Introduction to AiiDA

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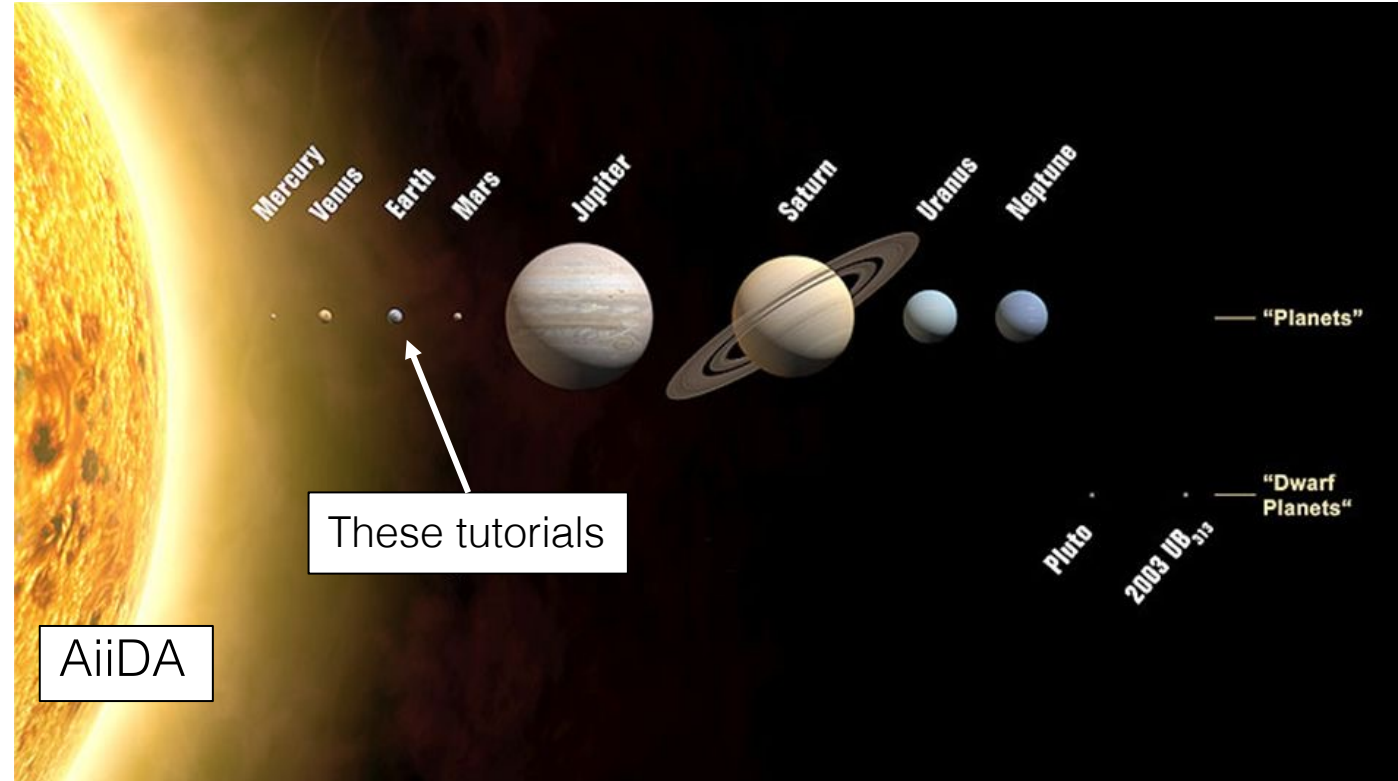
PHY90563

18 March 2022

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➢ T3 – data provenance

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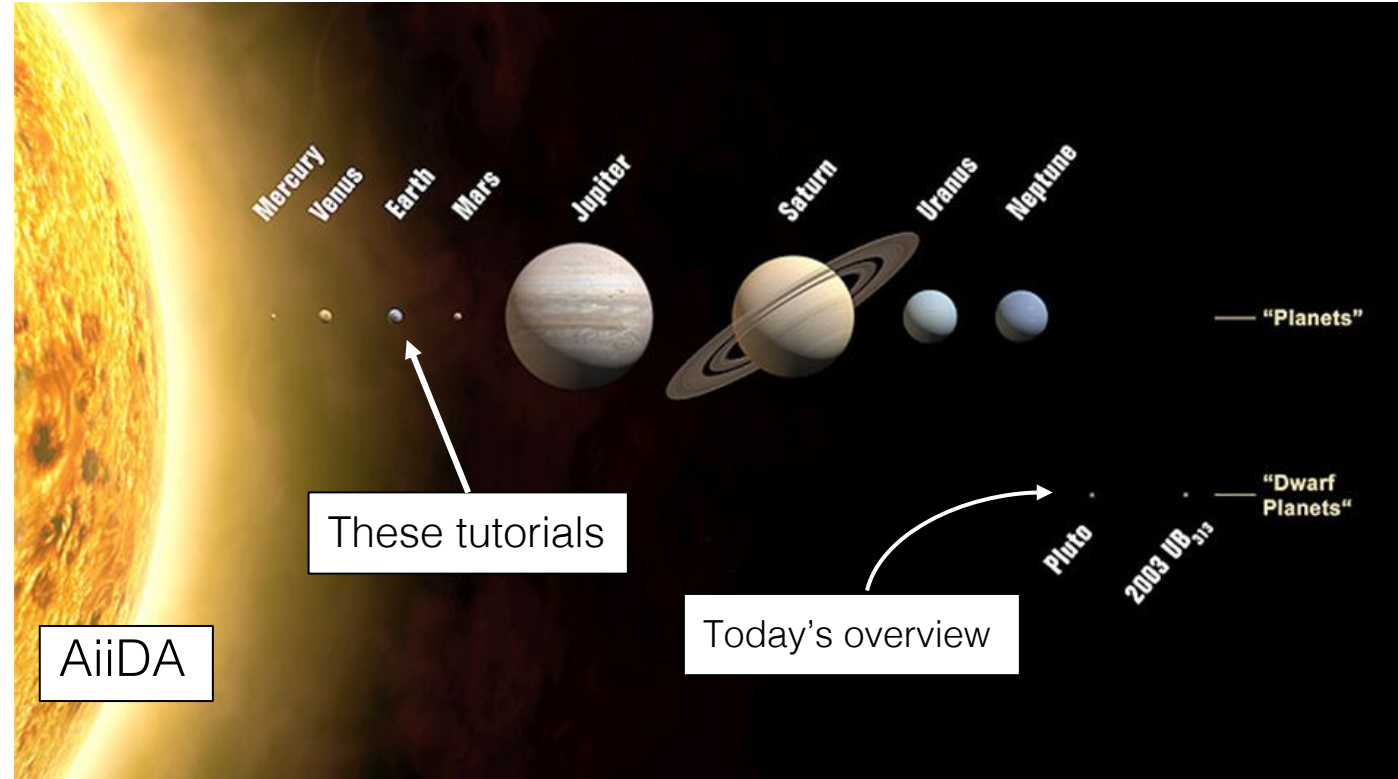
➢ Outlook – real use cases

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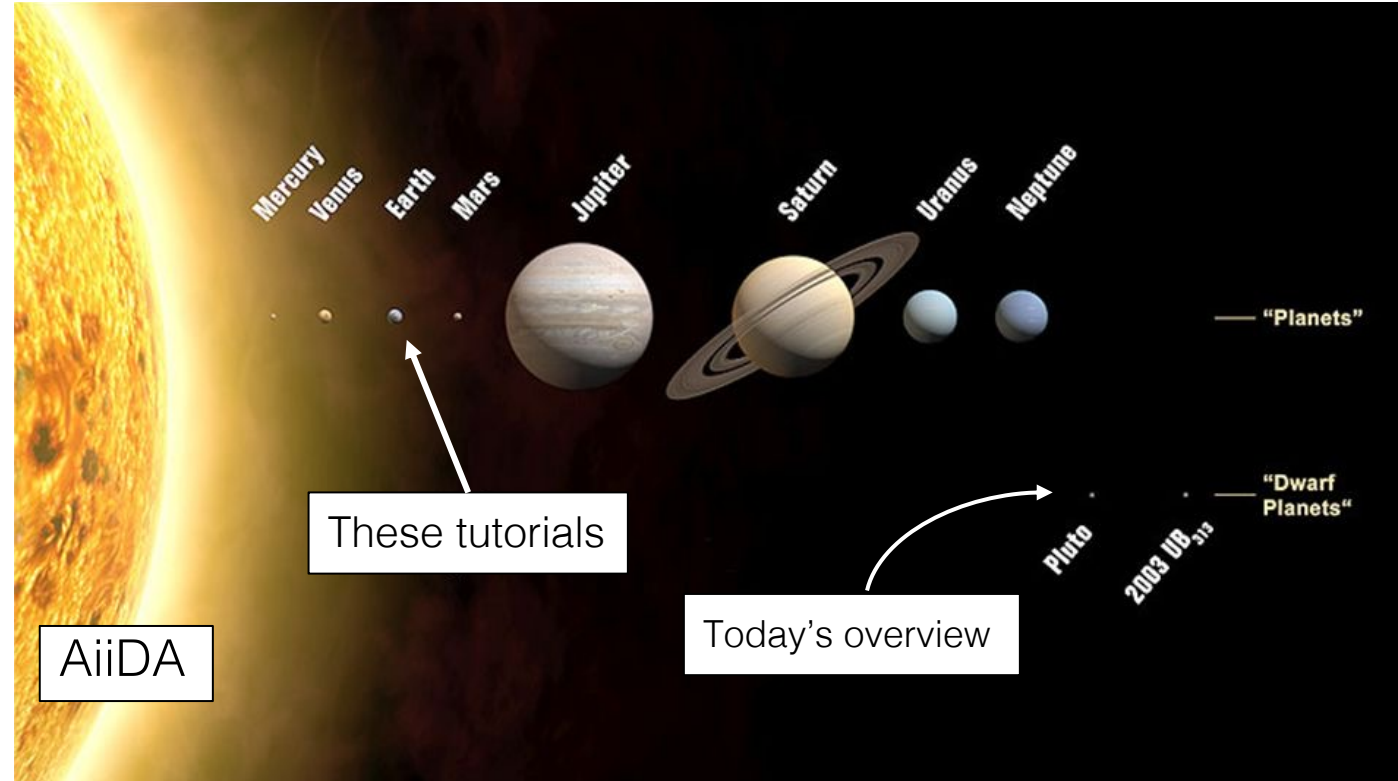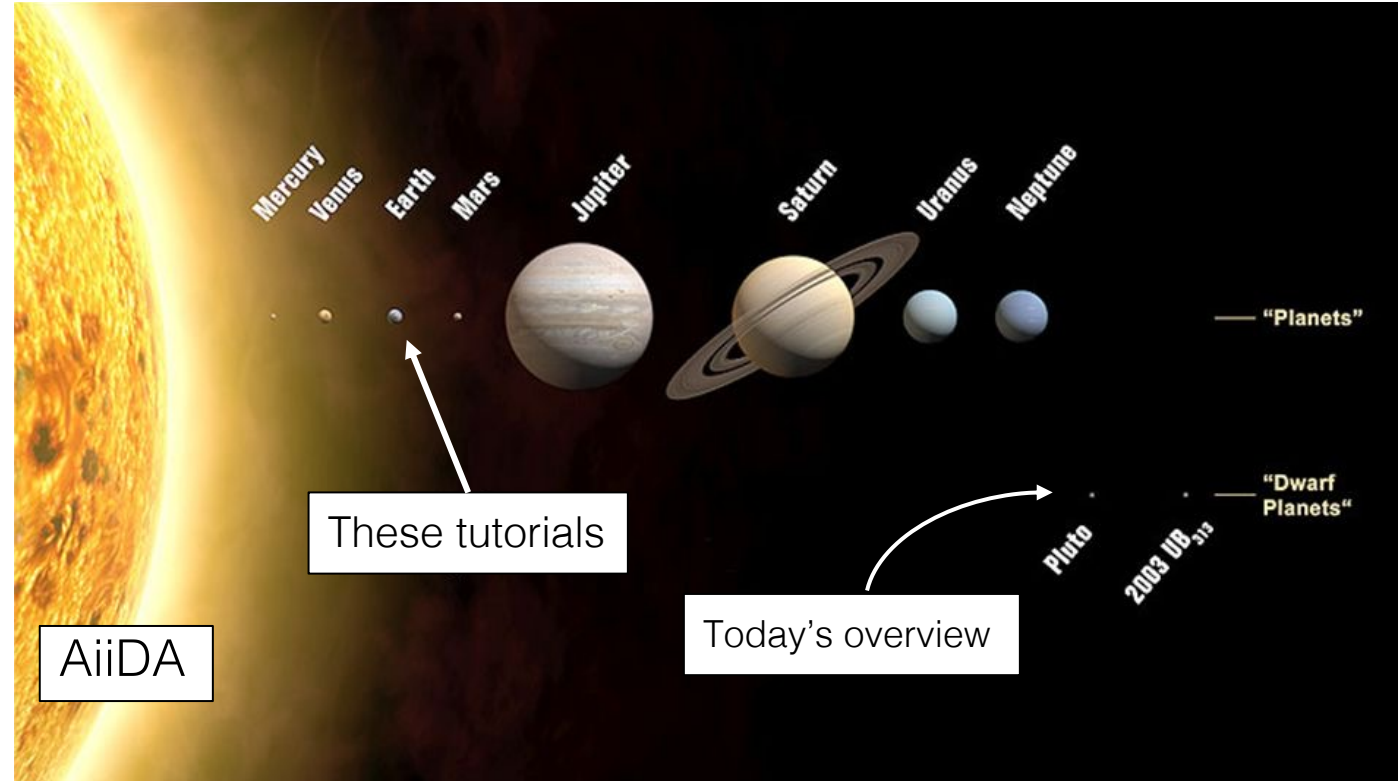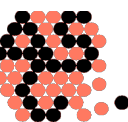
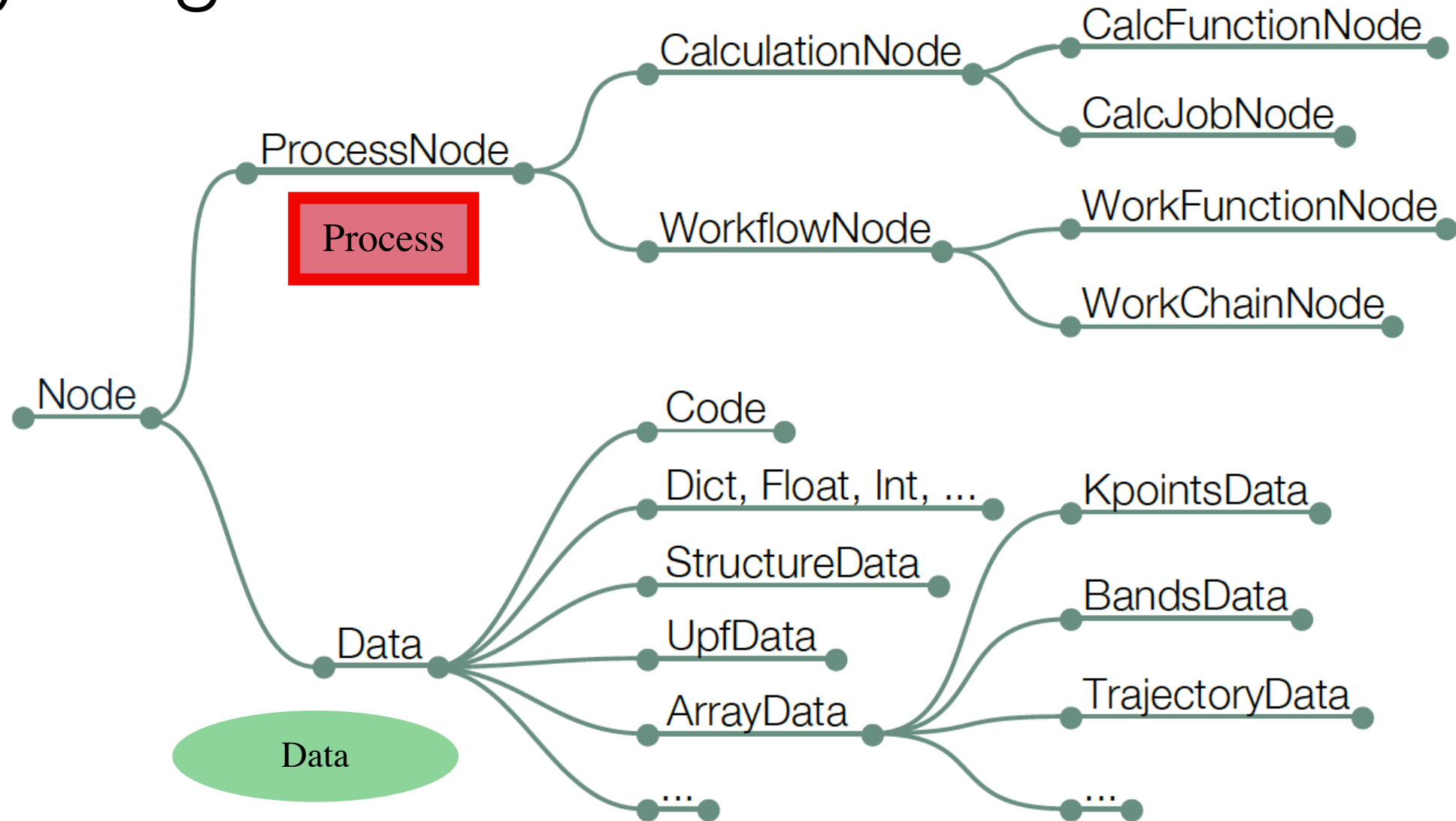- Outlook – real use cases

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These tutorials

AiiDA

Today's overview

Introduction

Introduction - What is AiiDA?

Introduction - What is AiiDA?

Everything is a Node

Example – one calculation
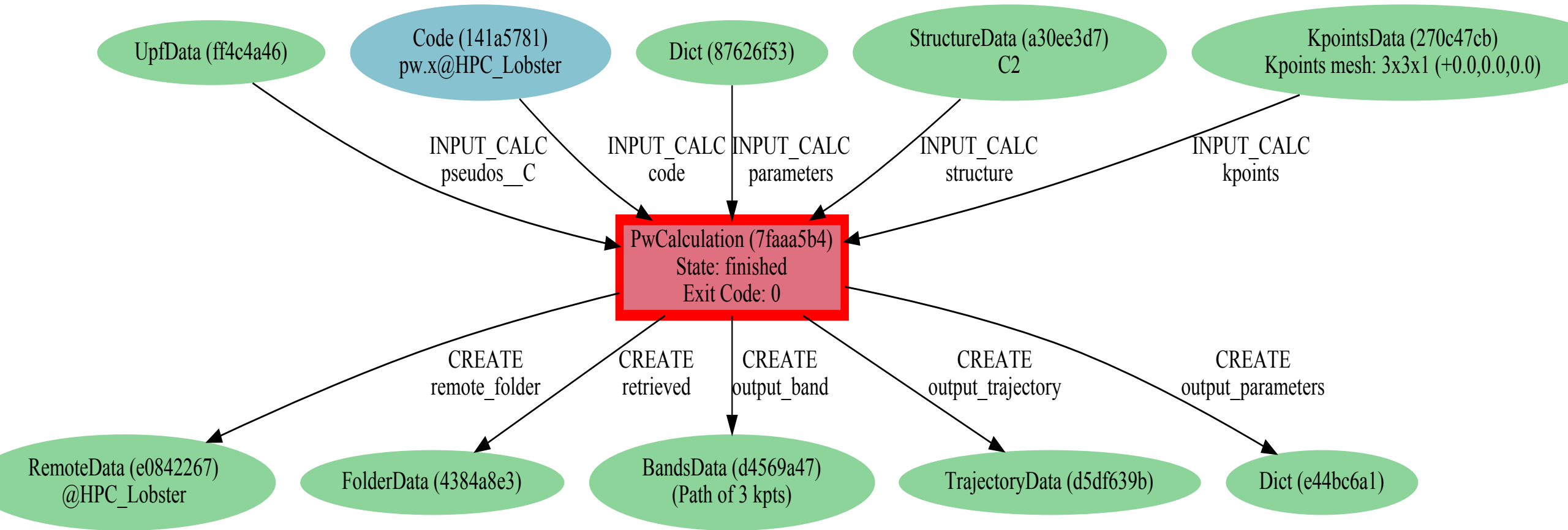
Basic benefits of AiiDA

1. Calculation management $\longrightarrow$ Tutorial 1

2. Workflows $\longrightarrow$ Tutorial 2

3. Data provenance $\longrightarrow$ Tutorial 3

1. Calculation Management

1. Calculation Management

Write input file

Write submission script

Copy files and PP to cluster

Login and submit job

Check status

scf

Parse the output

Perform arithmetic operations

1. Calculation Management

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Write submission script

Copy files and PP to cluster
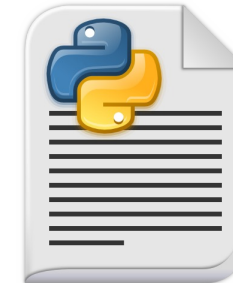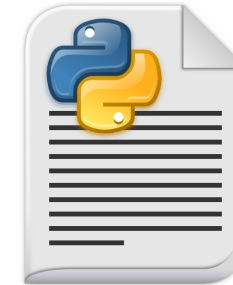
Login and submit job

Check status

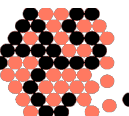Parse the output

Perform arithmetic operations

scf

➤ Single python script

➤ AiiDA executes all
steps automatically

1. Calculation Management

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➢ Single python script

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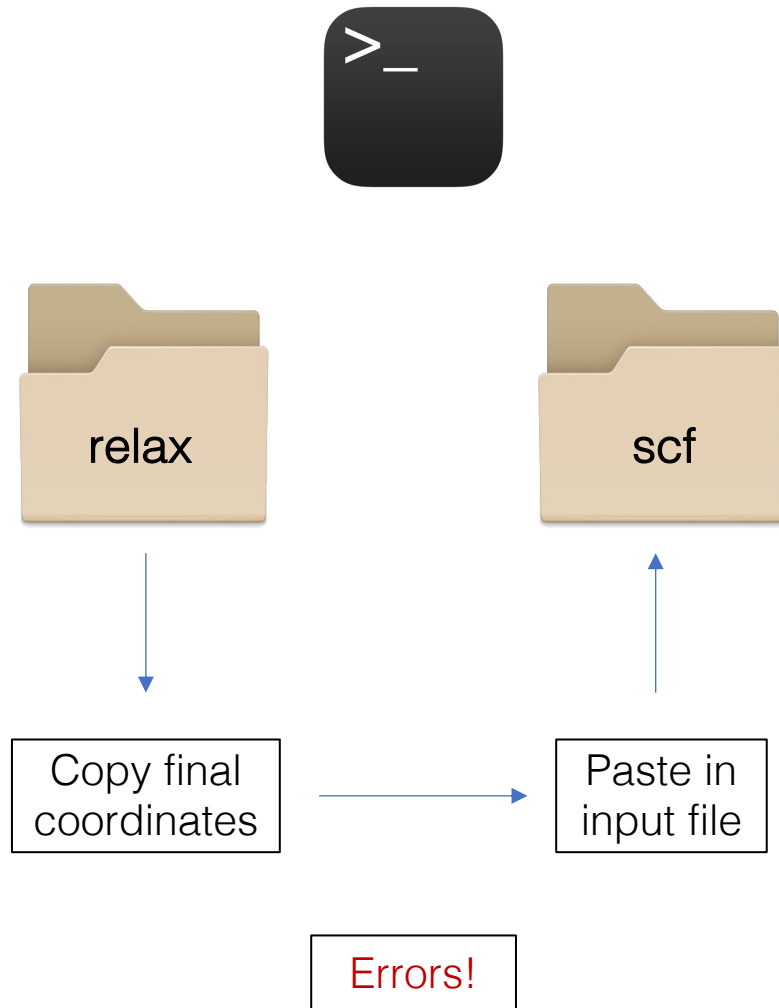
steps automatically
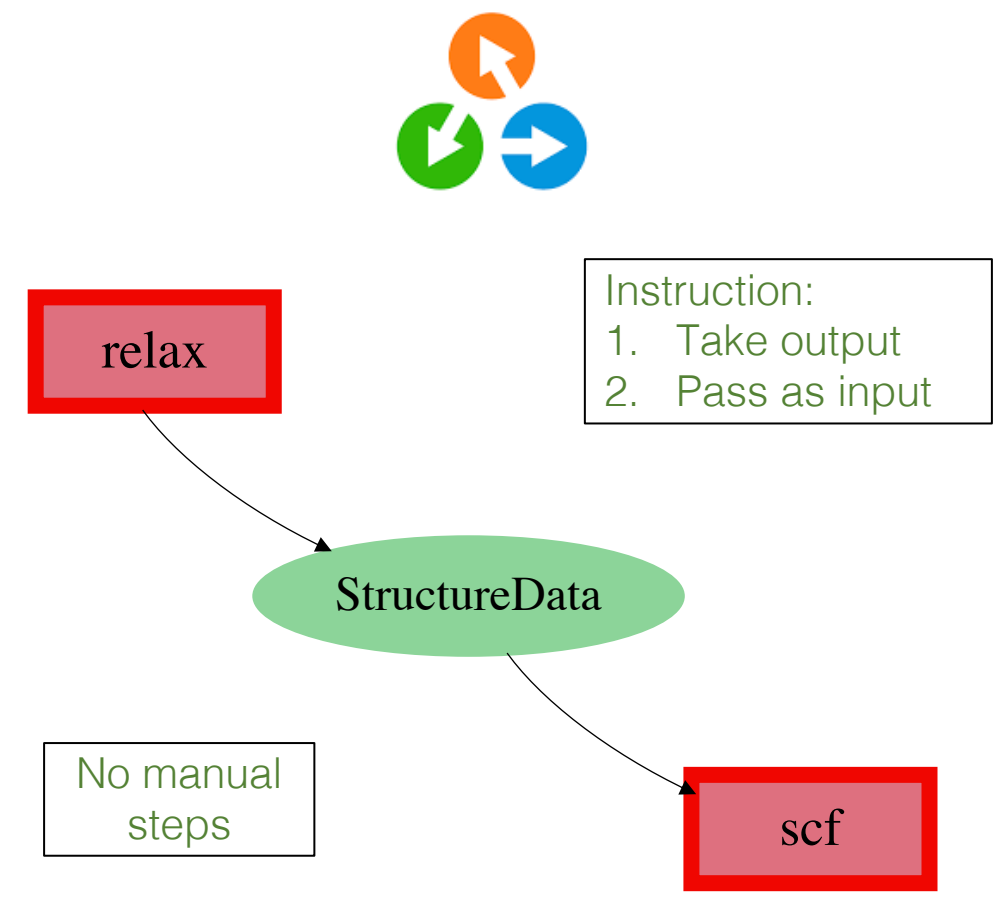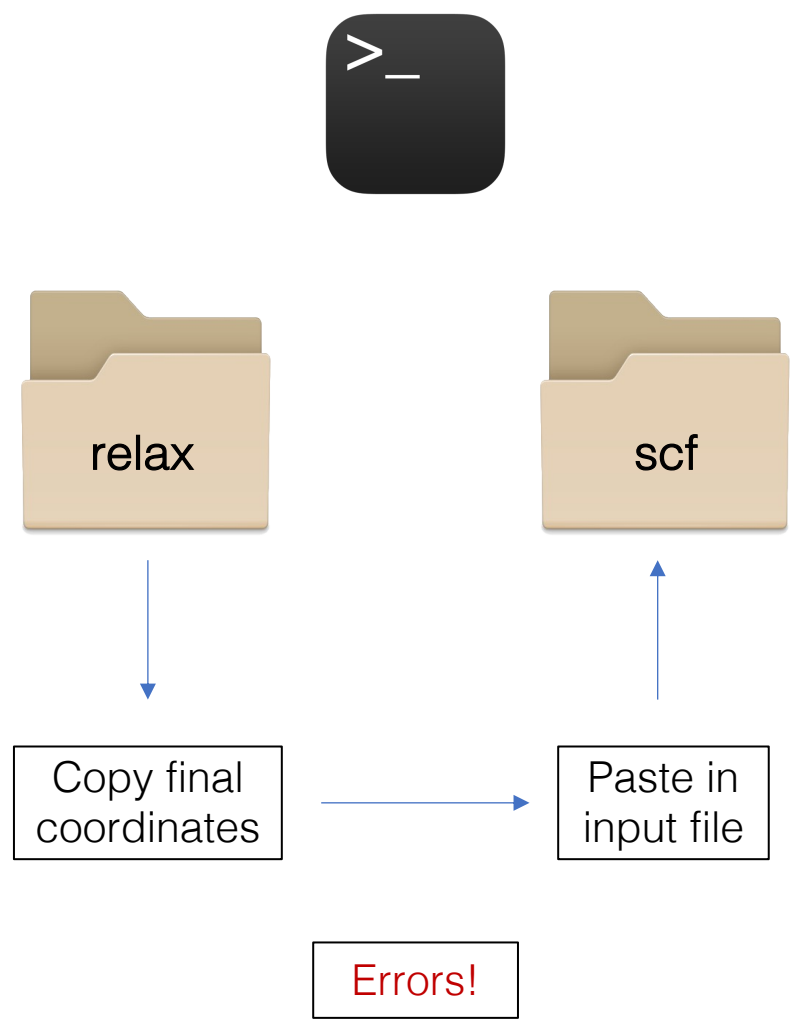
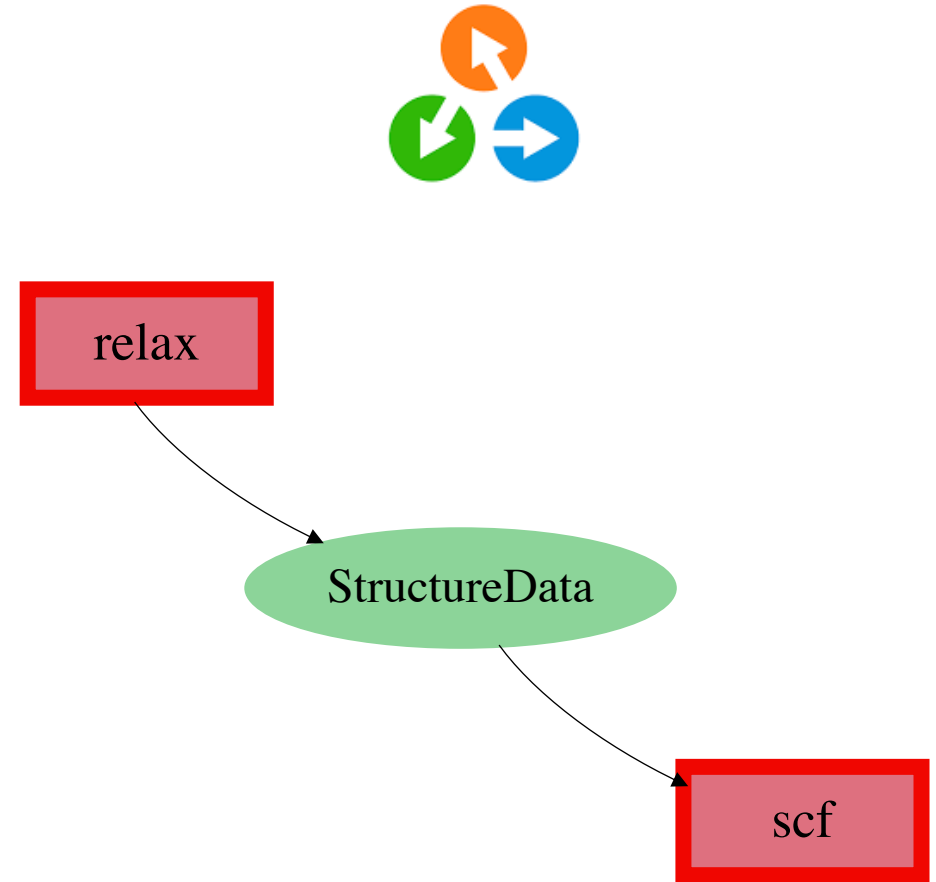Think of hundreds of calculations!

Think of automation!

2. Workflows

relax   scf

2. Workflows

relax

scf

Copy final coordinates → Paste in input file

Errors!

2. Workflows

relax

scf

Copy final coordinates → Paste in input file

Errors!

Instruction:
1. Take output
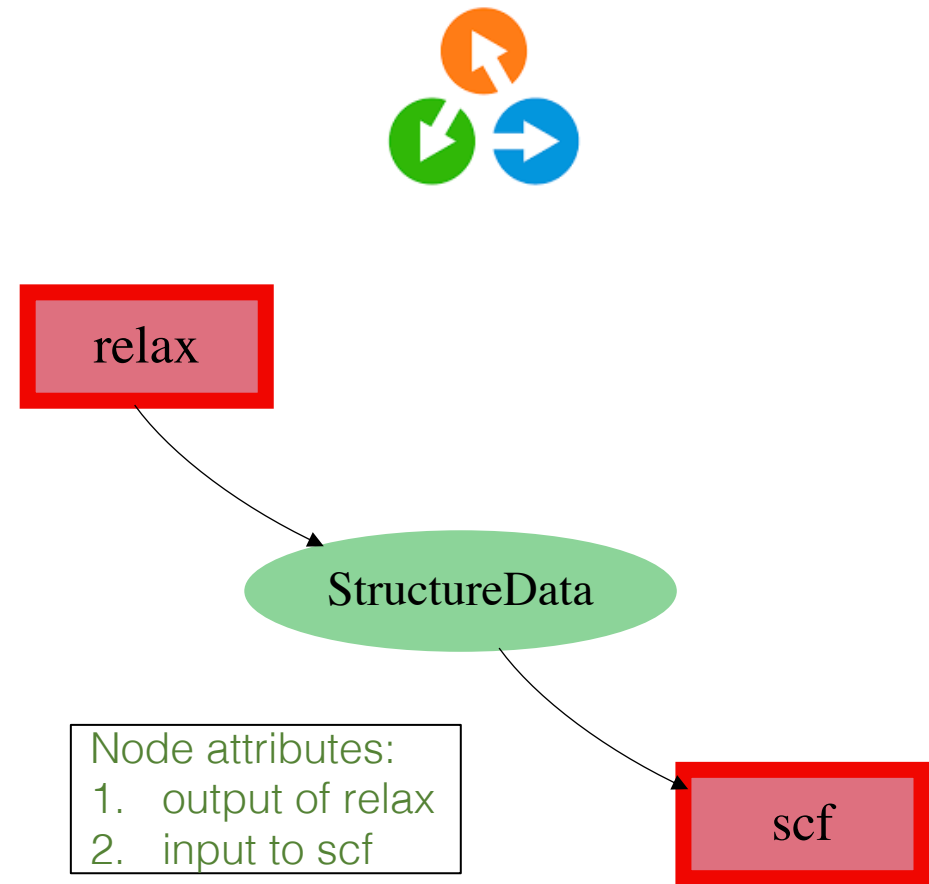2. Pass as input

relax → StructureData → scf
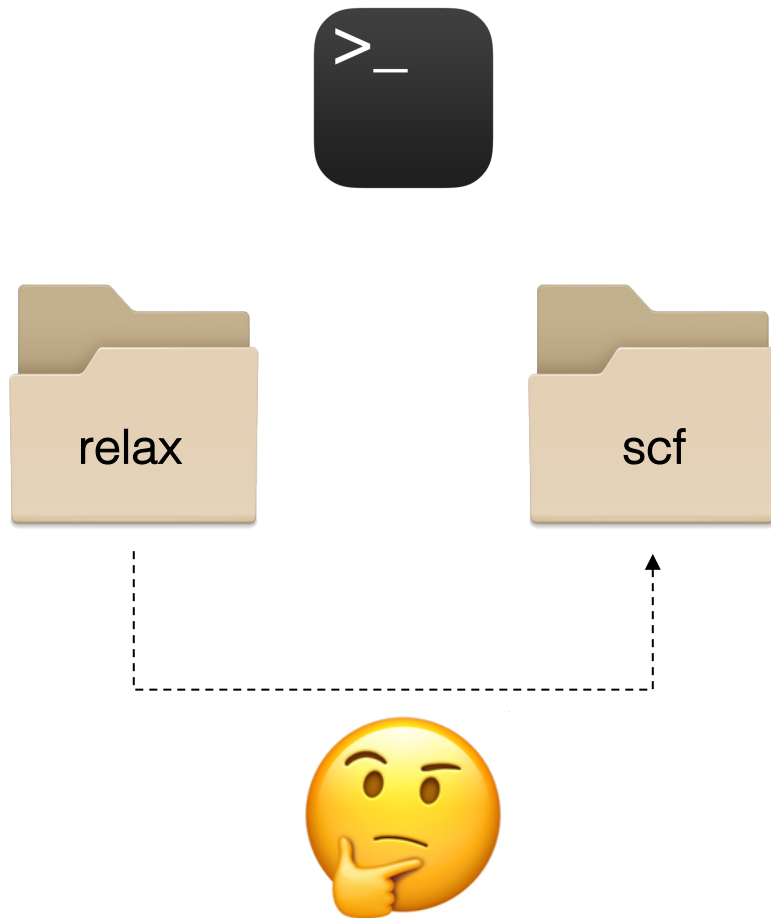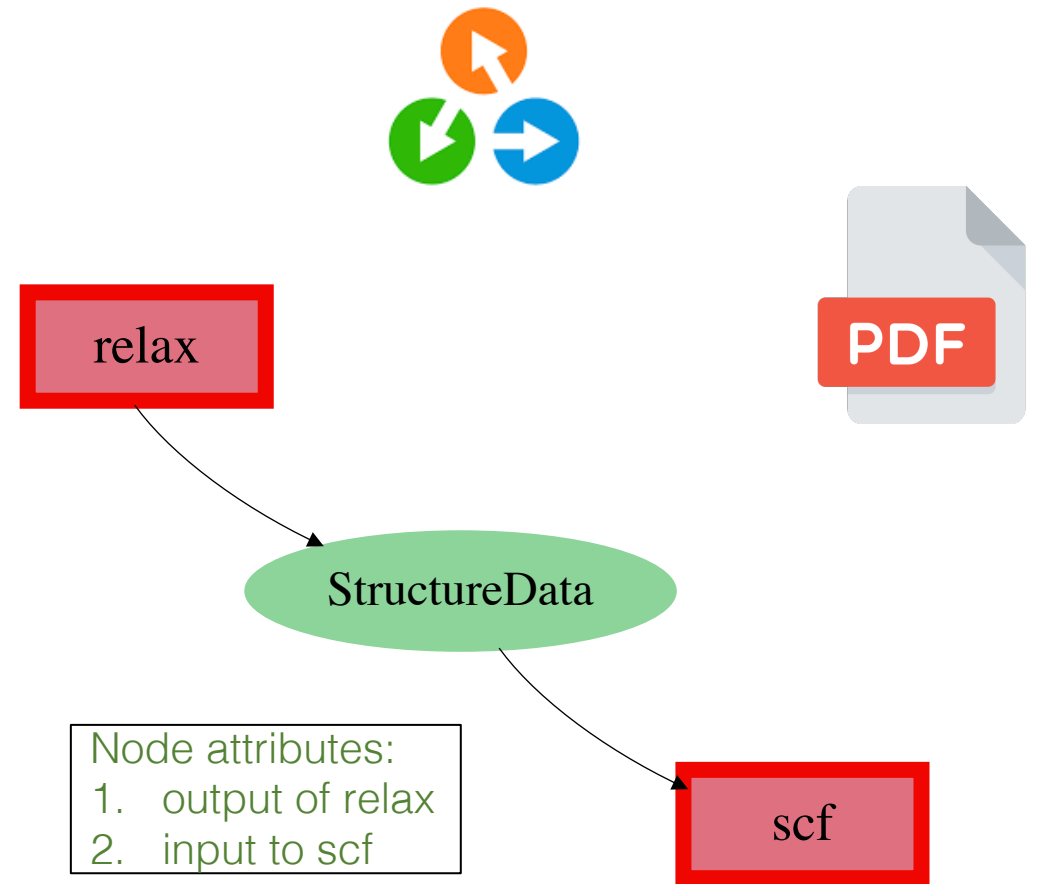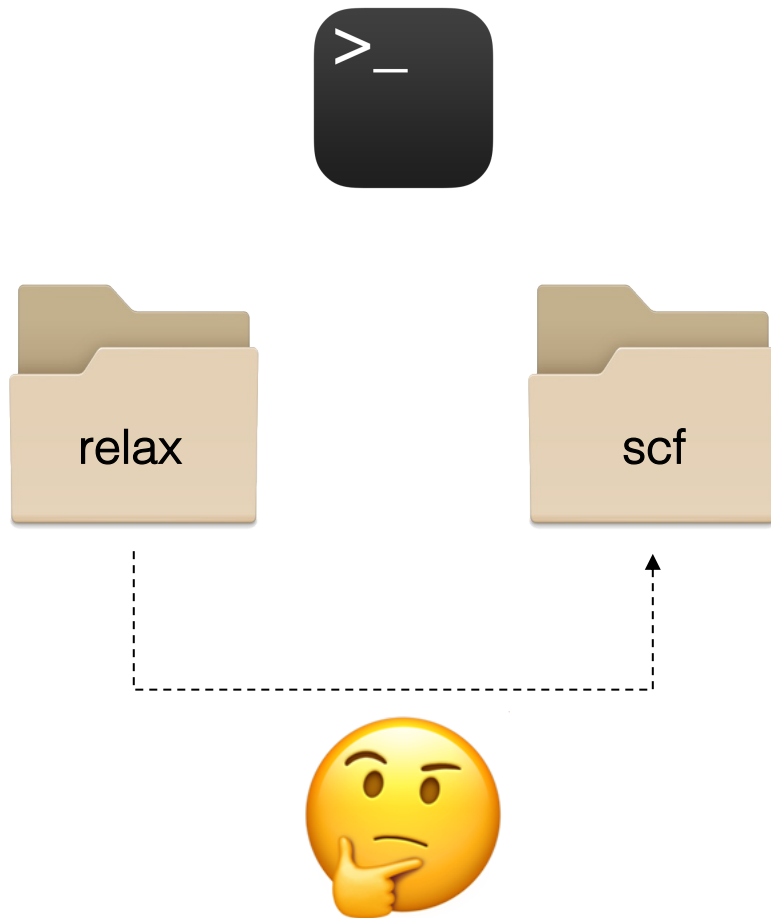
No manual steps

3. Provenance tracking

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relax   scf

Node attributes:
1. output of relax
2. input to scf
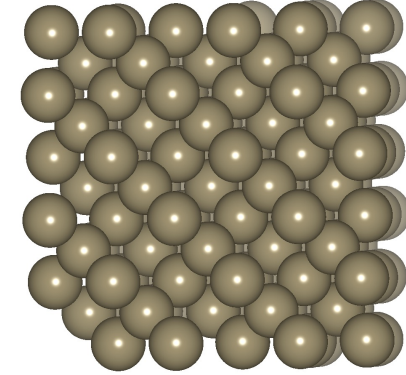
relax
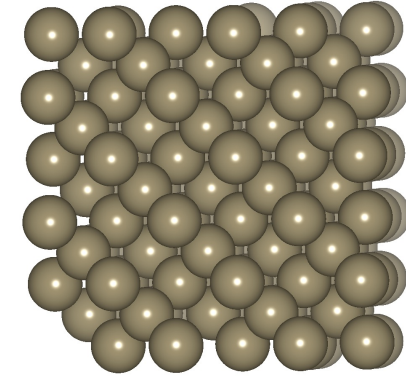
StructureData

scf

PDF
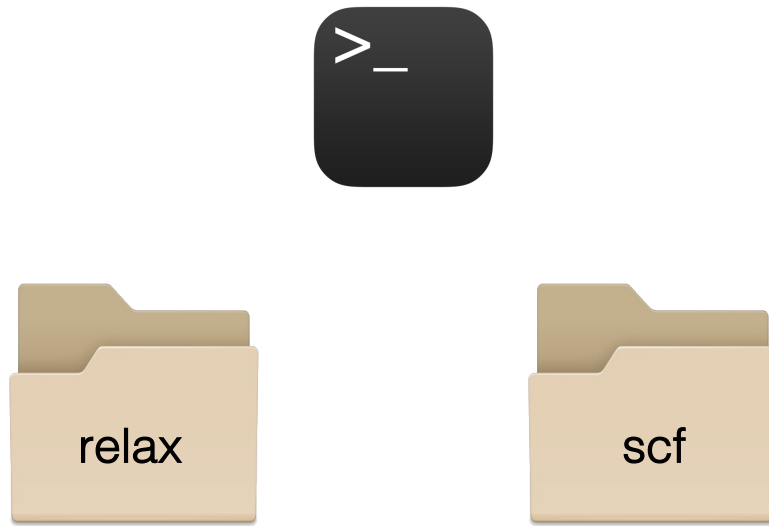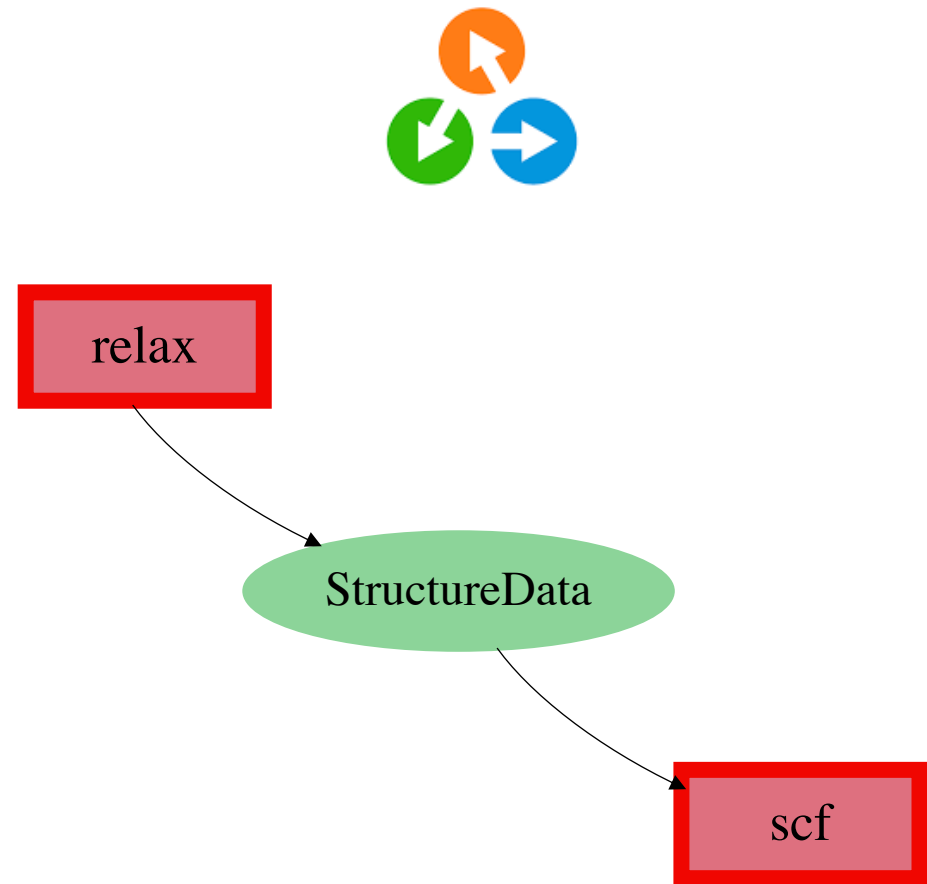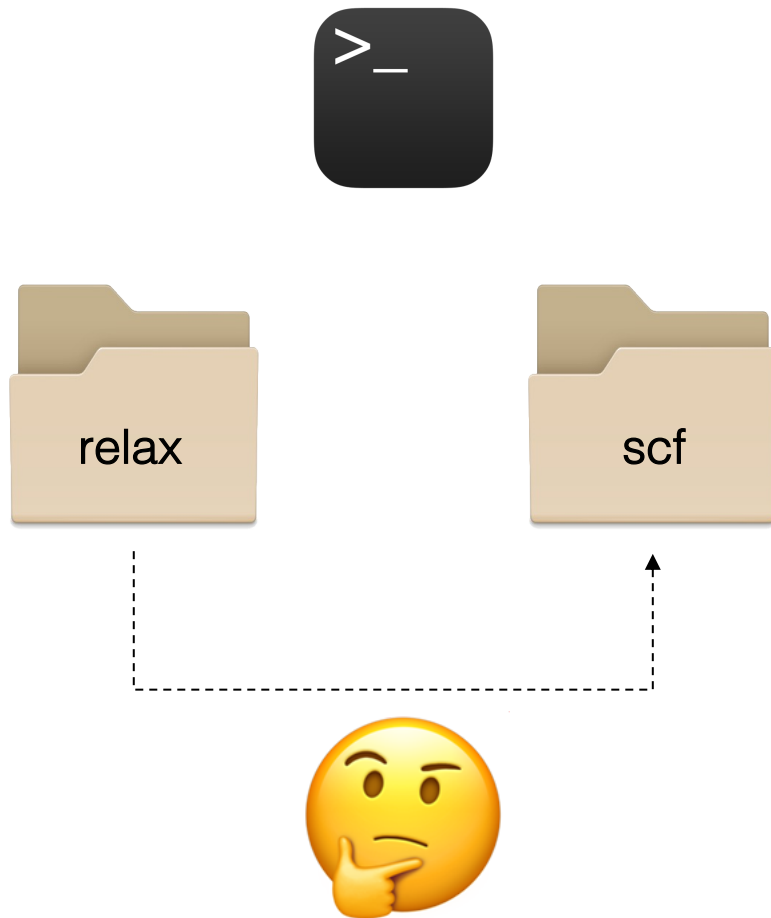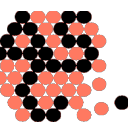
Tutorials

Tutorial 1 – calculation management
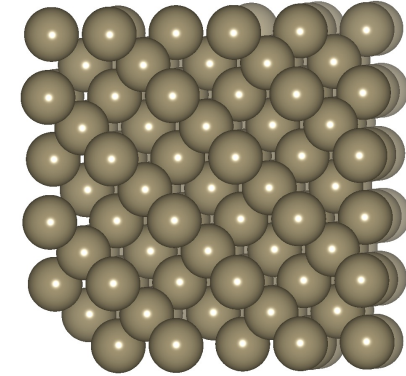
➢ Silicon PP and bulk structure

Tutorial 1 – calculation management

➢ Silicon PP and bulk structure

➢ Calculate energy

 ➢ of given structure (scf)

 ➢ of ground state structure (vc-relax)

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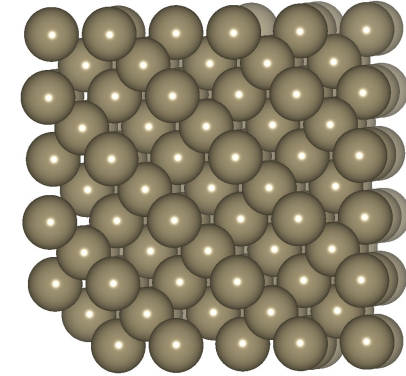➤ Print difference in meV

Tutorial 1 – calculation management

➤ Silicon PP and bulk structure

➤ Calculate energy

  ➤ of given structure (scf)

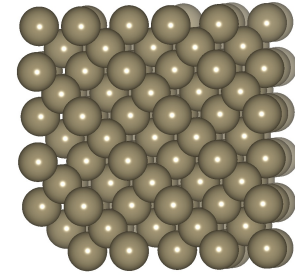 ➤ of ground state structure (vc-relax)

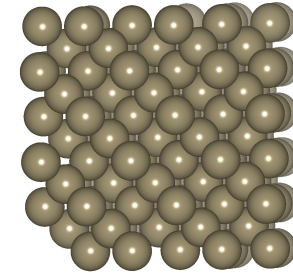➤ Print difference in meV

Bash
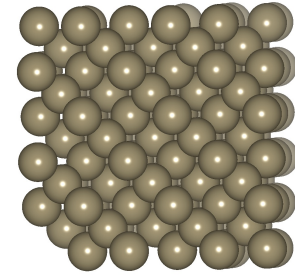
Aiida

Tutorial 1 – bash

➢ See files provided

Tutorial 1 – bash

➢ See files provided

➢ Common errors/shortcomings

    ➢ Writing QE input files

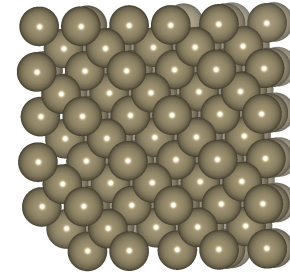   ➢ Parsing QE output files

    ➢ Interfacing with python

Tutorial 1 – AiiDA
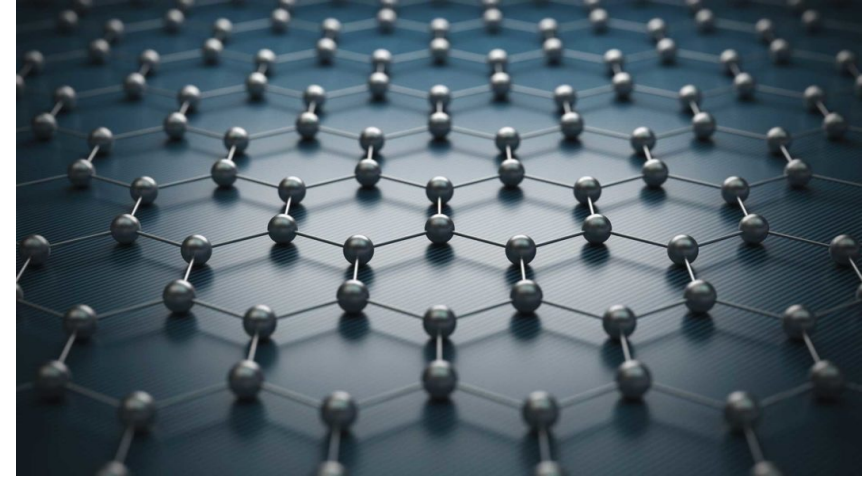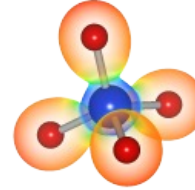
➢ See file provided

Tutorial 1 – AiiDA

➢ See file provided

➢ AiiDA can

  ➢ Write QE input files

  ➢ Parse QE output files

  ➢ Perform operations in Python
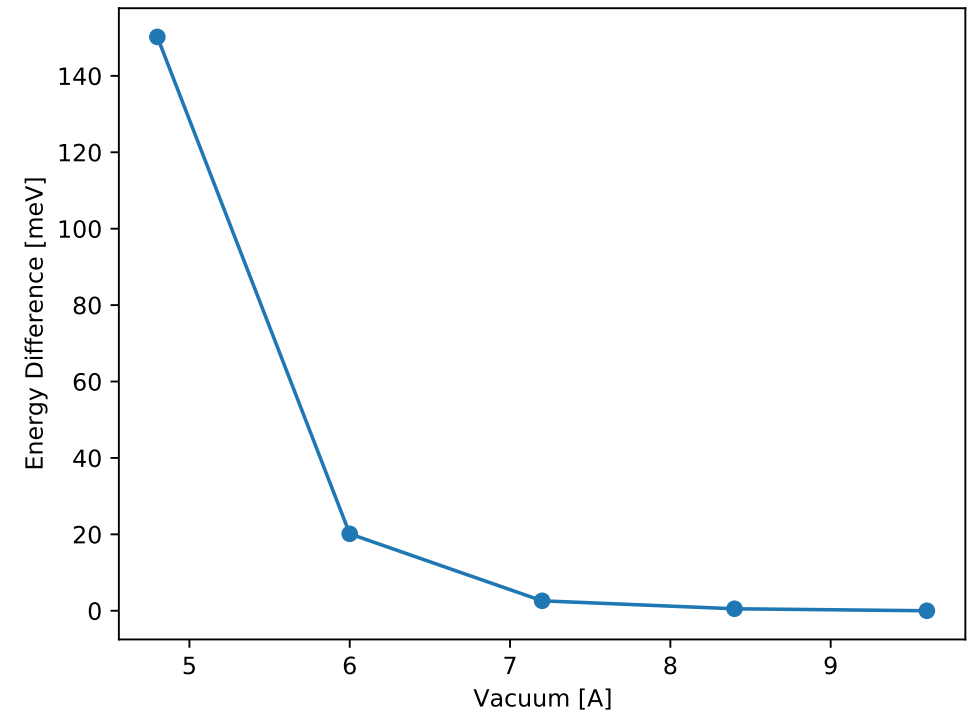
Tutorial 2 - workflow
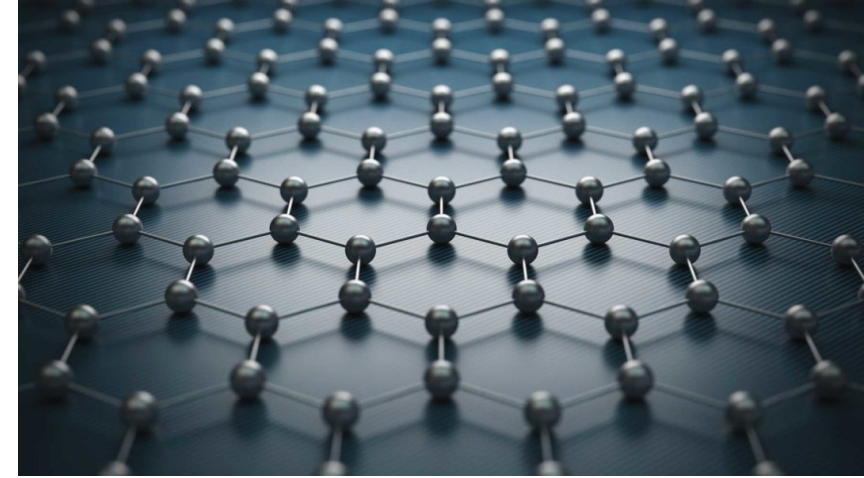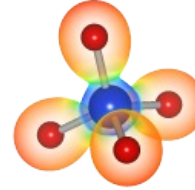
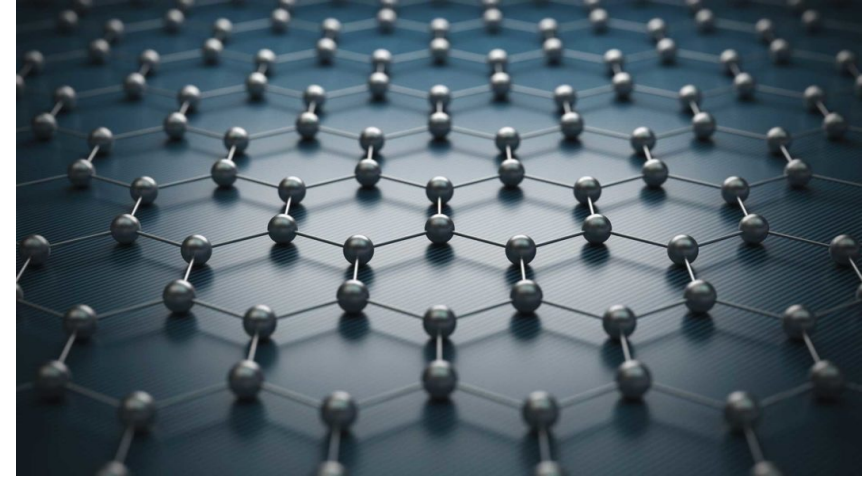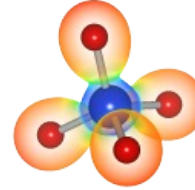> ➢ Converge the vacuum of graphene

Tutorial 2 - workflow

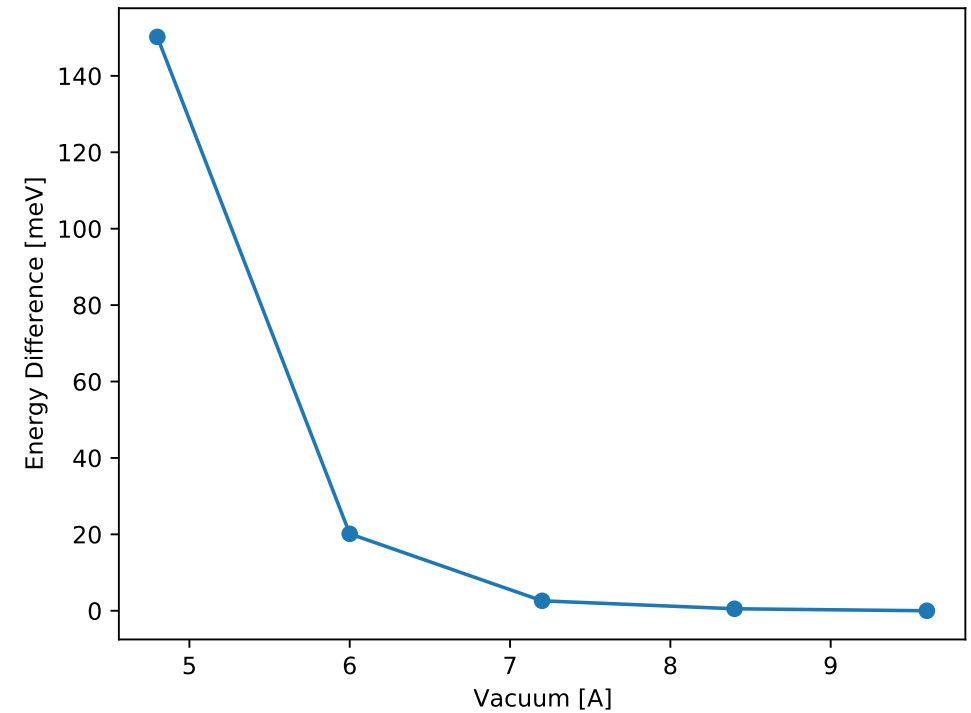➢ Converge the vacuum of graphene

Tutorial 2 - workflow

➤ Converge the vacuum of graphene

➤ Workflow

Tutorial 2 - workflow
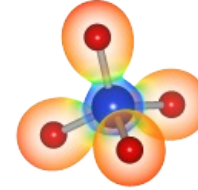

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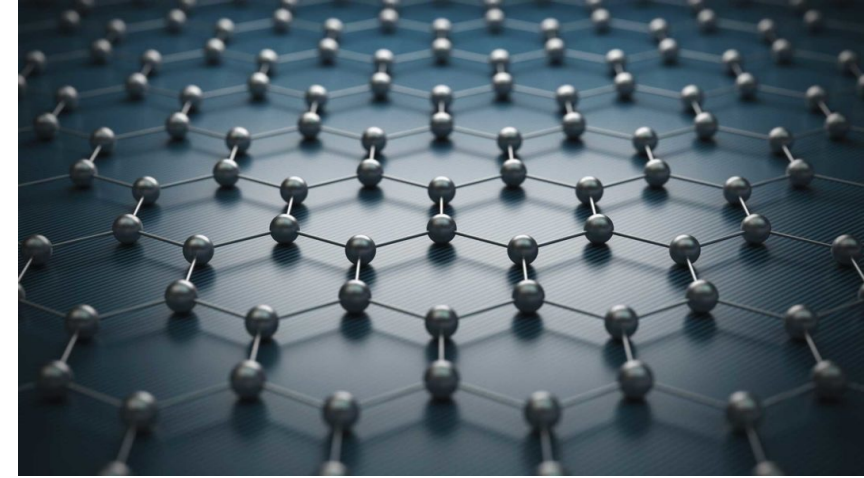
➢ Workflow

   1. Function to stretch structure

Tutorial 2 - workflow

➢ Converge the vacuum of graphene

➢ Workflow

1. Function to stretch structure

2. Function to create builder

Tutorial 2 - workflow
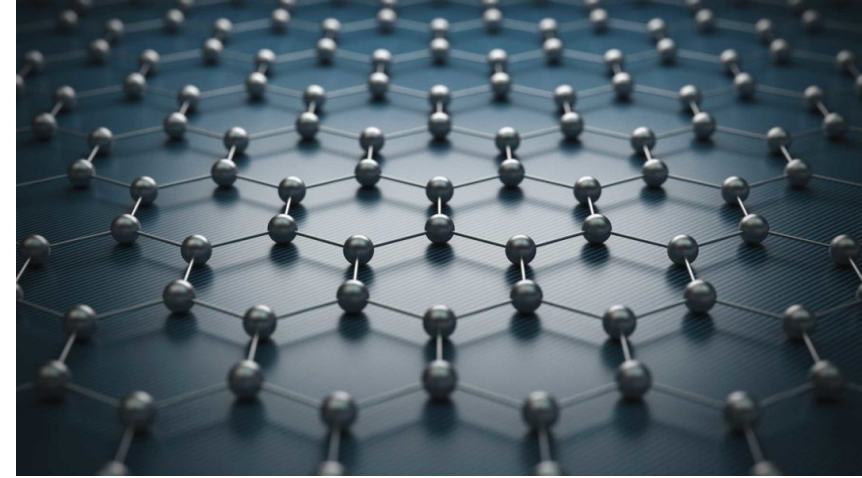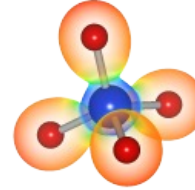
➢ Converge the vacuum of graphene

➢ Workflow

1. Function to stretch structure

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3. Function to call 1 and 2 in a loop
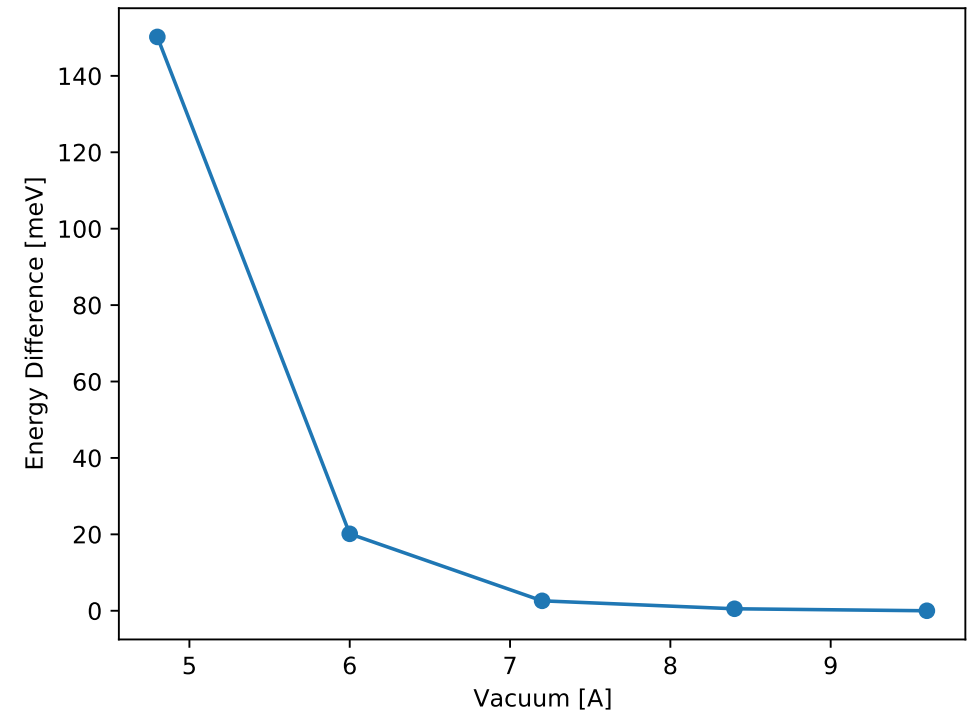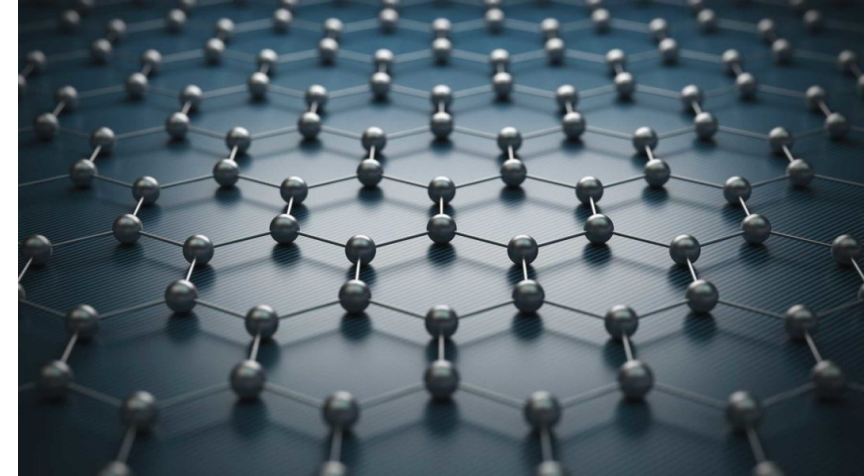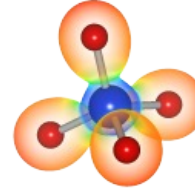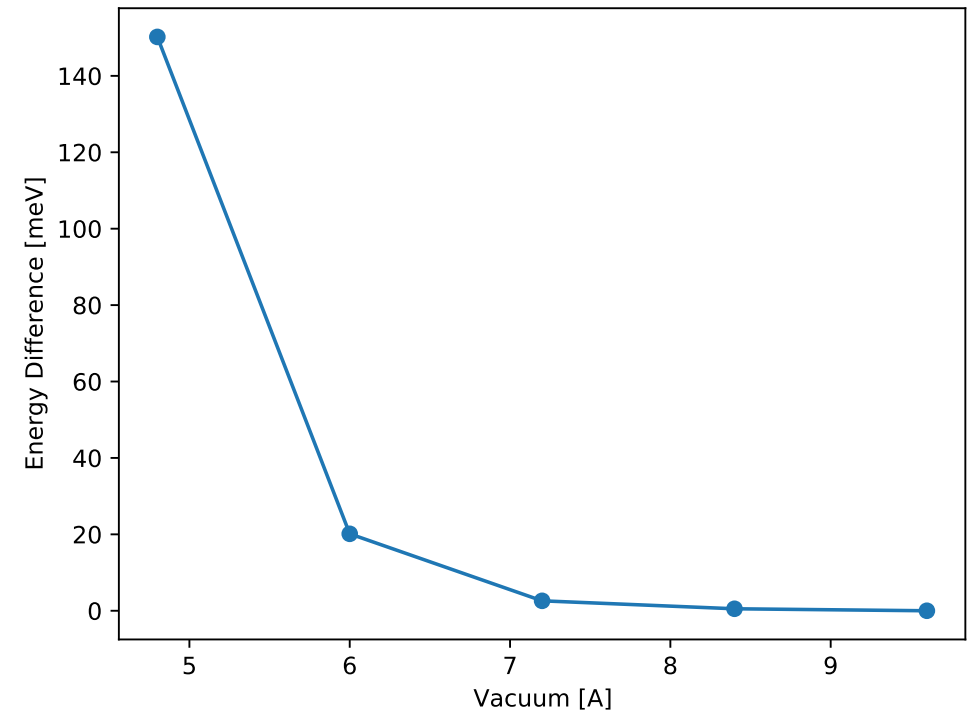
Tutorial 2 - workflow

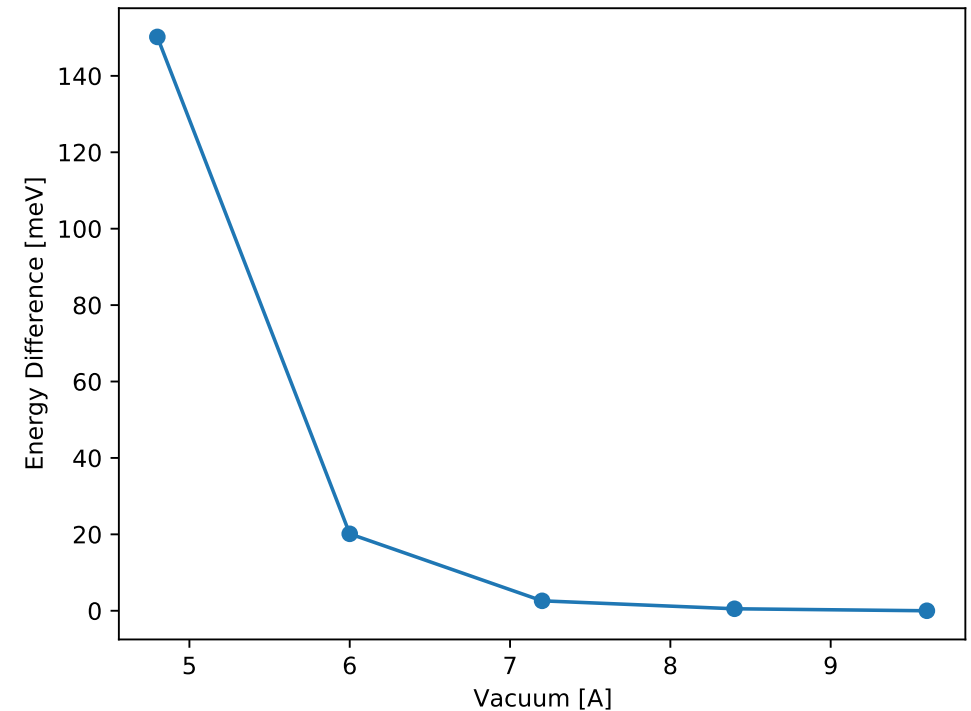➢ Converge the vacuum of graphene
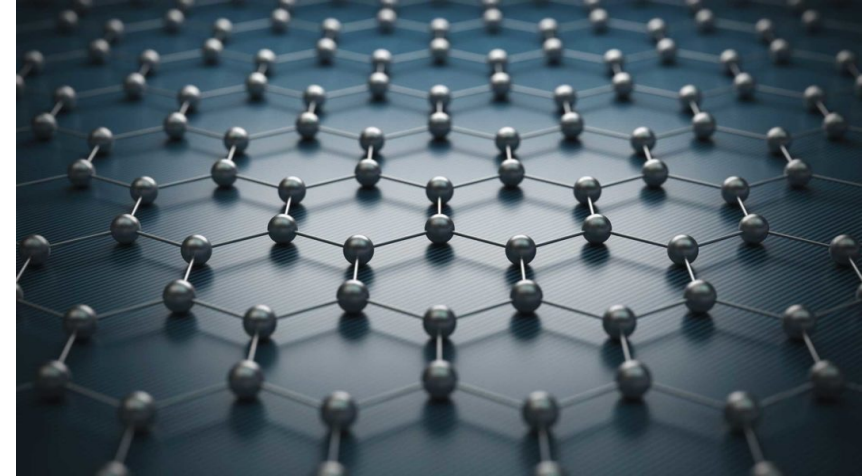
➢ Workflow

1. Function to stretch structure

2. Function to create builder

3. Function to call 1 and 2 in a loop

4. Plot results
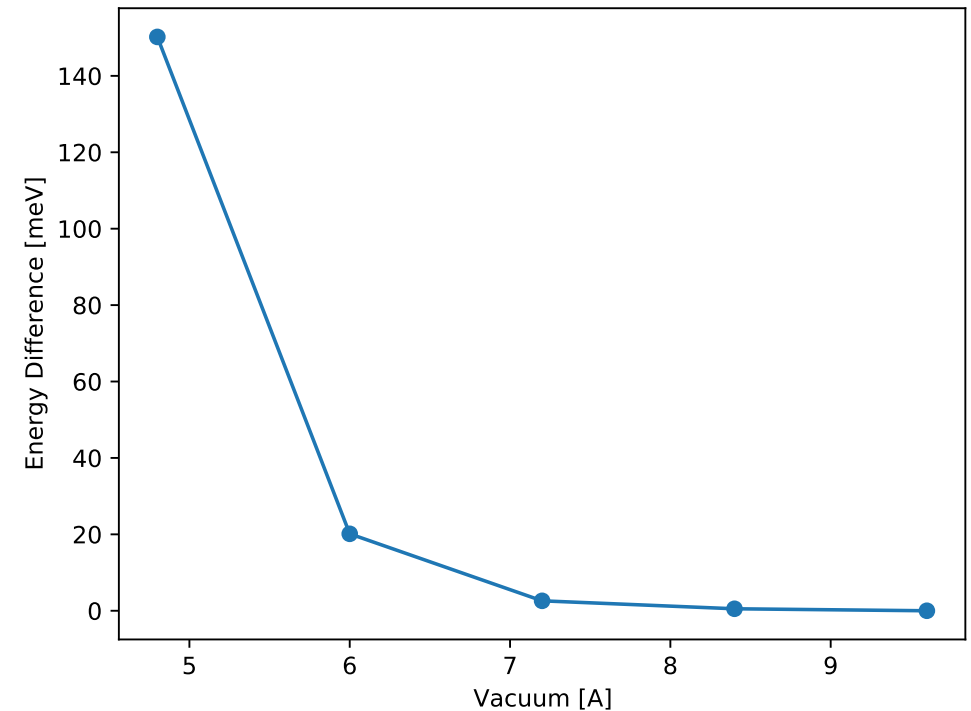
Tutorial 3 – data provenance
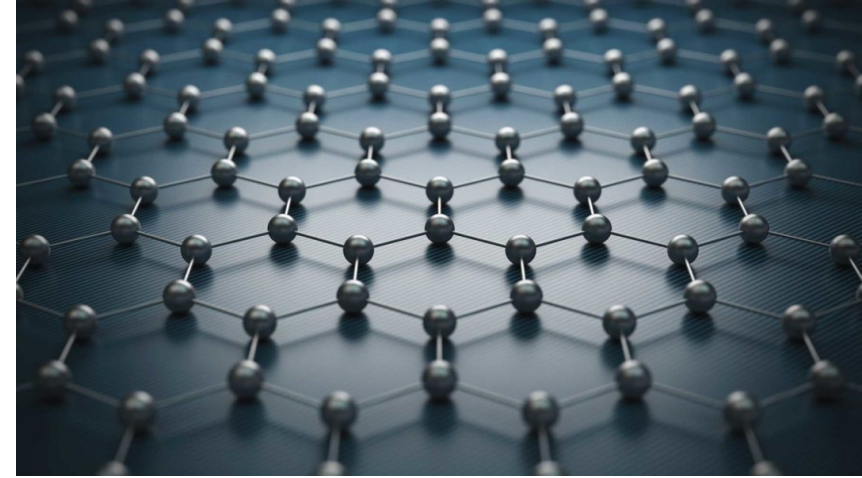
➢ What about the **provenance**?

Tutorial 3 – data provenance

- ➢ What about the **provenance**?

- ➢ Decorate python functions as

  - ➢ Calcfunctions (calculation node)

  - ➢ WorkFunctions (workflow node)

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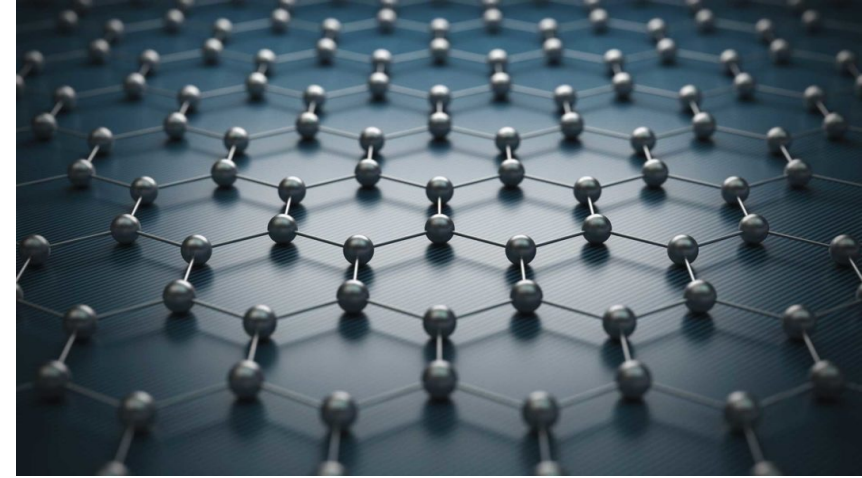
Tutorial 4 - WorkChains

➢ WorkFunctions run blockingly
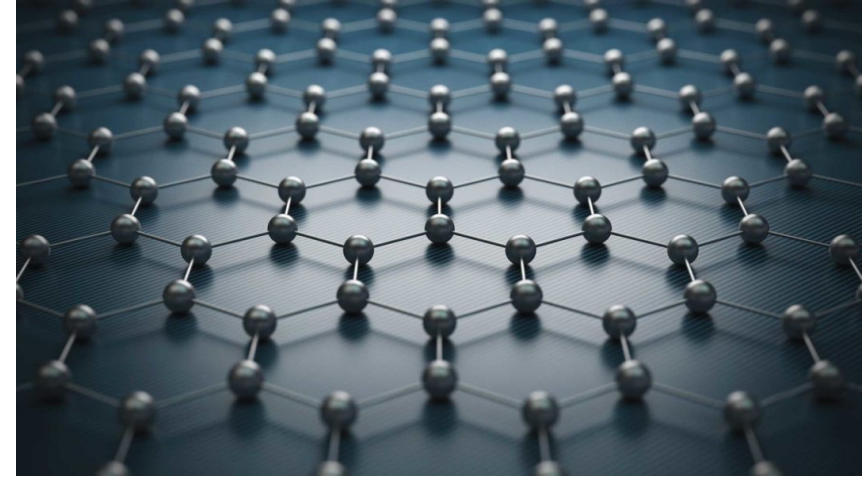
Tutorial 4 - WorkChains

➢ WorkFunctions run blockingly

➢ WorkChains

  ➢ Can be **submitted**

  ➢ Can use **To Context**
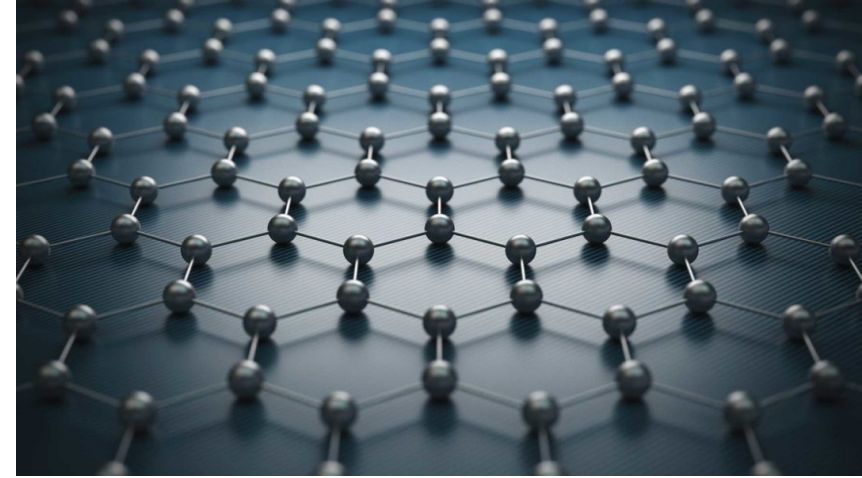
Conclusions & outlook

Conclusions

1. Automatic calculation management
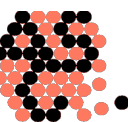
Conclusions

1. Automatic calculation management

2. Workflows (no provenance)

Conclusions

1. Automatic calculation management

2. Workflows (no provenance)

3. WorkFunctions (with provenance)
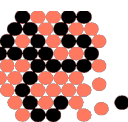
Conclusions

1. Automatic calculation management

2. Workflows (no provenance)

3. WorkFunctions (with provenance)

4. WorkChains (submit)
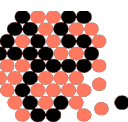
Outlook – Aiida plugins & tools

➢ Existing plugins for mainstream codes   [Aiida plugin registry](#)

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➢ Existing WorkChains for common uses

   ➢ PwBandsWorkChain

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➤ Existing WorkChains for common uses

  ➤ PwBandsWorkChain

➤ Restapi

Outlook – Aiida use cases
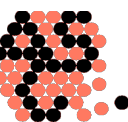
Outlook – Aiida use cases

➢ Reproducibility

Outlook – Aiida use cases

> Reproducibility

> > E.g., change the pseudopotentials

Outlook – Aiida use cases

➢ Reproducibility

    ➢ E.g., change the pseudopotentials

    ➢ Open-data publications

Outlook – Aiida use cases

- ➢ Reproducibility

  - ➢ E.g., change the pseudopotentials

  - ➢ Open-data publications

- ➢ High-throughput studies

  - ➢ Find the same property in thousands of

    materials

Computational discovery of materials

Outlook – want to use AiiDA?

➢ Complete these tutorials

➢ Complete official tutorials   www.aiida.net

➢ Read official documentation www.aiida.net

➢ Find the plugin of your code

    ➢ Use its WorkChains

    ➢ Write new WorkChains

Thank you