
data1 = times2(number=data0)
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```
cmd$ python procedure.py

     21
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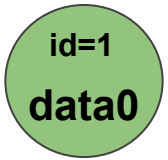

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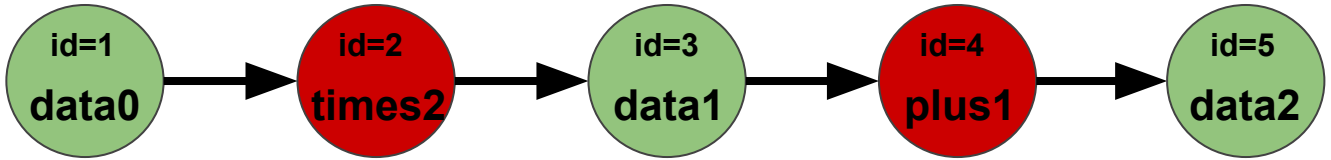

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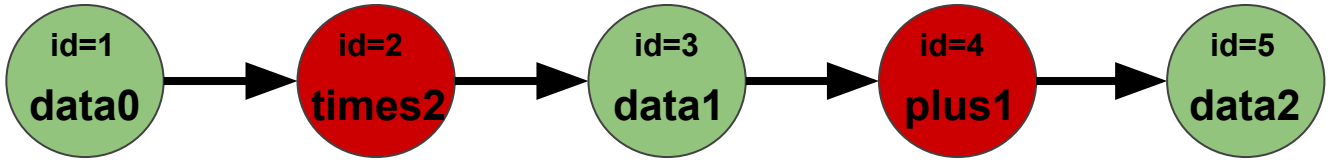

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Database:

How it works

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```
cmd$ verdi run procedure_tracked.py

cmd$ verdi process list -a

                  Process  Process
  Id    Created   Label    State
 ---- --------- -------- ----------
  2    2m ago    times2   Finished [0]
  4    2m ago    plus1    Finished [0]

cmd$
```

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```

Database:

How it works

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```
cmd$ verdi process show 2

   Property        Value
  ------------    -----------------
    type            times2
    state           Finished [0]
    (...)           (...)

   Inputs          Id       Type
  ------------    ------   --------
    number          1        Int

   Outputs         Id       Type
  ------------    ------   --------
    result          3        Int
```

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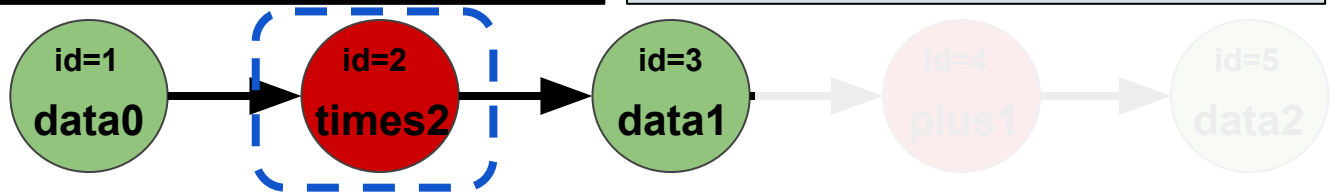

How it works

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```
cmd$ verdi node attributes 1

     “value”: 10

cmd$ verdi node attributes 3

     “value”: 20
```

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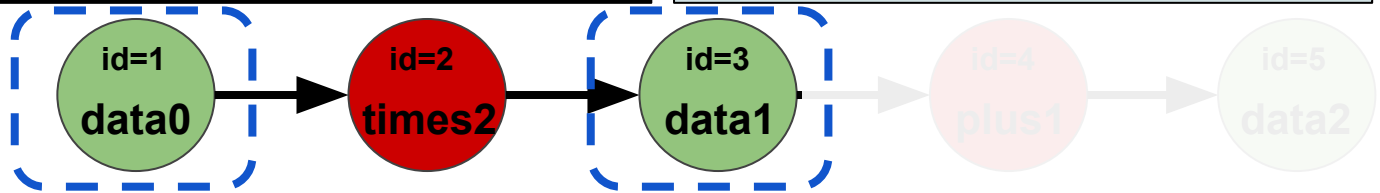

How it works

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```
cmd$ verdi node repo cat 2 src

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     (...)

cmd$
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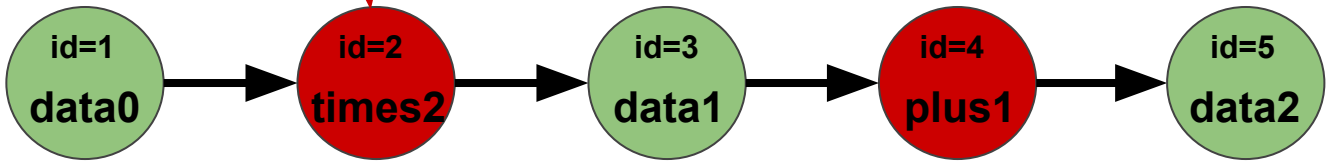
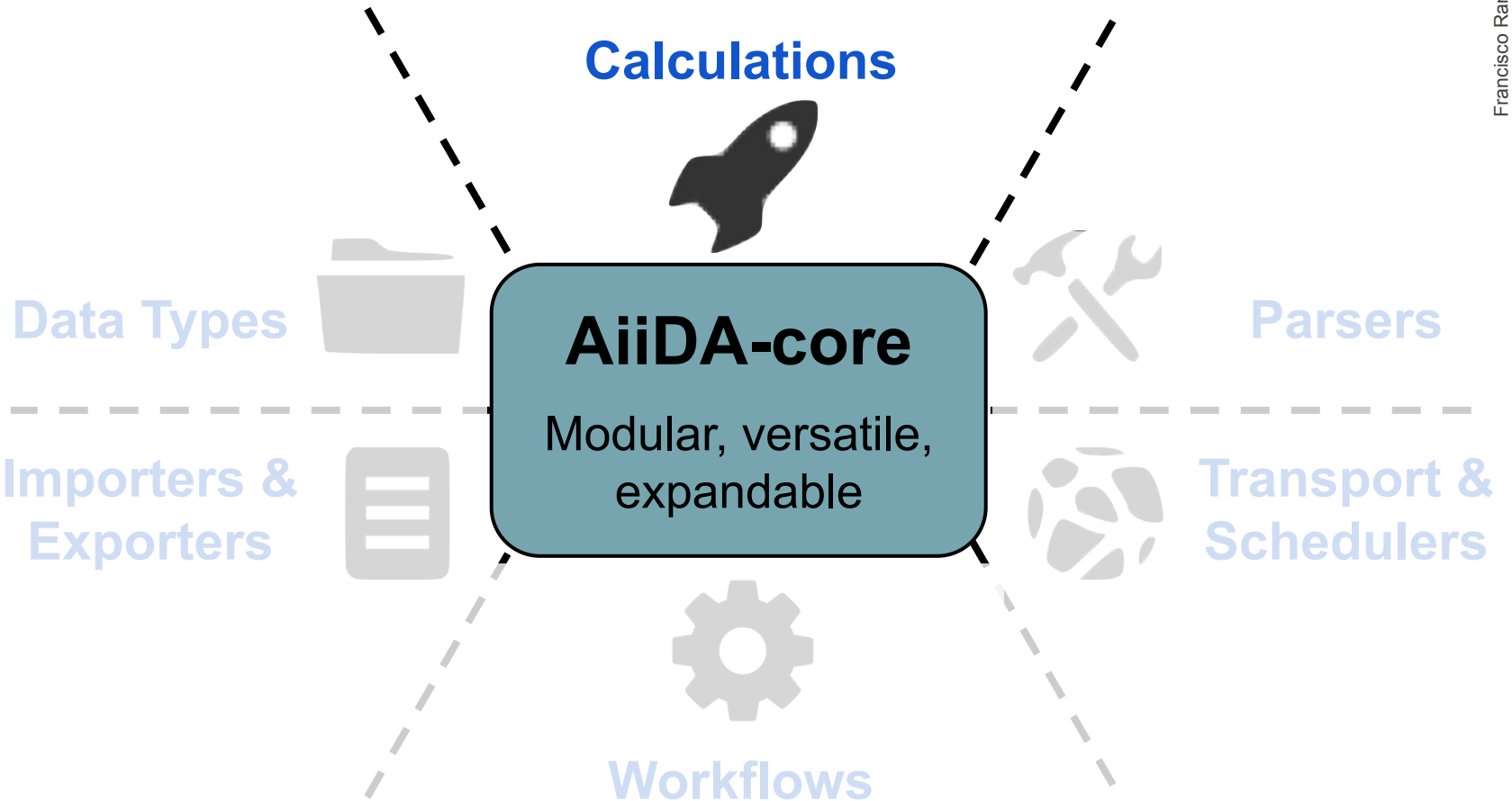


Extensibility & Plugins



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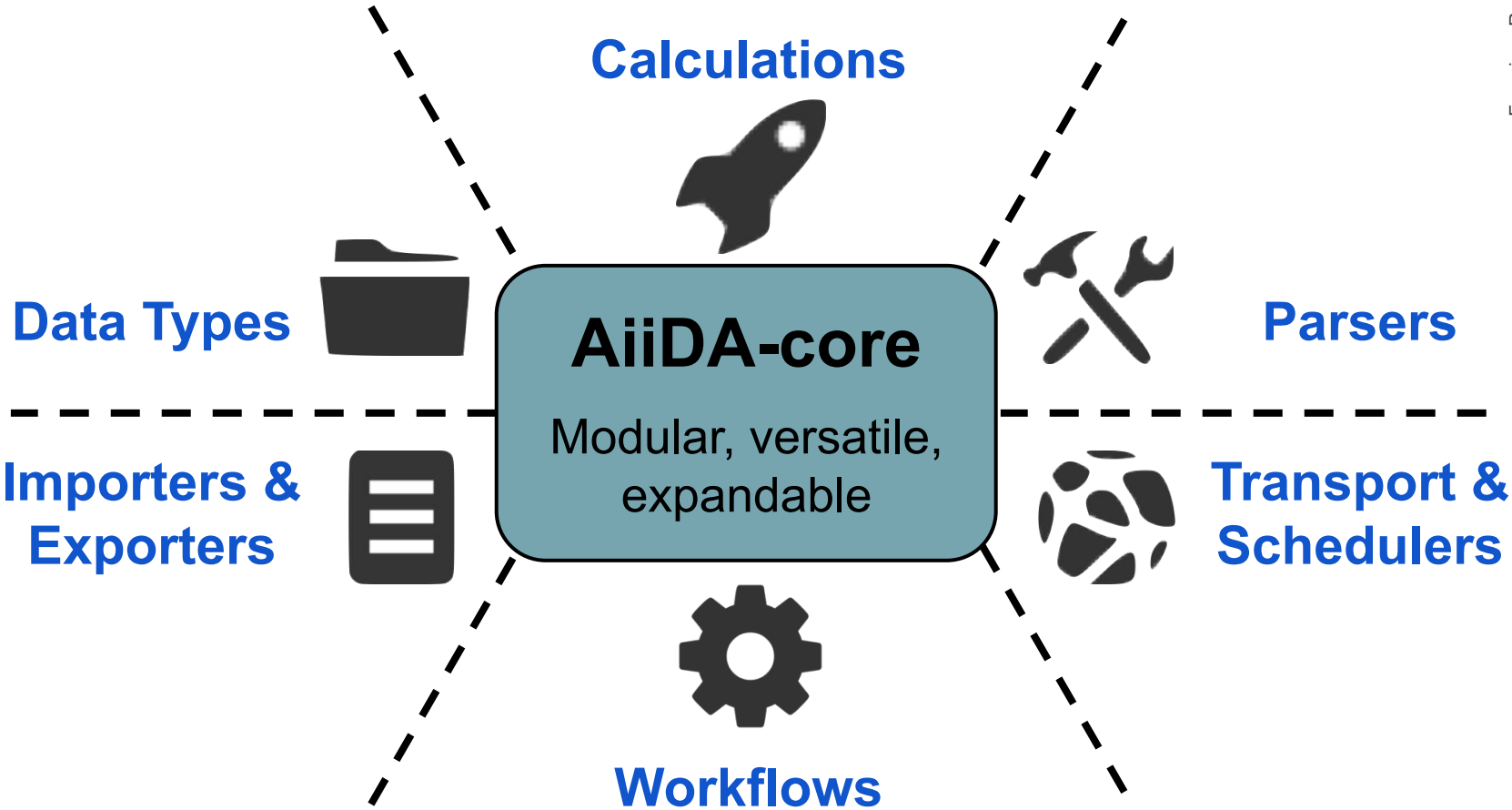

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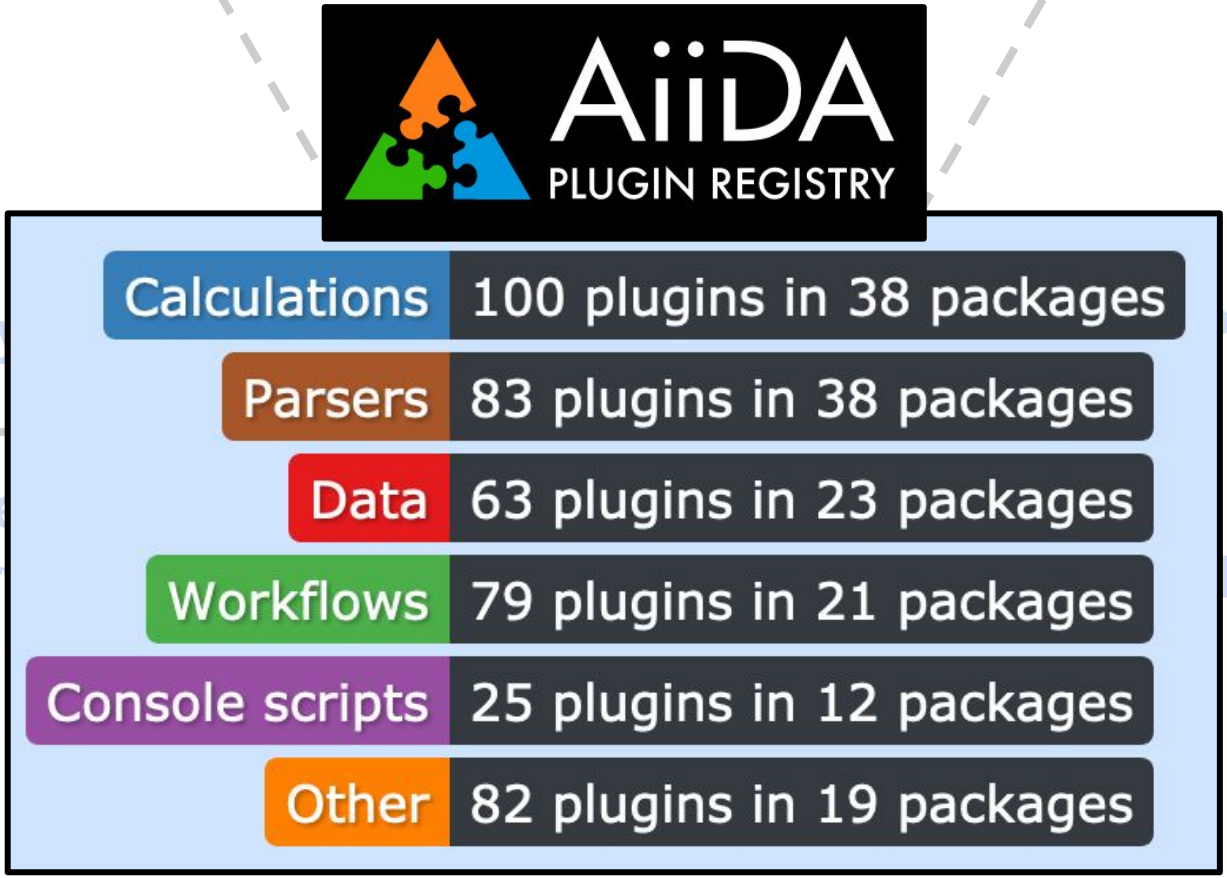

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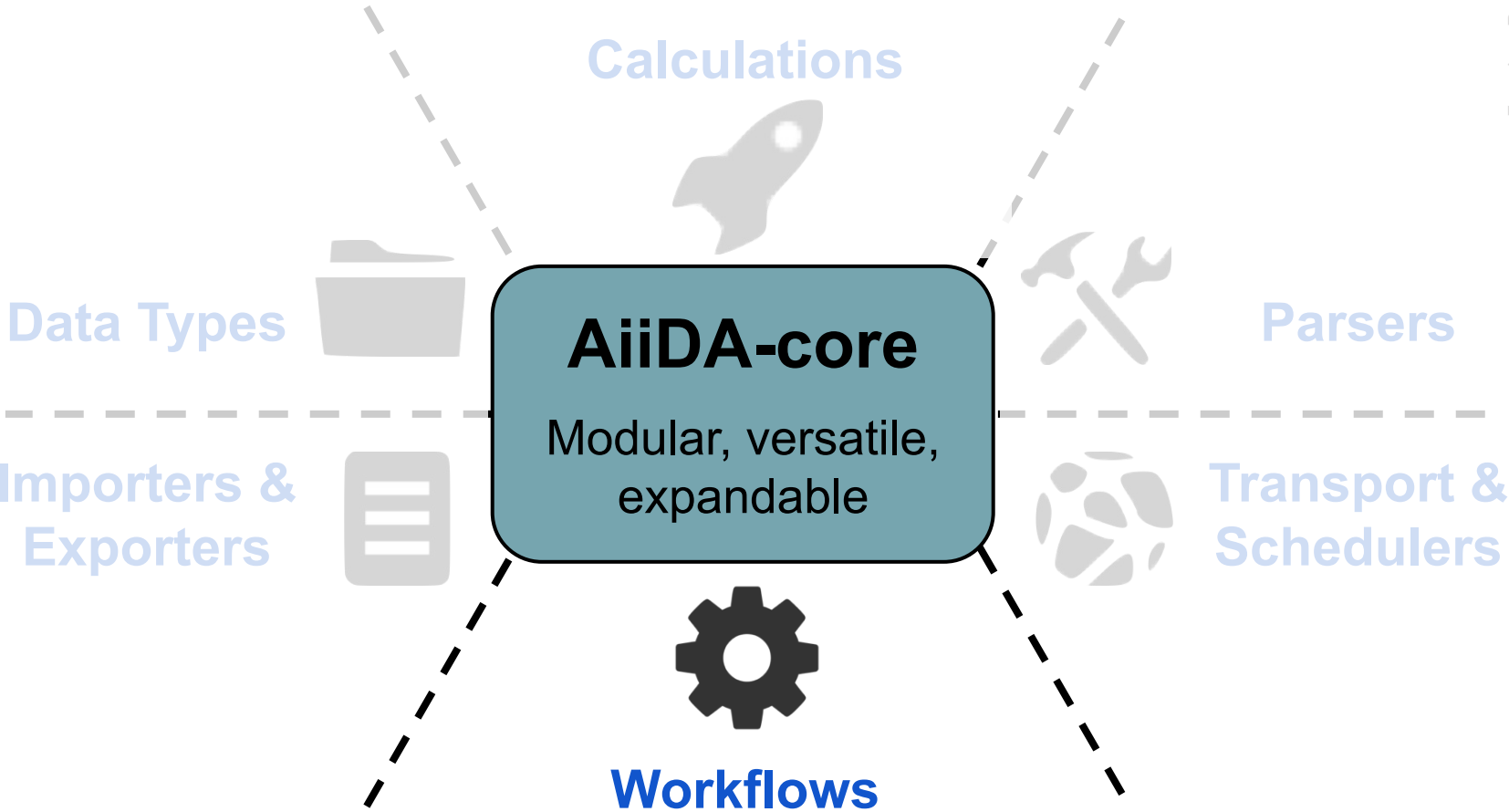

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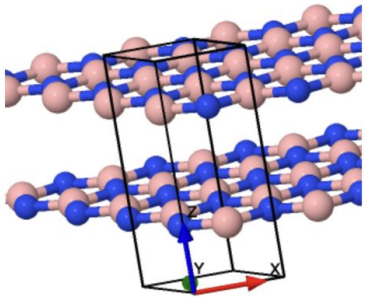
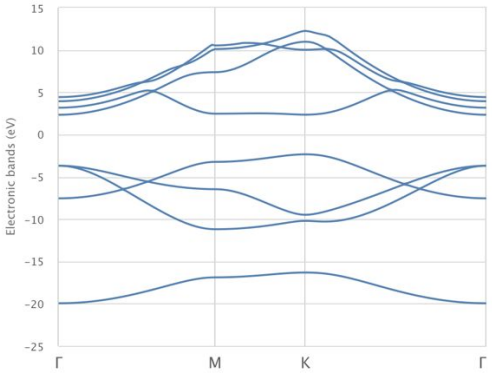
Introducing Workflows





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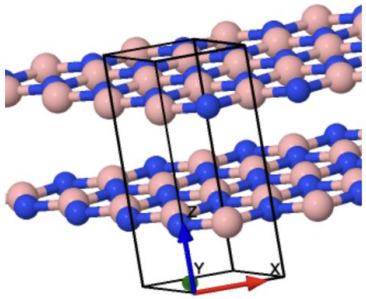

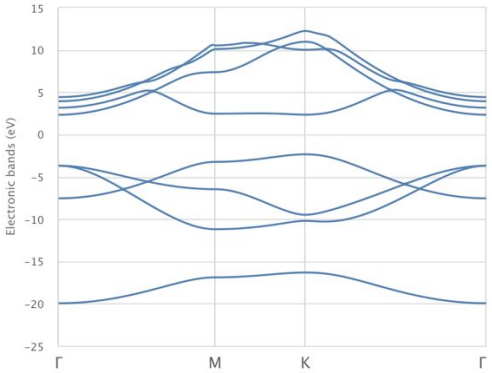

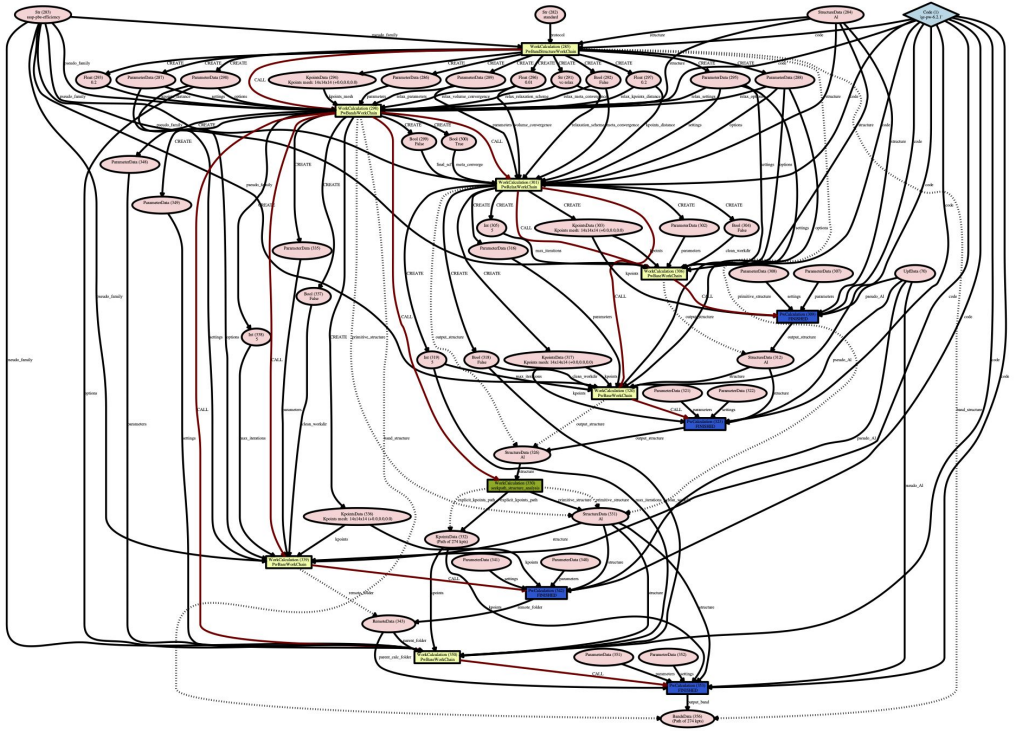

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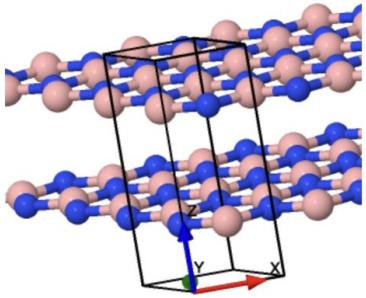

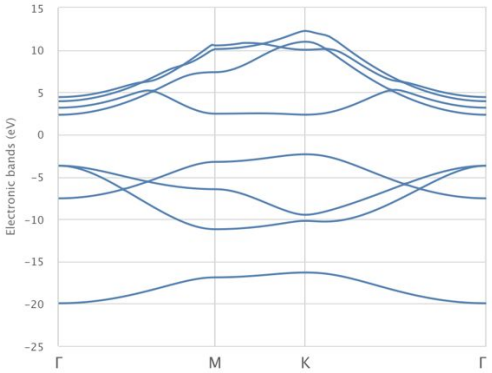

- Scripting environment: allows to automate the full process involved (optimizing a geometry, calculating a property, etc).
- Hide complexity (computational and scientific) from the end user, makes tools available for a wider audience.
- AiiDA supports Workflows nodes and the concept of logical provenance.

Introducing Workflows

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workflow.py

```
def workflow_x2p1( data0 ):
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        data2 = plus1(number=data1)
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procedure_tracked.py

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```
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```

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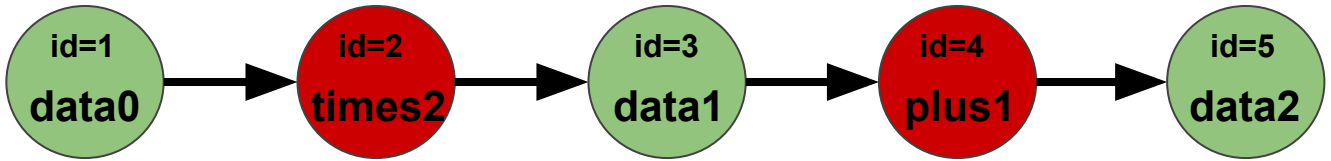

Introducing Workflows

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workfunc.py

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Introducing Workflows

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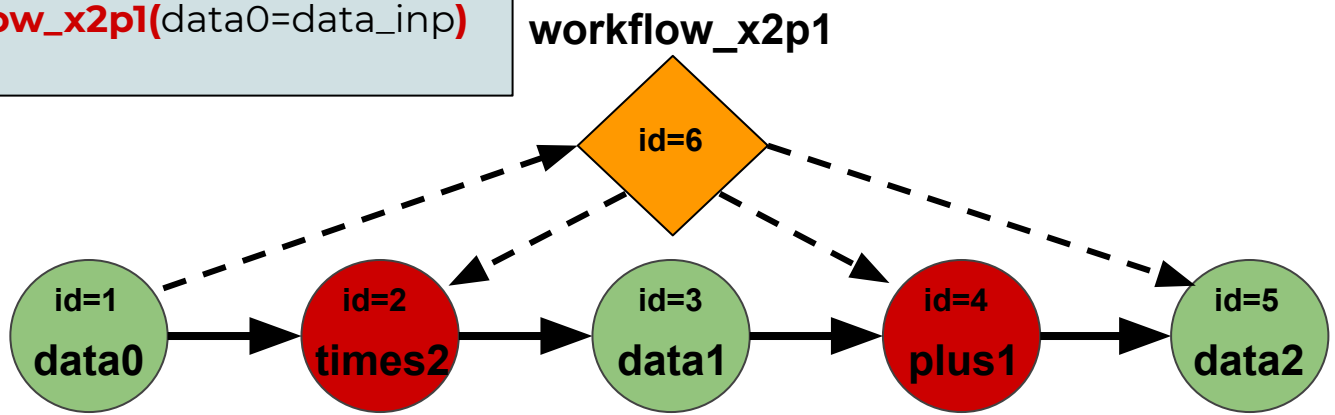
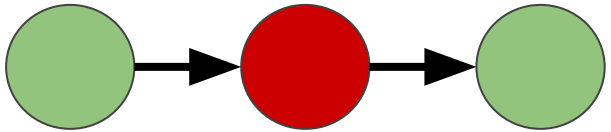


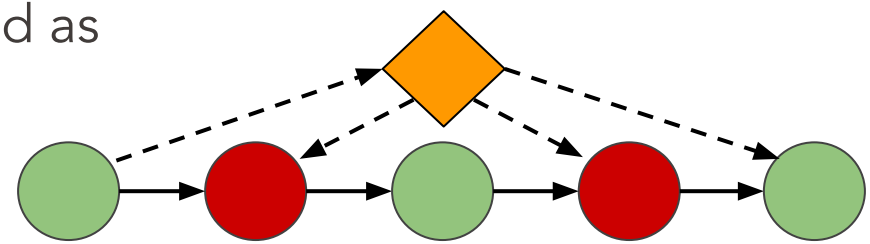
Summary of main features

- Locally controls remote resources, with an engine that centralizes its management.

- Automatically tracks the provenance and provides tools to explore it.



- Supports the implementation of high-level workflows to be used as turn-key solutions.



Funding and Online Resources

MARVEL

MARVEL National Centre for Competency in Research

MaX

European Centre of Excellence MaX

EPFL

École Polytechnique Fédérale de Lausanne

FNSNF

SWISS NATIONAL SCIENCE FOUNDATION

swissuniversities

MarketPlace

INTERSECT

erc

European Research Council

Established by the European Commission

European Research Council

pasc

Platform for Advanced Scientific Computing

PRACE

PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

nffa.eu

nanoscience foundries & fine analysis

EMMC

The European Materials Modelling Council

AiiDA 1.x

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WEBSITE
http://www.aiida.net

MATERIALS CLOUD
https://materialscloud.org

SOURCE CODE
github.com/aiidateam/aiida-core

DOCUMENTATION
https://aiida.readthedocs.io

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