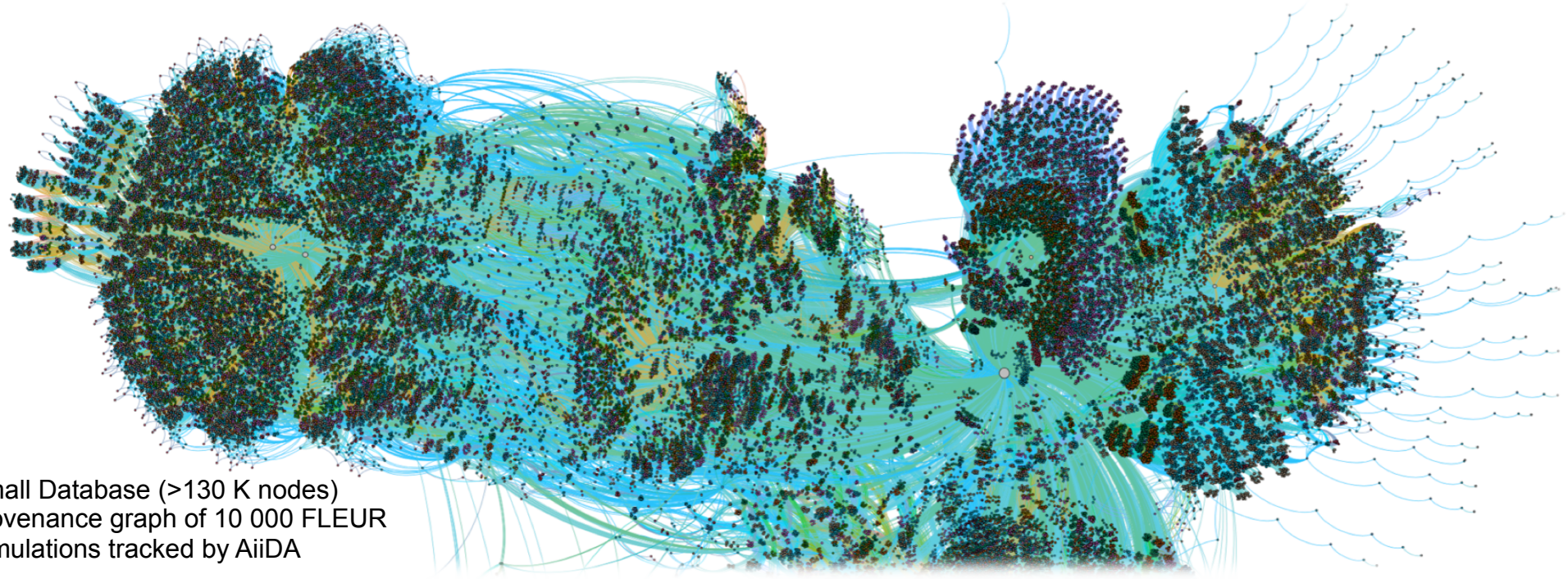

Small Database (>130 K nodes) provenance graph of 10 000 FLEUR Simulations tracked by AiiDA

AiiDA

www.flapw.de

fleur

INTRODUCTION INTO AIIDA-FLEUR:
MANAGING DATA AND (MANY) FLEUR SIMULATIONS

14.04.2021 I JENS BRÖDER (PGI-1/IAS-1), PICKING FLOWERS: HANDS-ON FLEUR

MAX DRIVING THE EXASCALE TRANSITION

Member of the Helmholtz Association

VMD JOINT LAB VIRTUAL MATERIALS DESIGN

cecam Centre Européen de Calcul Atomique et Moléculaire

JÜLICH Forschungszentrum

SHORT SUM UP OF AIIDA:

: scientist

Bringing FAIR data and high-throughput to the FLEUR community

Project size	Simulations steps	Job Management	Data	Limited by
$\mathcal{O}(1-100)$ Hand selected	+	+		People
$\mathcal{O}(1-1.000.000)$ from databases	Workflows: Task 1, ..., Task N → Result	AiiDA $\mathcal{O}(1000)$ jobs/day	FAIR [1]	Infrastructure

[1] M. D.Wilkinson. Scientific Data 3 (2016), pp. 1–9., also see www.go-fair.org

OUTLINE

1. Motivation: Connecting Fleur to AiiDA

- AiiDA sum up. How do we do simulations?

2. The AiiDA-Fleur plugin

- Calculation plugins
- Basic and advanced Workflows
- Command line interface

3. Application: Use case examples

- Material screening (high-throughput) with FLEUR
- Periodic table of FLAPW parameters
- Screening of 5000 binary metals

www.flapw.de

fleur

2. THE AIIDA-FLEUR PLUGIN:

14.04.2021 I JENS BRÖDER (PGI-1/IAS-1), PICKING FLOWERS: HANDS-ON FLEUR

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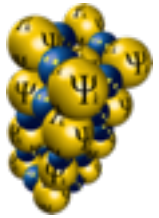

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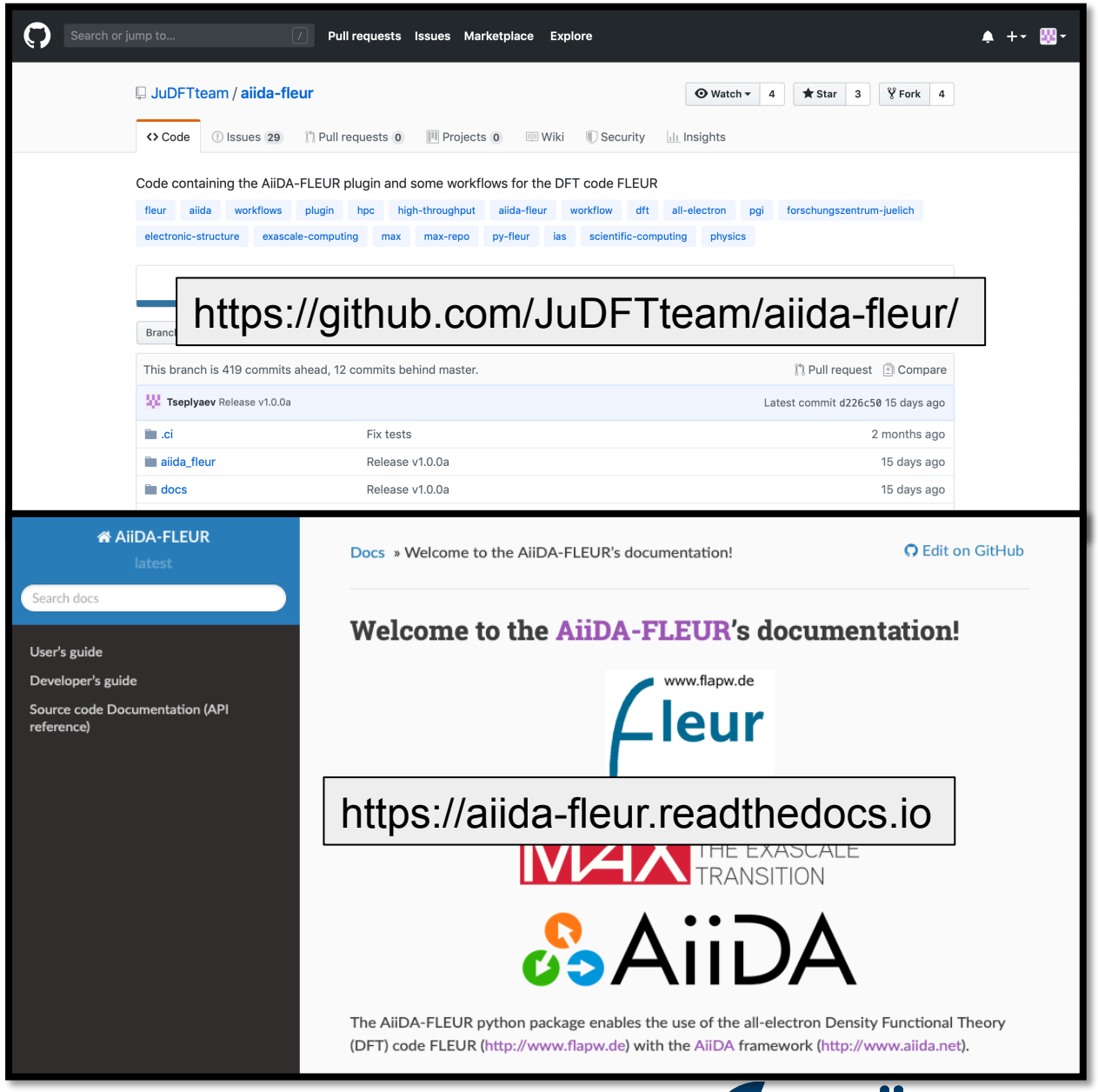
AiiDA-FLEUR PACKAGE [1]

Open source (MIT license)

- Fleur and inpgen calculation plugins
- Parsers, tools
- Fleur specific workflows/workchains
- Enables high-throughput with Fleur
- Connects Fleur to python universe
- Easy interoperability with other electronic structure codes and data sources

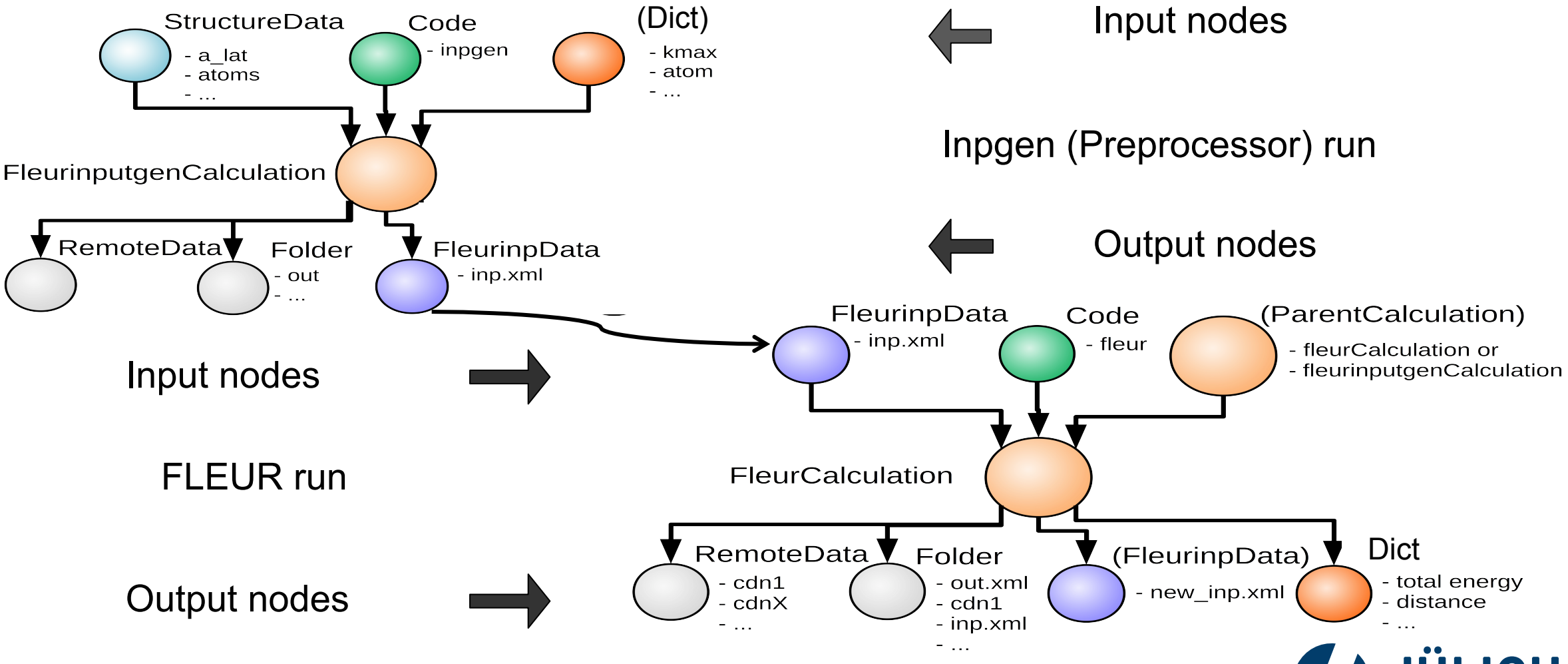


Feel free to give feedback and contribute in any way!
Checkout: https://github.com/JuDFTteam

[1] J. Bröder, D.Wortmann and S. Blügel,
In Extreme Data Workshop 2018 Proceedings, 2019, vol 40, p 43-48

AiiDA-FLEUR CALCULATION PLUG-INS

Connecting FLEUR and inpgen to AiiDA.



EXAMPLE OF PARSED CALCULATION OUTPUTS

Inpgen

Parsed inp.xml (a part is shown)

```
'files': ['inp.xml'],
'inp_dict': {
   'cell': {'filmLattice': {
     'dVac': 10.31,
     'scale': 1.0,
     'dTilda': 13.62,
     'latnam': 'any',
     'bravaisMatrix': {
       'row-1': '5.3011797029 .0000000000 .0000000000',
       'row-2': '.0000000000 7.4970000330 .0000000000',
       'row-3': '.0000000000 .0000000000 11.3011800234'},
     'vacuumEnergyParameters': {
       'spinUp': '-.25000000',
       'vacuum': '2',
       'spinDown': '-.25000000'}},
    'symmetryOperations': {
       'symOp': {'row-1': '-1 0 0 .0000000000',
                 'row-2': '0 -1 0 .0000000000',
                 'row-3': '0 0 1 .0000000000'}}}
```

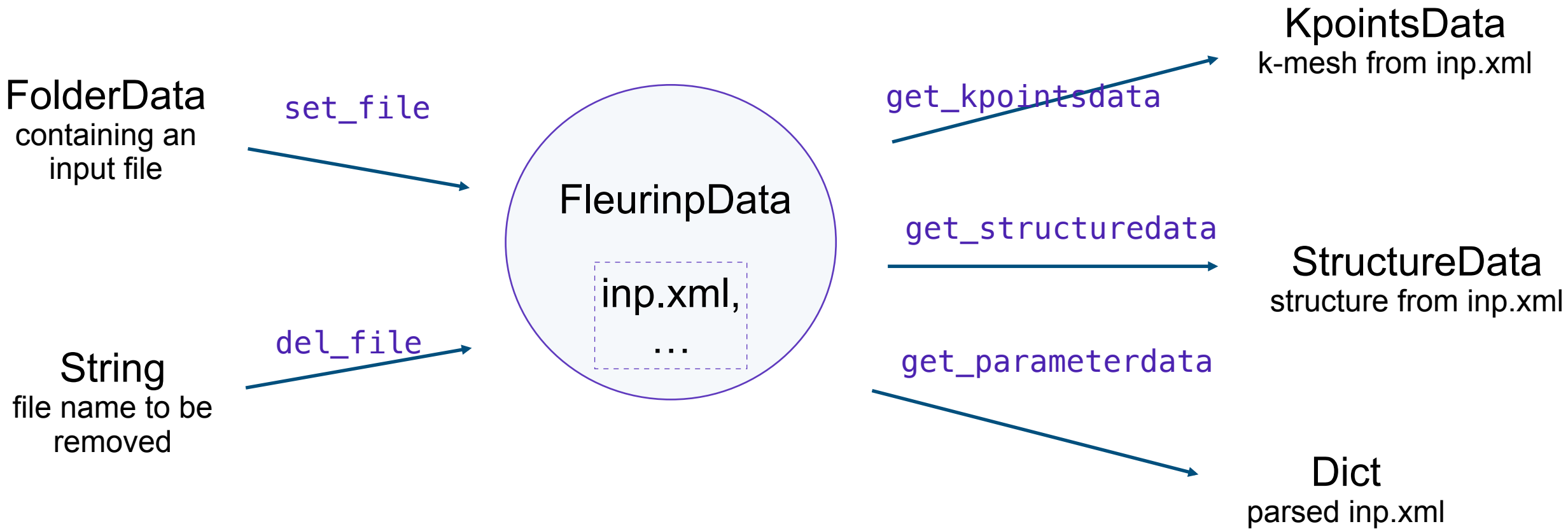
FLEUR

Parsed out.xml (a part is shown)

```
'energy': -536262.57517656,
'bandgap': 0.0014428048,
'end_date': {'date': '2019/08/26', 'time': '13:19:38'},
'unparsed': [],
'walltime': 276,
'start_date': {'date': '2019/08/26', 'time': '13:15:02'},
'energy_units': 'eV',
'fermi_energy': 0.2355843143,
'spin_density': 1.10861e-05,
'bandgap_units': 'eV',
'force_largest': 0.0,
'energy_hartree': -19707.286309577,
```

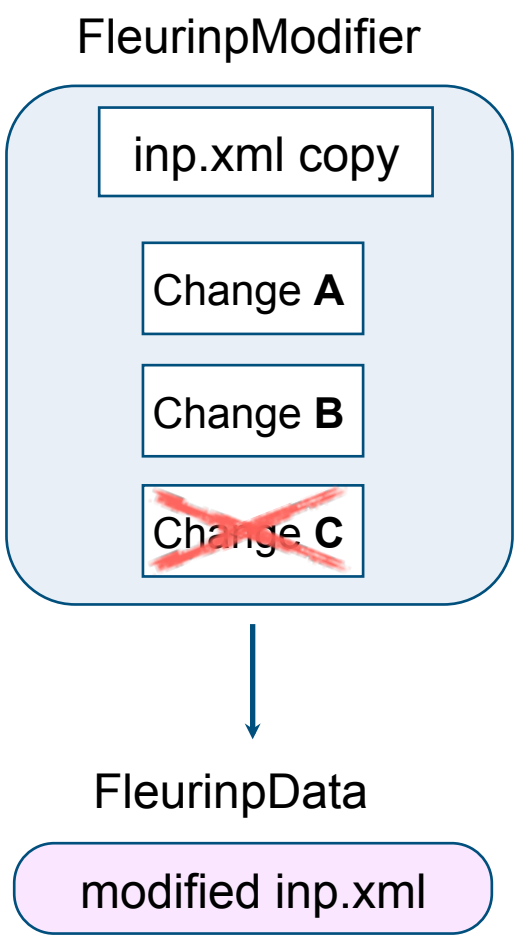
DATASTRUCTURE: FLEURINPDATA

Representing Fleur input files



INPUT MODIFICATIONS

Stored FleurinpData is sealed ➔ one needs to create a new one



1. Initialise FleurinpModifier object:

```
from aiida_fleur.data.fleurinpmodifier import FleurinpModifier
modification = FleurinpModifier(fleurinp)
```

2. Register modifications:

```
modification.set_inpchanges({'phi': 0.33079})

modification.set_inpchanges({'theta': 1.57079})

modification.set_species('W-1', {'mtSphere' : {'radius' : 3.5}})
modification.undo()
```

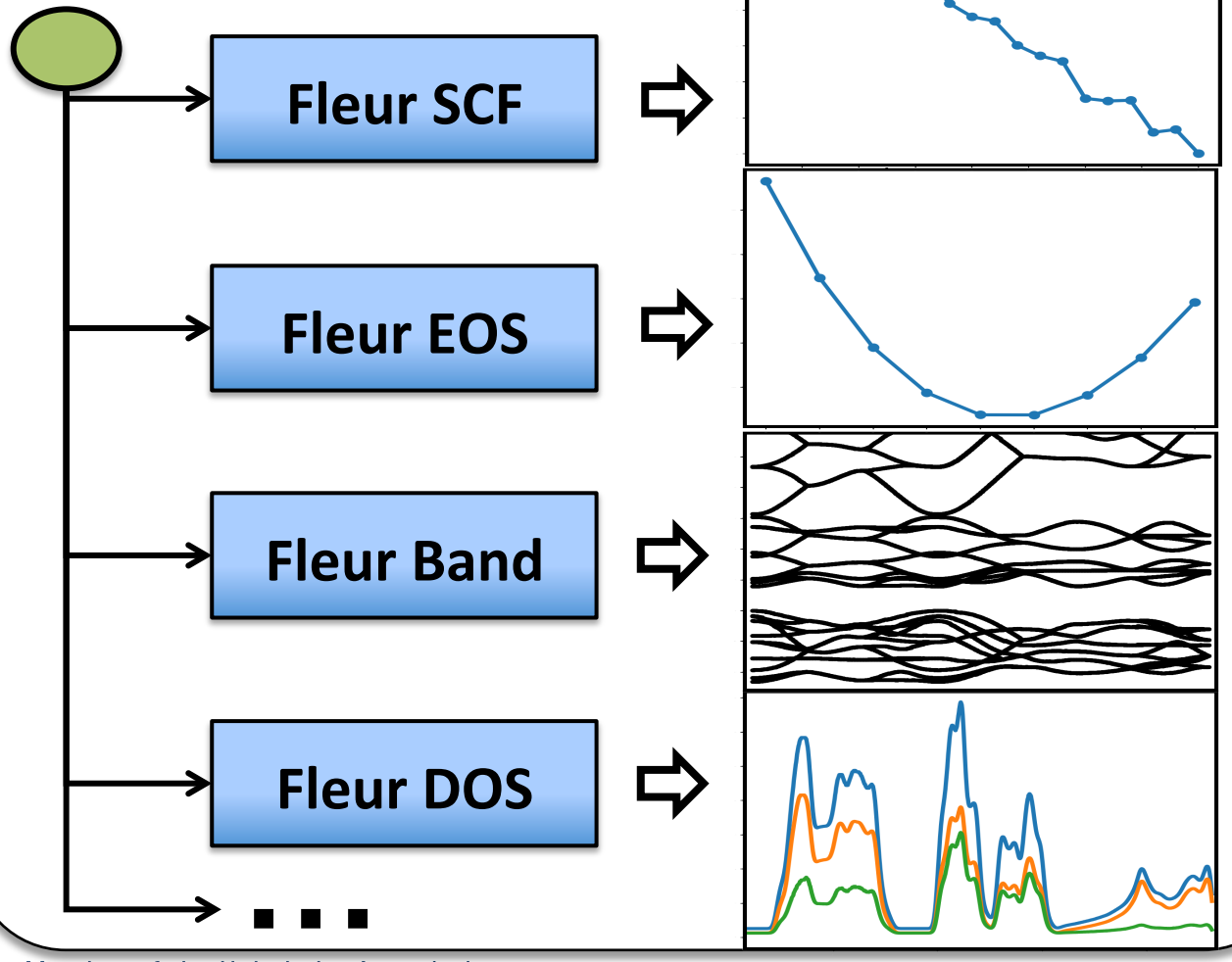
3. Apply modifications:

```
modified_fleurinp = modification.freeze()
```

AIIDA-FLEUR WORKFLOWS

Basic Fleur workflows

Structure, any source




```
from aiida.orm import WorkflowFactory,load_group,Code
from aiida.work.launch import submit
fleur_scf = WorkflowFactory('fleur.scf')

inpgen = Code.get_from_string('inpgen@otherhost')
fleur = Code.get_from_string('fleur@cluster')

strucs = load_group(label='oqmd_strucs').nodes.dbnodes
paras = load_group(label='oqmd_paras').nodes.dbnodes

for i,struc in enumerate(strucs):
    res = submit(fleur_scf, structure=struc,
                 calc_parameter=paras[i],
                 fleur=fleur, inpgen=inpgen)
```

Advanced workflows:

- Relaxation, MAE, SSdisp, (DMI)
- Core-hole, initial_cls

Wishlist (in progress):

- EELS, Phonons, Jijs, LDA+U, Magnons, …

COMMAND LINE INTERFACE

```
broeder@iffaiida:~/$ aiida-fleur -h
Usage: aiida-fleur [OPTIONS] COMMAND [ARGS]…

   CLI for the `aiida-fleur` plugin.

Options:
      -p, --profile PROFILE    Execute the command for this profile

      -h, --help               Show this message and exit.

Commands:
      data        Commands to create and inspect data nodes.
      launch      Commands to launch workflows and calcjobs of aiida-fleur.
      plot        Invoke the plot_fleur command on given nodes
      workflow    Commands to inspect aiida-fleur workchains.
```

➡ You can use parts of aiida-fleur inside (shell) scripts, without any python.

LAUNCH WORKFLOWS

```
broeder@iffaiida:~/$ aiida-fleur launch scf -h
Usage: aiida-fleur launch scf [OPTIONS]

   Launch a scf workchain

Options:
  -s, --structure STRUCTUREFILE     StructureData node, given by pk or uuid or file in any format
  -i, --inpgen CODE                 A code node or label for an inpgen executable. [default: (dynamic)]

  -calc_p, --calc-parameters DATA   Dict with calculation (FLAPW) parameters to build, which will be
                                    given to inpgen.

  -set, --settings DATA             Settings node for the calcjob.
  -inp, --fleurinp DATA             FleurinpData node for the fleur calculation.
  -f, --fleur CODE                  A code node or label for a fleur executable.
  -wf, --wf-parameters DATA         Dict containing parameters given to the workchain.
  -P, --parent-folder DATA          The PK of a parent remote folder
  -d, --daemon                      Submit the process to the daemon instead of running it locally
  -set, --settings DATA             Settings node for the calcjob
  -opt, --option-node DATA          Dict, an option node for the workchain
```

LAUNCH WORKFLOWS EXAMPLE

More in the Hands-on session

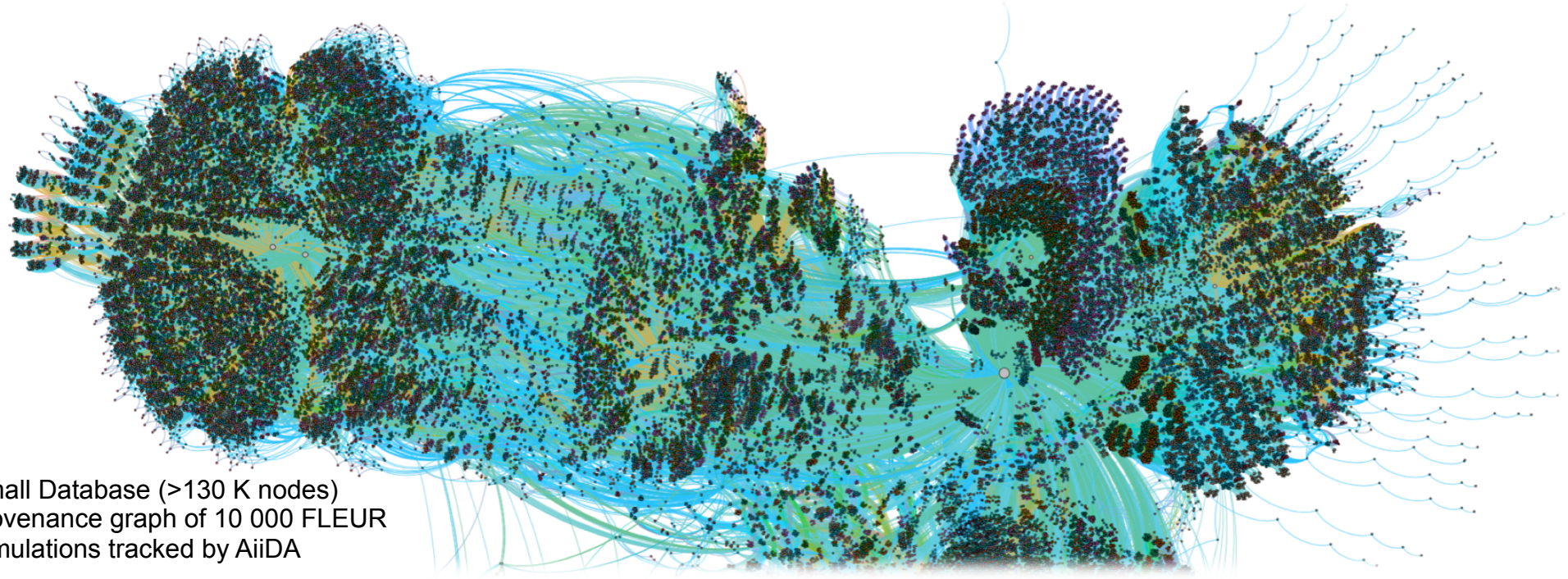
```
$ verdi code list | grep cluster
* pk 71041 -  inpgen_m4@cluster
* pk 71042 -  fleur_m4@cluster

$ aiida-fleur launch scf -d –f 71042 –i 71041 –S NdNiO2.cif
Submitted FleurScfWorkChain<98232> to the daemon
$ aiida-fleur launch relax -d -f 71042 –i 71042 –S NdNiO2.cif
Submitted BaseRelaxWorkChain<98235> to the daemon
```

Further check with (verdi) commands on status and results of these workchains

There is are also common workflow interfaces between (10 DFT codes, see Quantum-mobile)

```
$ aiida-common-workflows launch relax –d –p moderate -S NdNiO2.cif fleur
Submitted FleurRelaxWorkChain<123> to the daemon
$ aiida-common-workflows launch relax –d –p moderate -S NdNiO2.cif –r atom_cell quantum_expresso
Submitted QuantumEspressoRelaxWorkChain<124> to the daemon
```

Paper coming up. (https://github.com/aiidateam/aiida-common-workflows)
Baseline of larger Delta DFT project, teaching, web apps



Small Database (>130 K nodes)
provenance graph of 10 000 FLEUR
Simulations tracked by AiiDA

AiiDA

www.flapw.de
fleur

3. APPLICATION: USE CASE EXAMPLES
WHAT CAN YOU DO WITH AIIDA-FLEUR?

14.04.2021 I JENS BRÖDER (PGI-1/IAS-1), PICKING FLOWERS: HANDS-ON FLEUR

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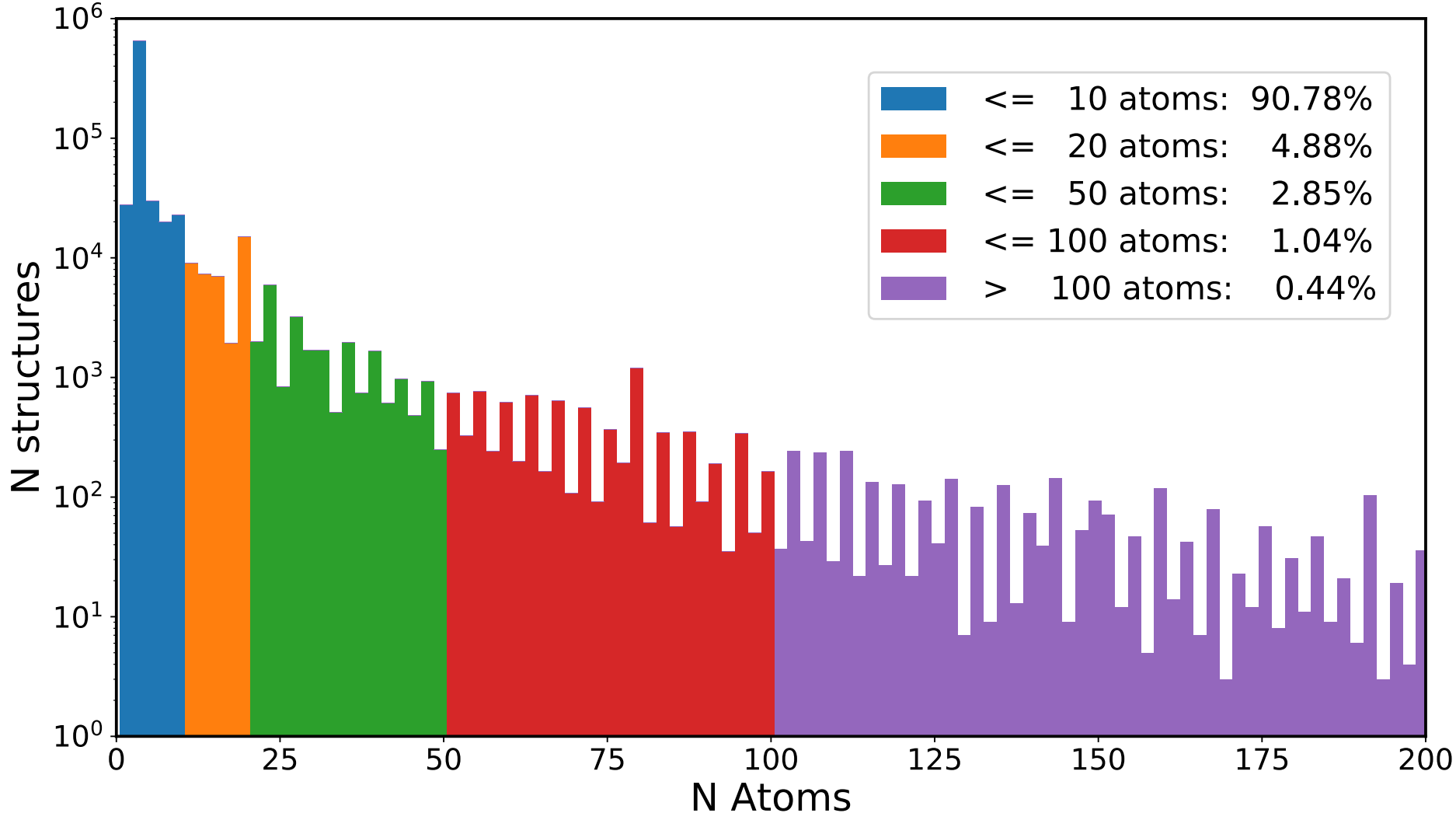
1. TEST INPGEN ON OVER 800 K STRUCTURES

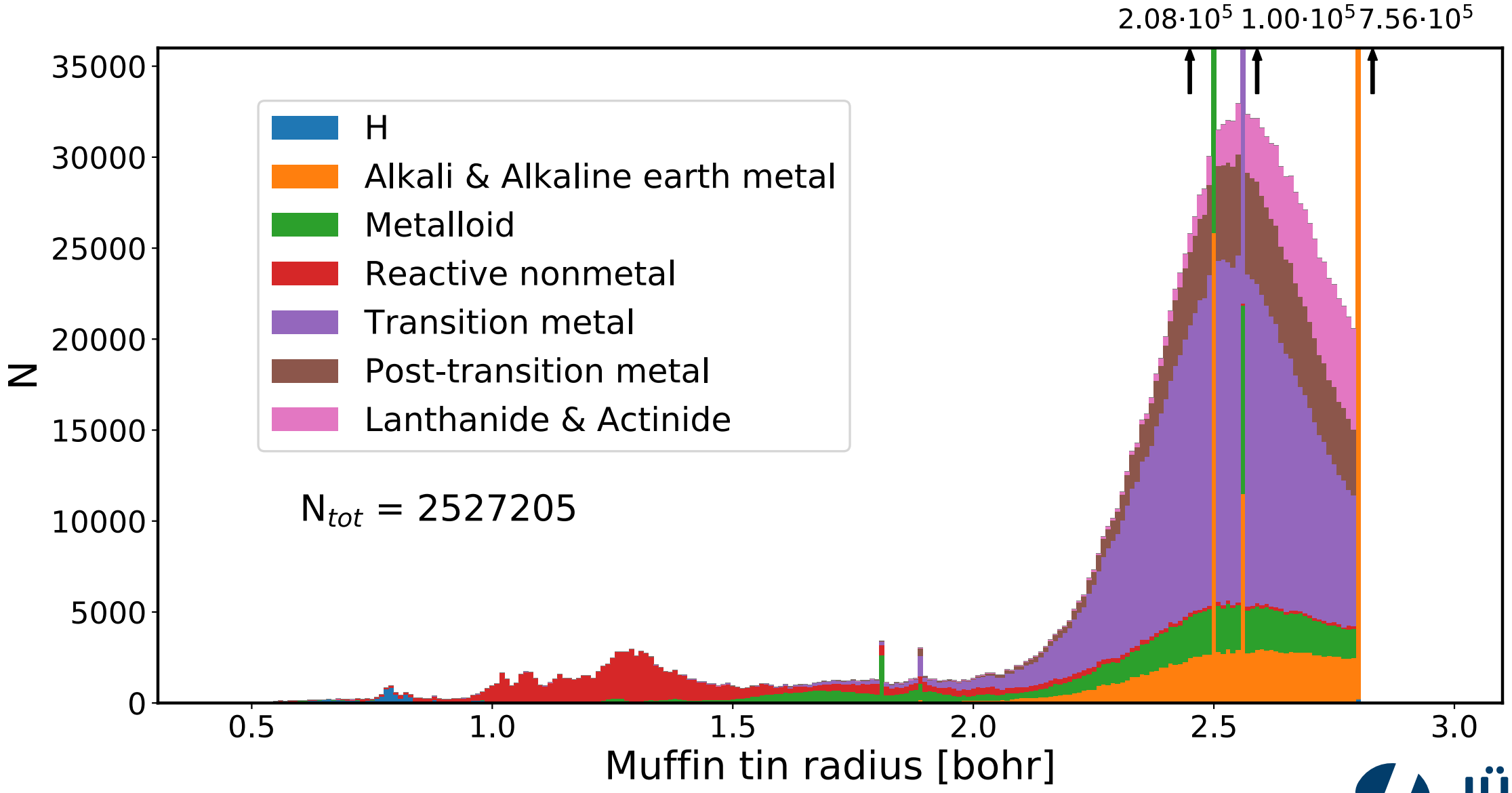
To improve defaults and robustness; structures from OQMD http://www.oqmd.org/



All symmetry groups in set.

80 % cubic

RMTS OF OQMD STRUCTURES

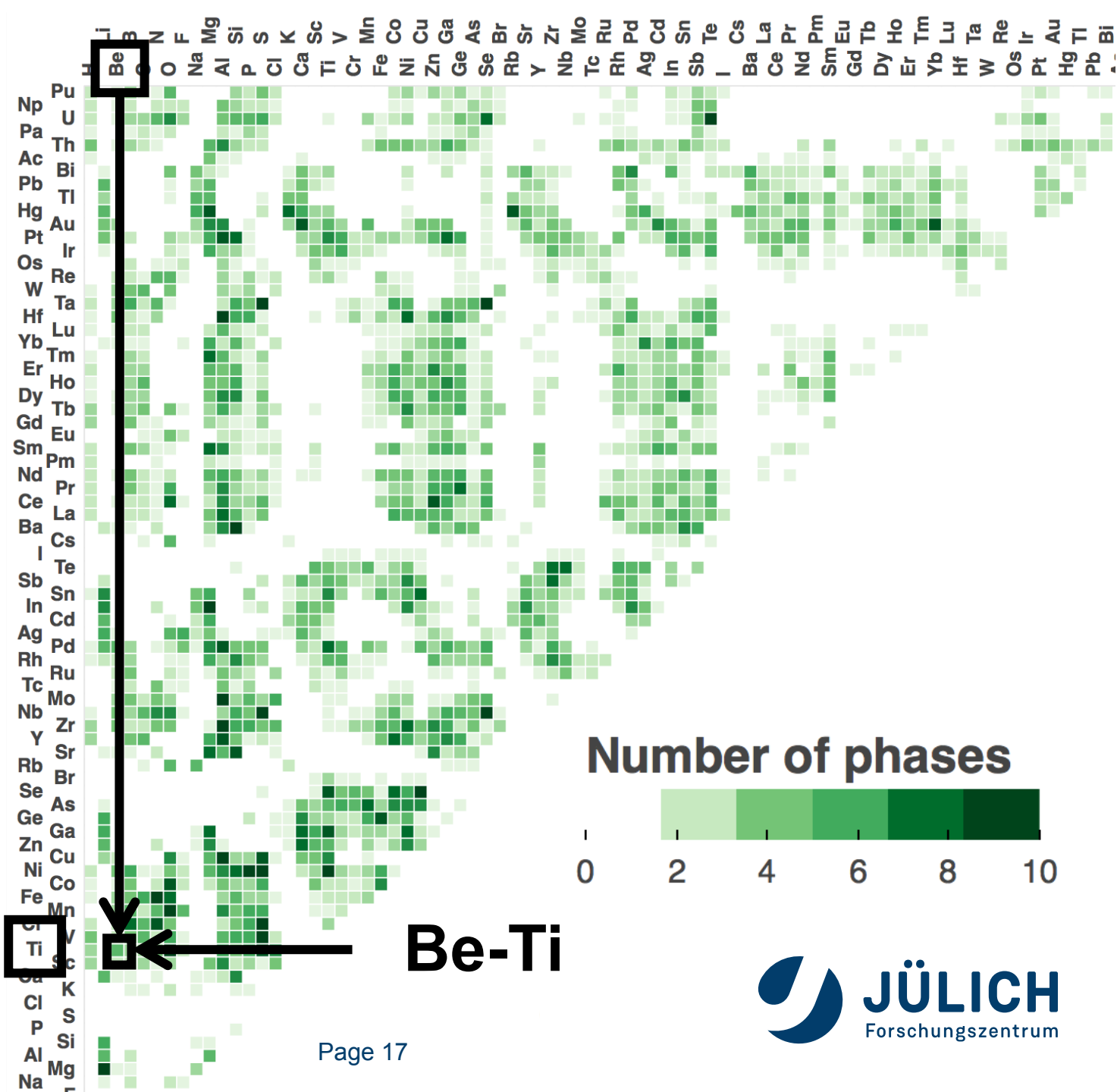


2. HTC PROJECT:

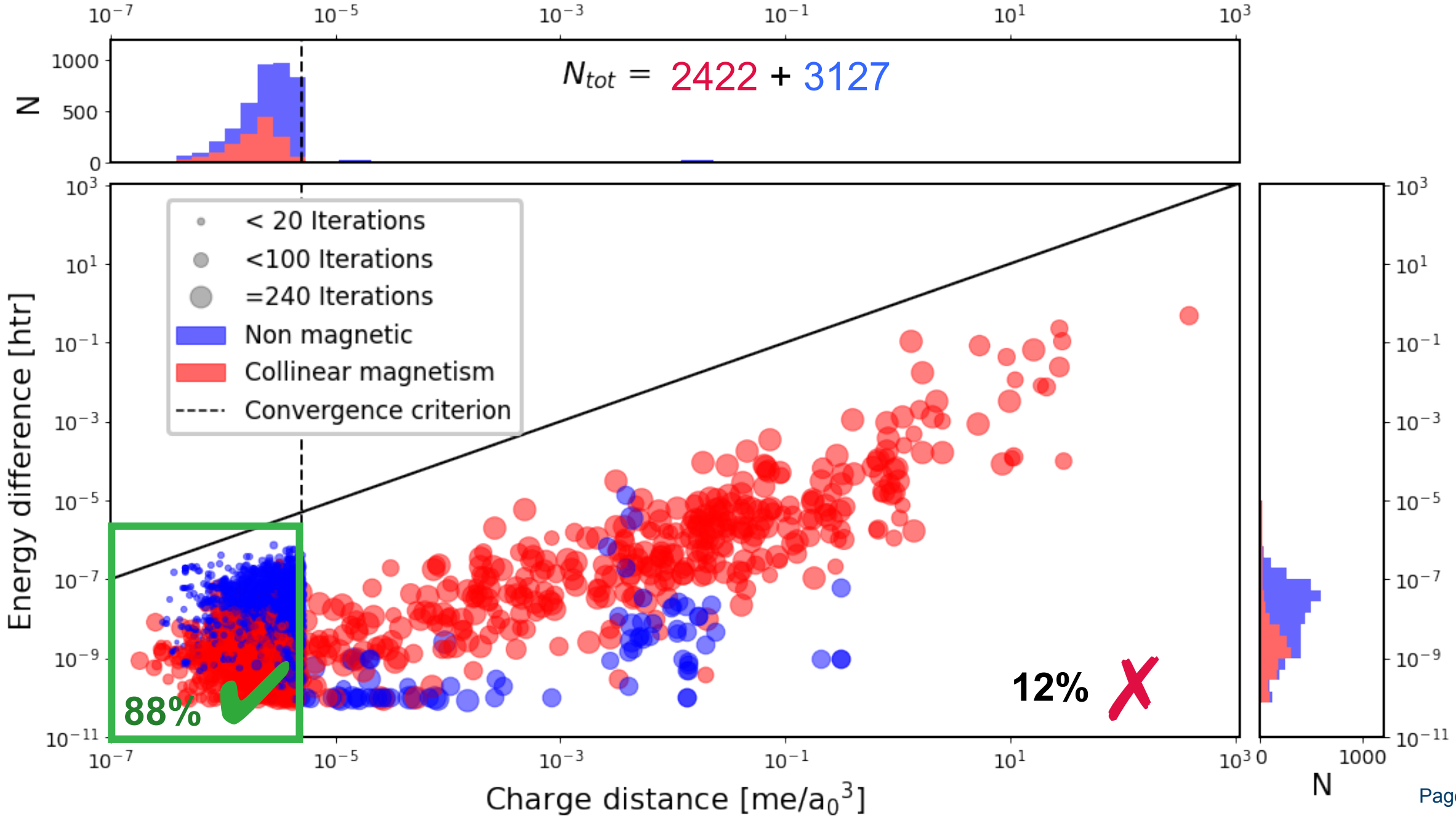
Create a database of core-level shifts

1. **Structure set:**
   - 1271 elements (ICSD)
   - 5058 stable binary metals from the Materials Project database
2. **Prepare FLAPW parameters**
3. **Launch:** > 6000 SCFs workflows
   Run time about two weeks
4. **Data Evaluation**

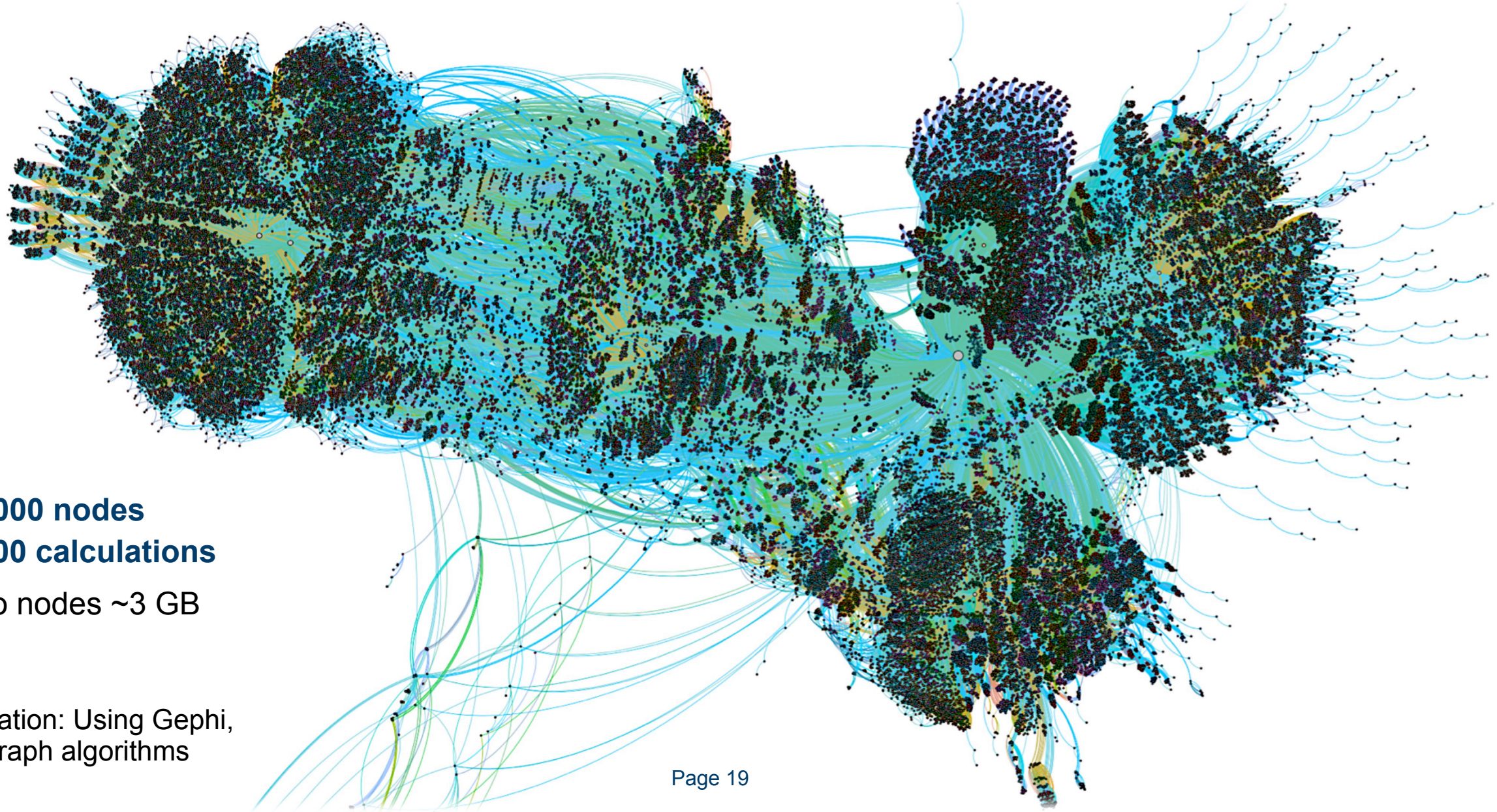
➡ First high-throughput project
at Peter Grünberg Institute (PGI);
with FLEUR;
with the FLAPW method



CONVERGENCE OF ALL FLEUR CALCULATIONS



VISUALIZING A SMALL AIIDA DATABASE GRAPH



> 130 000 nodes

> 10 000 calculations

1 Mio nodes ~3 GB

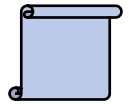
Visualization: Using Gephi,
Force-graph algorithms

TAKE HOME MESSAGE

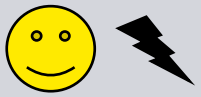
www.flapw.de

1. Introduction into the AiiDA Fleur Plugin package

- Fleur is connected to AiiDA via a plugin python package
- It parses and stores results of all simulations in a database
- Further it contains tools, workflows/workchains, turn-key solutions.

→ More details about some advanced workflows in an other talk 

2. Screening through larger material sets possible

- With great power comes great responsibility
- FLAPW high throughput possible, but lots to think about
  i.e optimal FLAPW parameter choice, optimal execution, …
- AiiDA scales to around 100 000 jobs per day
  → (do not try this on your virtual machines for the tutorial!) 

ACKNOWLEDGEMENTS

The FLEUR community:
D. Wortmann, G. Michalicek,
U. Alekseeva, G. Bihlmayer,
M. Redies, C. R. Gerhorst,
S. Blügel, …

Virtual materials design team:
A. Chandran, R. Kovacik,
P. Rüßmann, V. Tseplyaev

From the AiiDA community:
G. Pizzi, S. Huber, L. Talirz, M. Uhrin,
L. Kahle, N. Mounet, S. Zoupanos,
A. Cepellotti, N. Marzari, …

IT: N. Heimbach, D. Kaiser

And the open source community!

Computational resources from
JARA project jara0172 on CLAIX and JURECA.

Funding:

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Thank you!

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SOFTWARE STACK, REPOSITORIES

↑ := depends on

Dependency graph https://github.com/JuDFTteam

Masci-tools:

- AiiDA independent
- Parsers for files (Fleur and KKR)
- Writers for files
- Plot methods, matplotlib interactive bokeh
- Band structure tool
- Other tools …

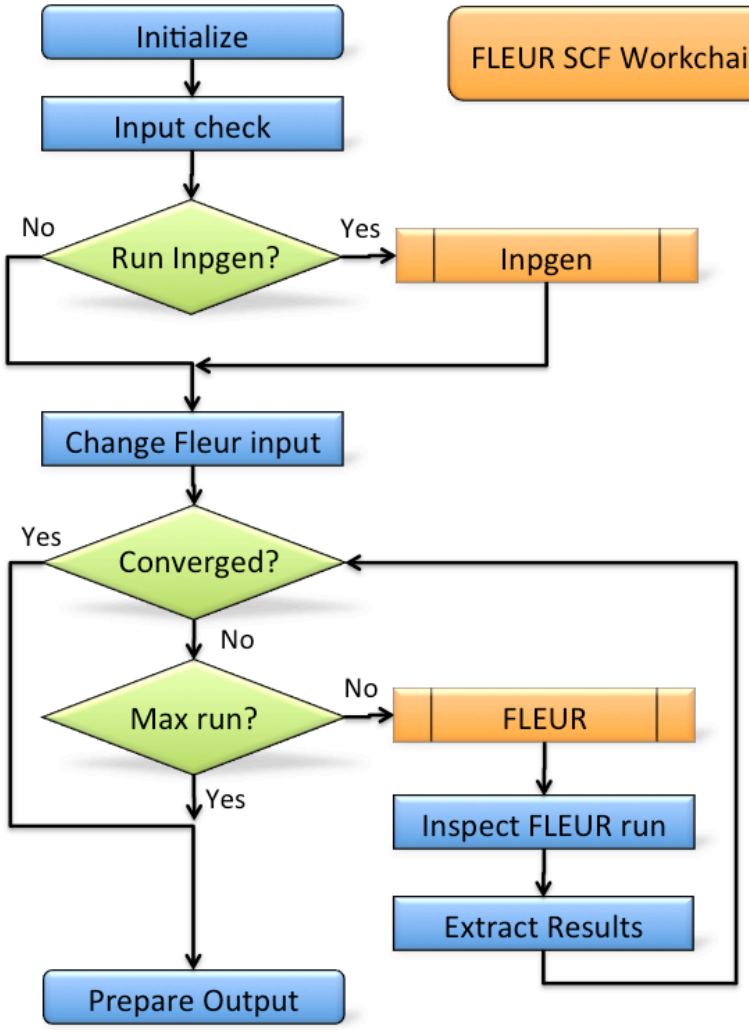
aiida-jutools: Aiida depended tools

aiida-kkr: Aiida-plugin for the KKR codes

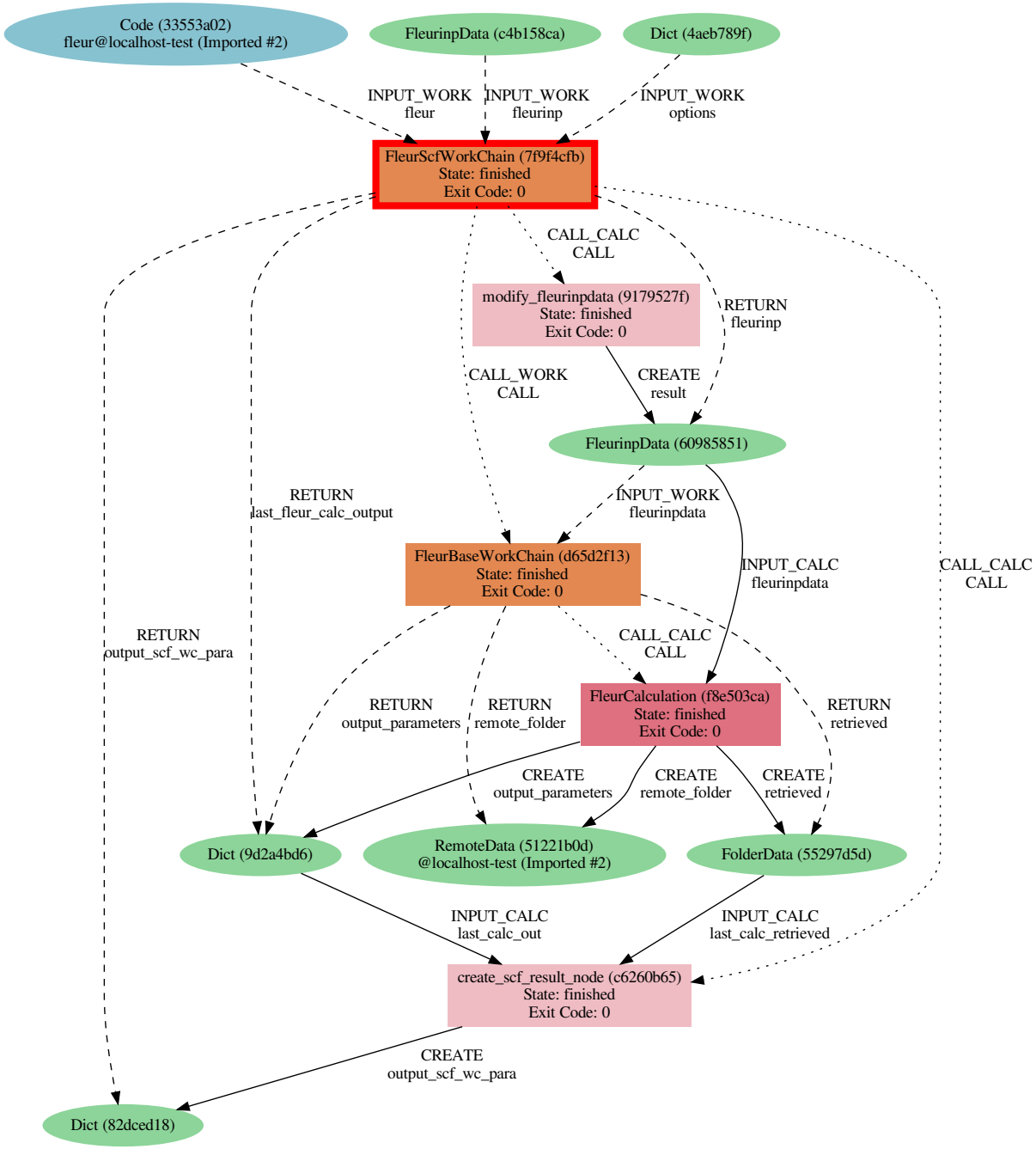
aiida-fleur: Aiida-plugin for the Fleur code

aiida-spex: Aiida-plugin for the Spex code

Feel free to contribute in any way!


Initialize
FLEUR SCF Workchain
Input check
No
Run Inpgen?
Yes
Inpgen
Change Fleur input
Yes
Converged?
No
Max run?
No
FLEUR
Yes
Inspect FLEUR run
Extract Results
Prepare Output

graph:


Code (33553a02)
fleur@localhost-test (Imported #2)
FleurinpData (c4b158ca)
Dict (4aeb789f)
INPUT_WORK
fleur
INPUT_WORK
fleurinp
INPUT_WORK
options
FleurScfWorkChain (7f9f4cfb)
State: finished
Exit Code: 0
CALL_CALC
CALL
modify_fleurinpdata (9179527f)
State: finished
Exit Code: 0
RETURN
fleurinp
CALL_WORK
CALL
CREATE
result
FleurinpData (60985851)
RETURN
last_fleur_calc_output
INPUT_WORK
fleurinpdata
FleurBaseWorkChain (d65d2f13)
State: finished
Exit Code: 0
INPUT_CALC
fleurinpdata
CALL_CALC
CALL
RETURN
output_scf_wc_para
CALL_CALC
CALL
RETURN
output_parameters
RETURN
remote_folder
FleurCalculation (f8e503ca)
State: finished
Exit Code: 0
RETURN
retrieved
CREATE
output_parameters
CREATE
remote_folder
CREATE
retrieved
Dict (9d2a4bd6)
RemoteData (51221b0d)
@localhost-test (Imported #2)
FolderData (55297d5d)
INPUT_CALC
last_calc_out
INPUT_CALC
last_calc_retrieved
create_scf_result_node (c6260b65)
State: finished
Exit Code: 0
CREATE
output_scf_wc_para
Dict (82dced18)

CONVERGENCE OF ALL FLEUR CALCULATIONS