



AIIDA-FLEUR WORKCHAINS

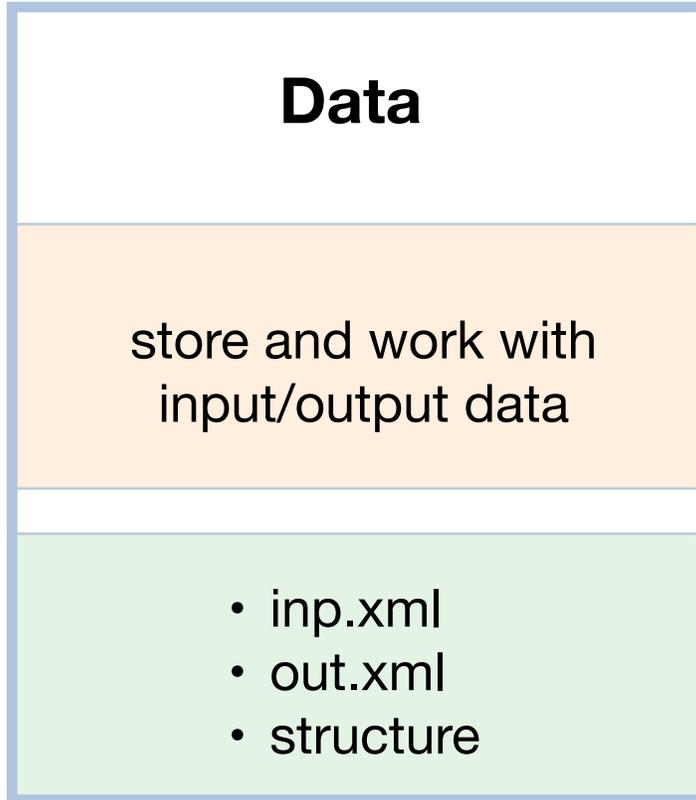
Key-turn solutions for your FLEUR calculations

14. APRIL 2021 | VASILY TSEPLYAEV

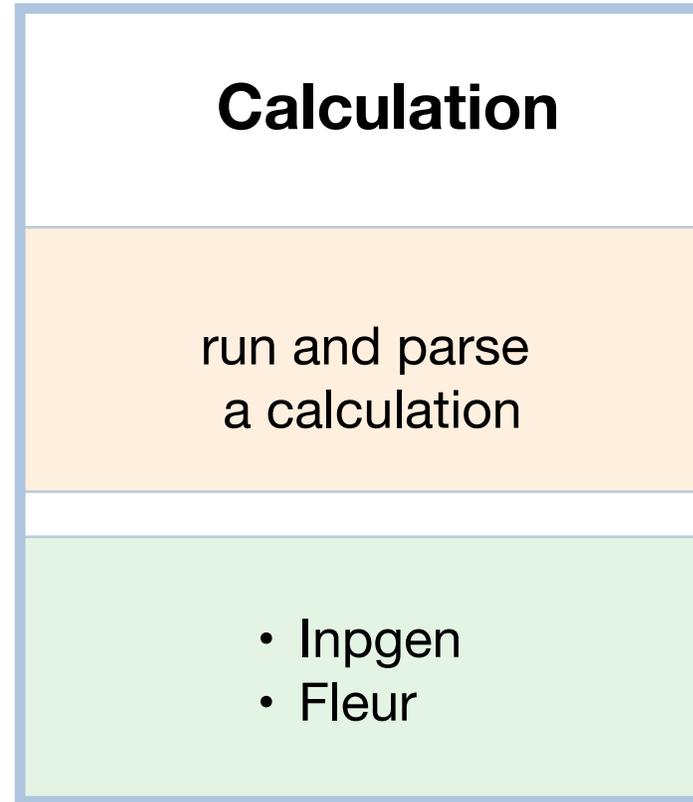
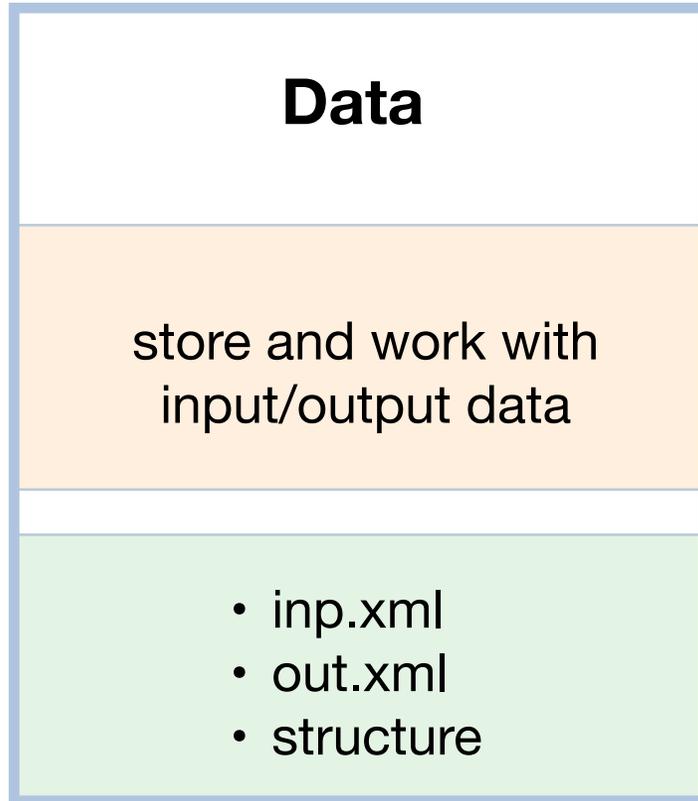


Plugin Structure

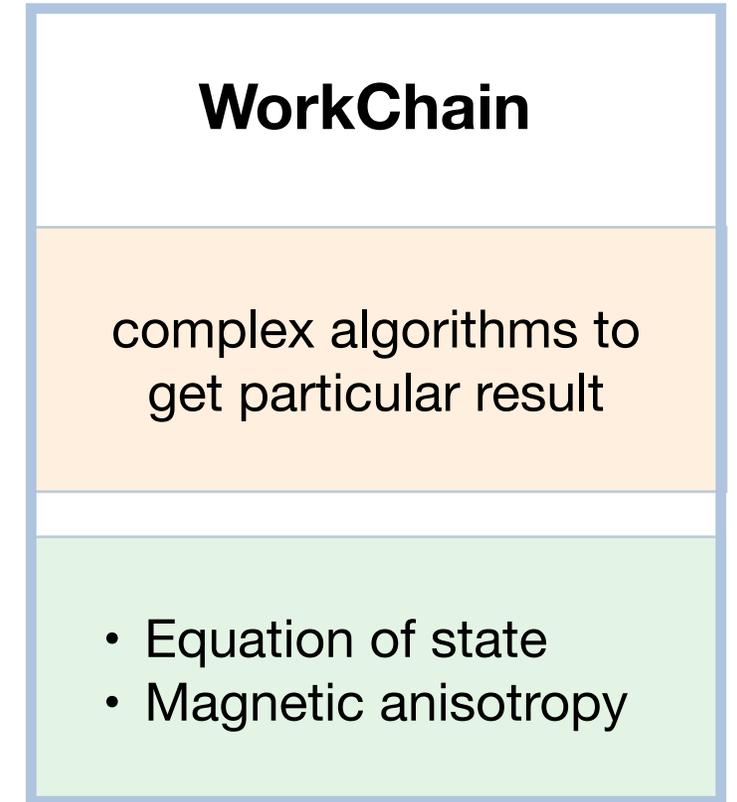
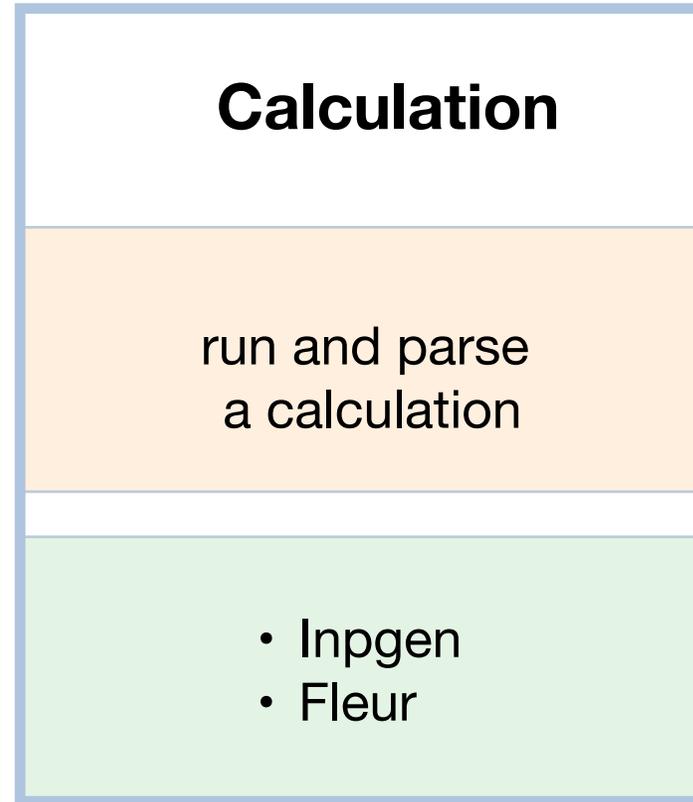
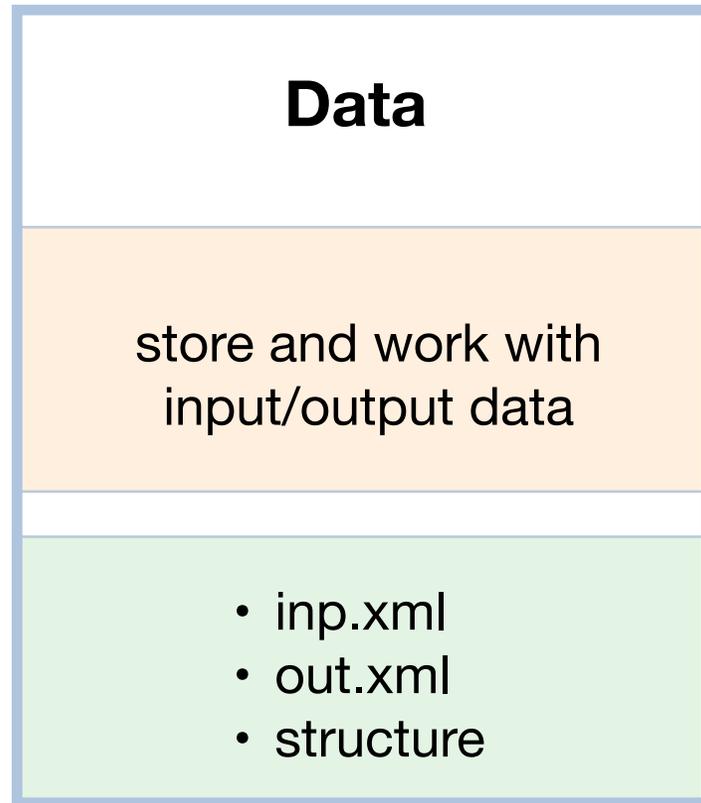
Plugin Structure



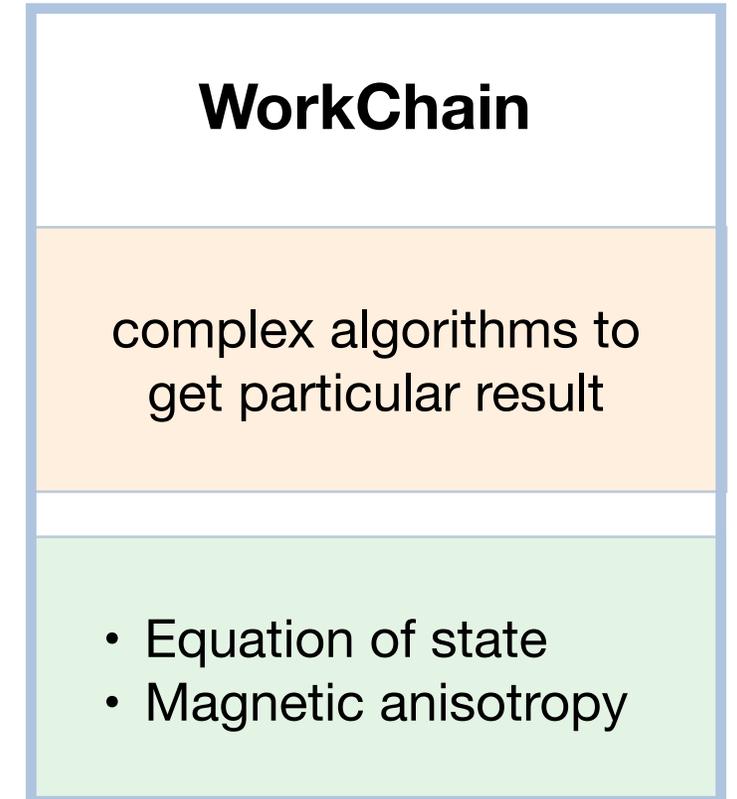
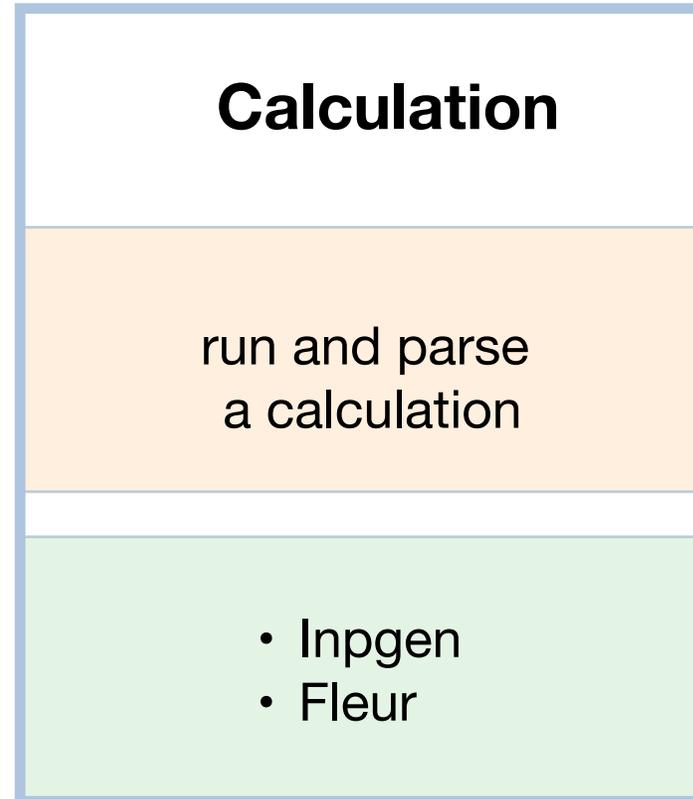
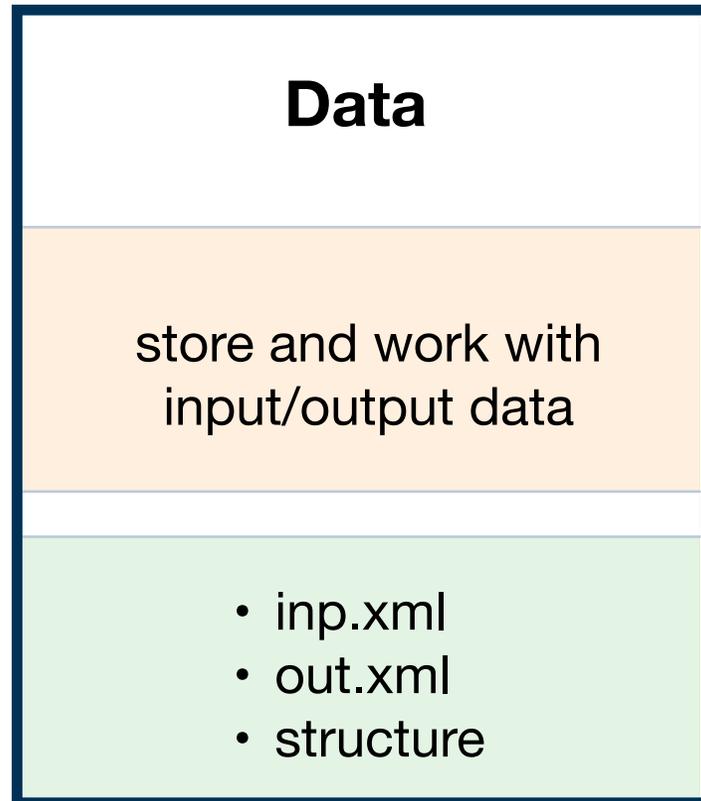
Plugin Structure



Plugin Structure



Plugin Structure



AiiDA data types

AiiDA data types

Python-like types

Int

Float

Str

Dict

a nested set of **key**: **value** pairs

```
{'conv_mode': 'density',  
 'loop_count': 1,  
 'total_energy': -90511.187617666,  
 'force_largest': 0.0,  
 'workflow_name': 'FleurScfWorkChain'}
```

AiiDA data types

Python-like types

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Float

Str

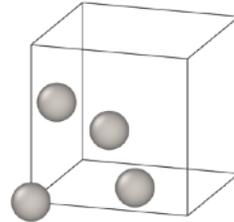
Dict

a nested set of **key**: **value** pairs

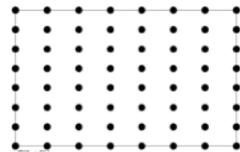
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 'workflow_name': 'FleurScfWorkChain'}
```

Structure types

StructureData



KpointsData



k-point grid

AiiDA data types

Python-like types

Int

Float

Str

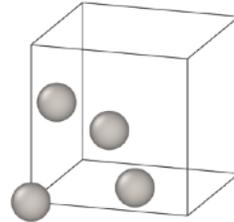
Dict

a nested set of **key: value** pairs

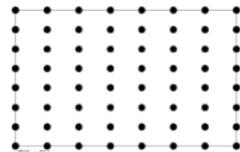
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```

Structure types

StructureData



KpointsData



k-point grid

File types

FolderData



a local folder

RemoteData

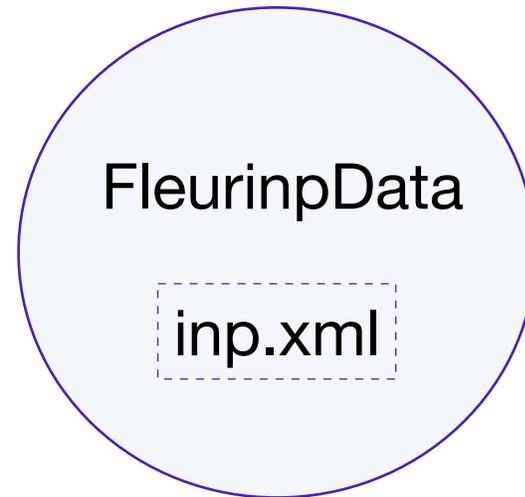


a remote folder

SinglefileData

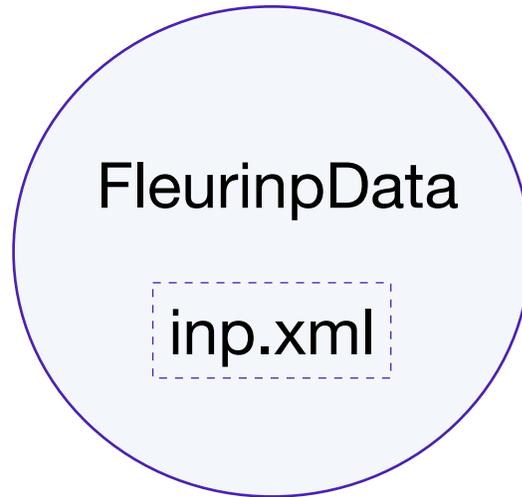


AiiDA-Fleur input files



AiiDA-Fleur input files

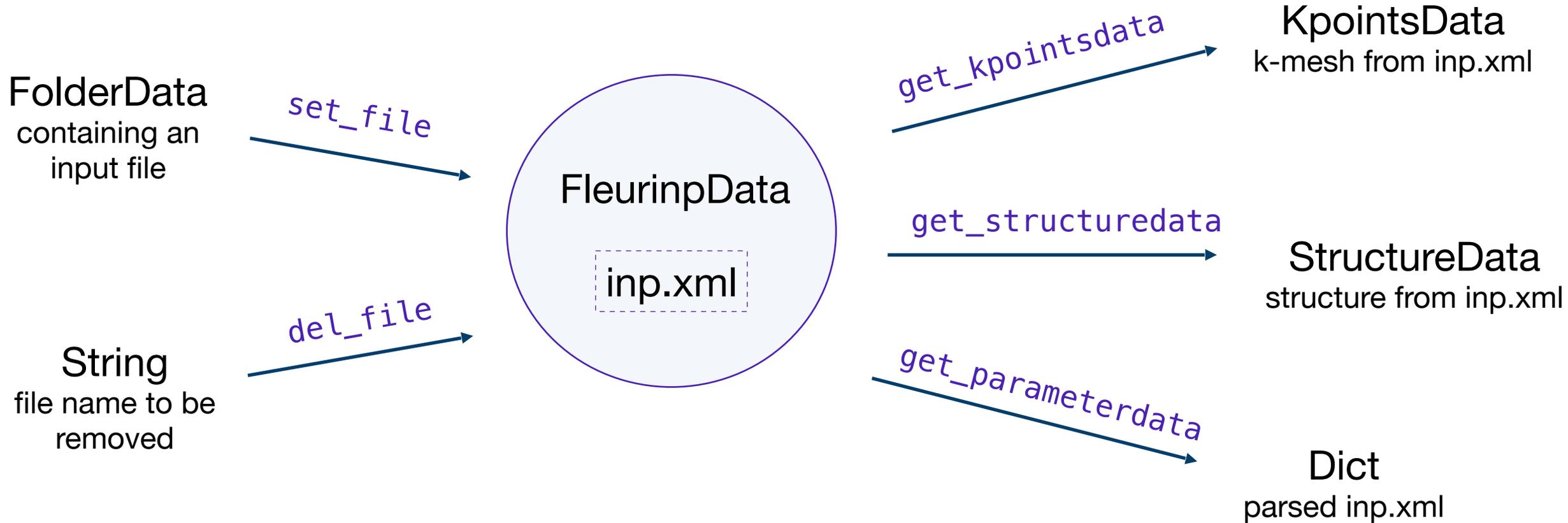
FolderData
containing an
input file



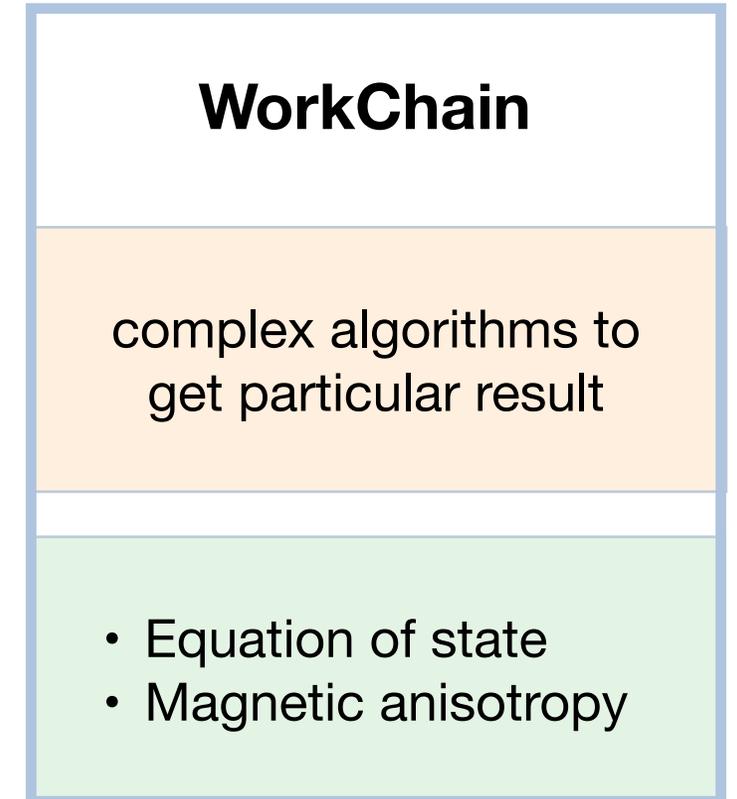
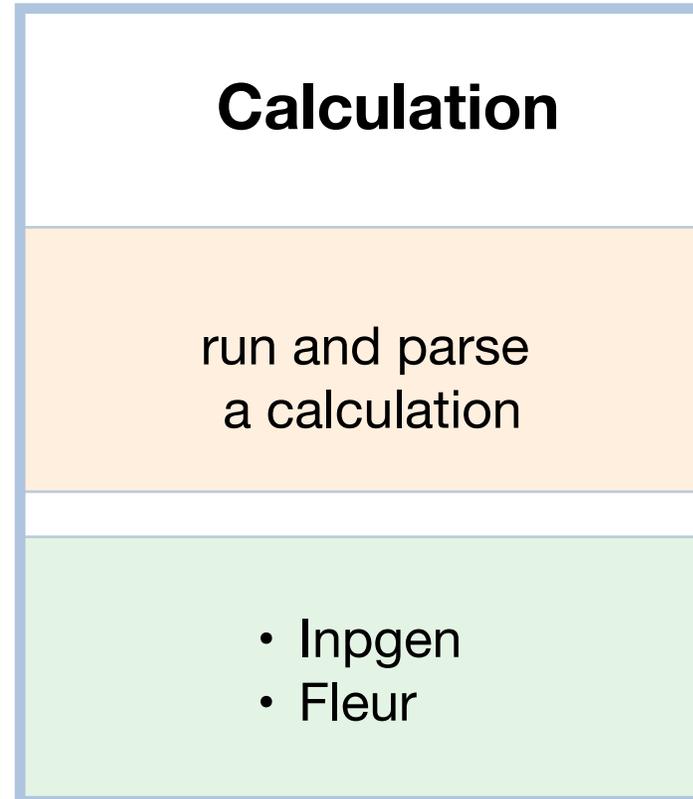
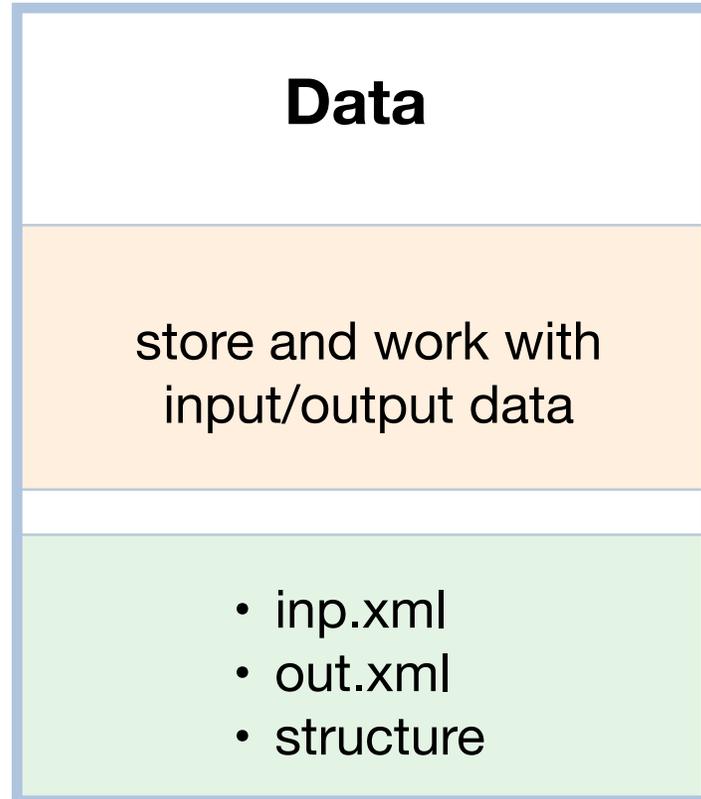
String
file name to be
removed



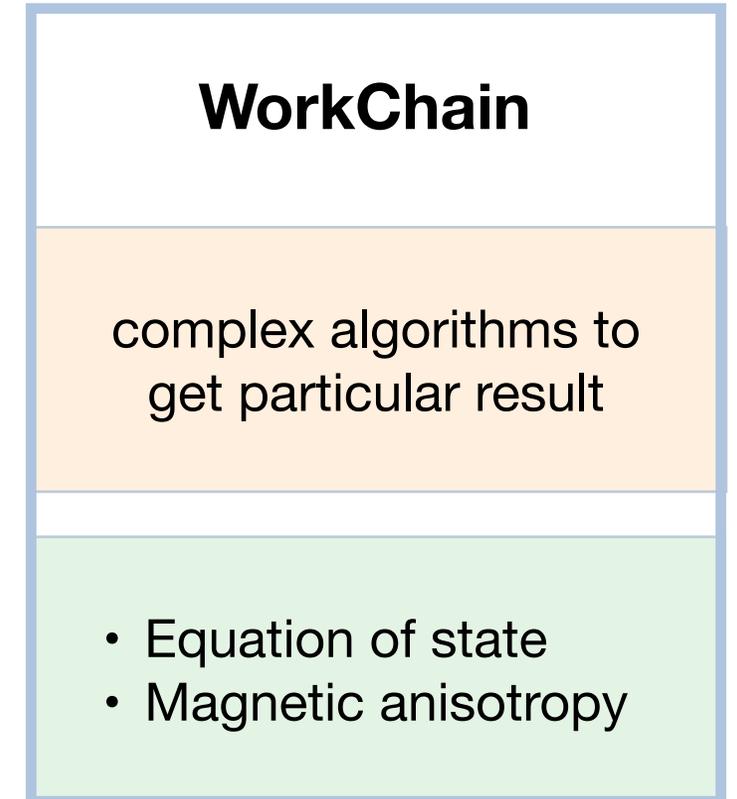
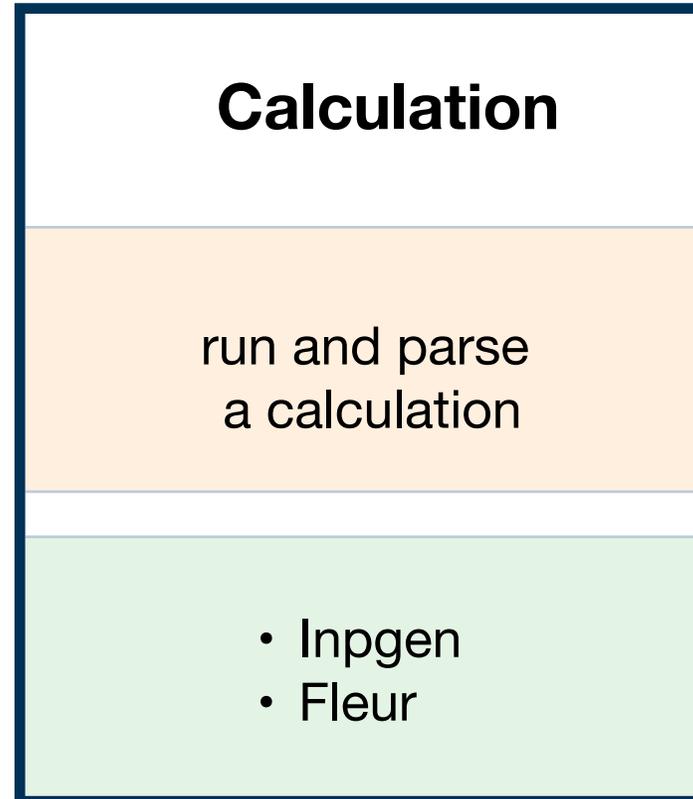
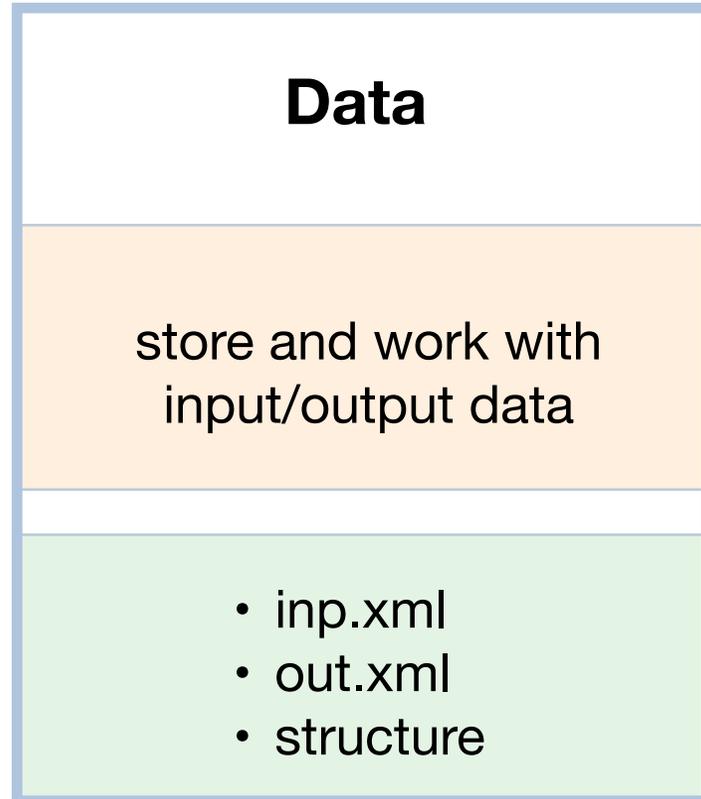
AiiDA-Fleur input files



Plugin Structure



Plugin Structure



AiiDA engine types

Code

Executable



Used by calculations

AiiDA engine types

Code

Executable



Used by calculations

```
(base) jovyan@6668aa26739f:~$ verdi code show 2
```

```
-----  
PK                2  
UUID              dfae82d2-d687-42f8-be36-8277f3d06bd7  
Label             fleur  
Description       FLEUR, FLAPW code based on DFT compiled with HDF5  
Default plugin    fleur.fleur  
Type              remote  
Remote machine    localhost  
Remote absolute path /usr/bin/fleur_MPI  
Prepend text  
Append text  
-----
```

AiiDA engine types

Code

Executable



Used by calculations

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AiiDA engine types

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the reference

how to submit and parse

AiiDA engine types

Code

Executable



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Default plugin    fleur.fleur  
Type              remote  
Remote machine    localhost  
Remote absolute path /usr/bin/fleur MPI  
Prepend text  
Append text  
-----
```

the reference

how to submit and parse

which computer

where to find the executable

AiiDA engine types

AiiDA engine types

CalcJob

Calculation *process*



Runs a single Fleur calculation and parses results

AiiDA engine types

Calculation *process*

CalcJob



Runs a single Fleur calculation and parses results

```
(base) jovyan@6668aa26739f:~$ verdi node show 196
Property      Value
-----
type          FleurCalculation
state         Finished [0]
pk            196
uuid          7f12f811-ae9b-4dcf-83a3-c5fb590e384b
label         scf: fleur run 1
description   |fleur_scf_wc| fleur run 1 on Fe
ctime         2021-01-19 12:05:15.247012+00:00
mtime         2021-01-19 12:07:43.087097+00:00
computer      [2] iffslurm

Inputs          PK  Type
-----
code            324 Code
fleurinpdata    216 FleurinpData
settings        257 Dict

Outputs          PK  Type
-----
output_parameters  253 Dict
remote_folder     343 RemoteData
retrieved         104 FolderData

Caller      PK  Type
-----
CALL        34  FleurBaseWorkChain
```

AiiDA engine types

Calculation *process*

CalcJob



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when created?

AiiDA engine types

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where executed?

AiiDA engine types

Calculation process

CalcJob



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what are the inputs?

AiiDA engine types

Calculation *process*

CalcJob



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the reference

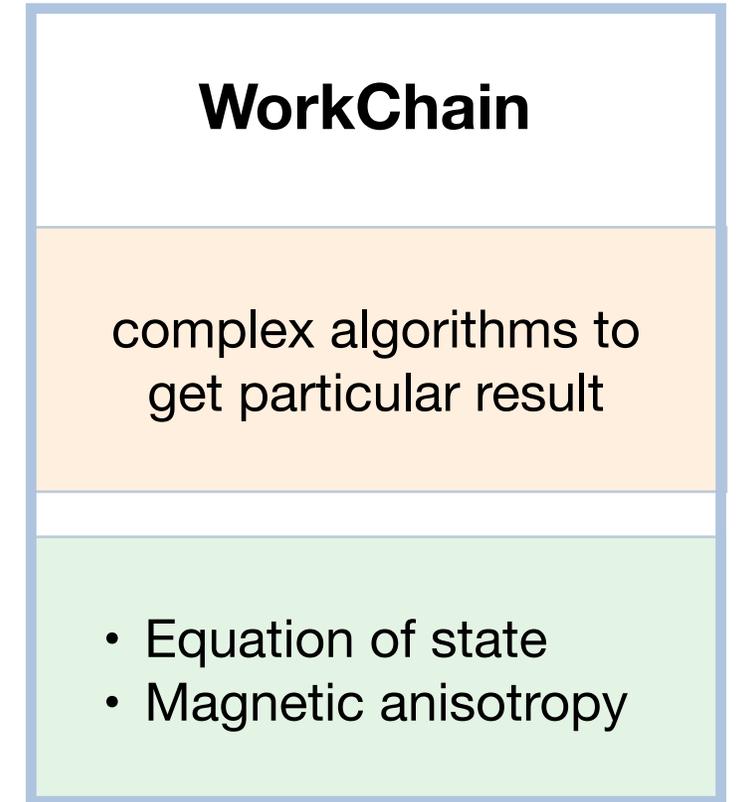
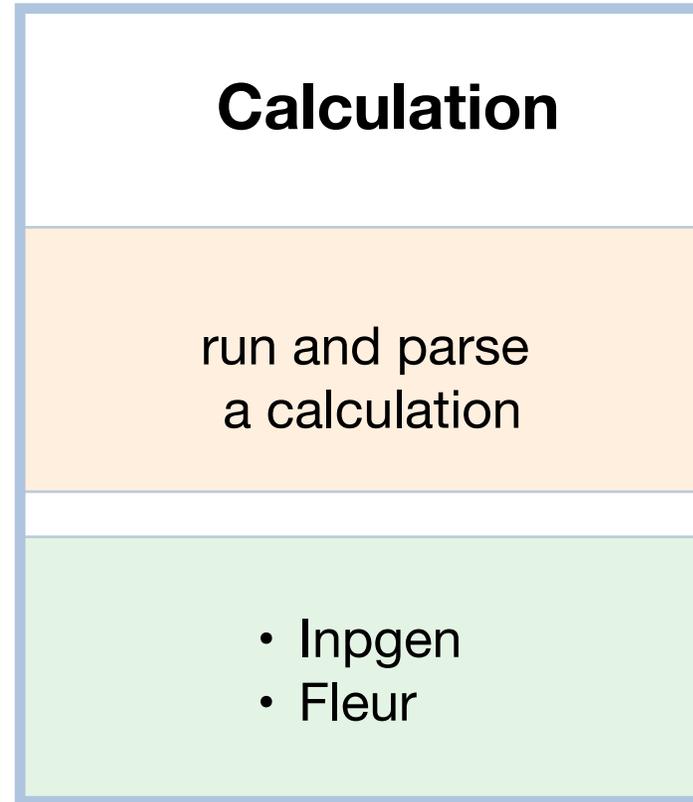
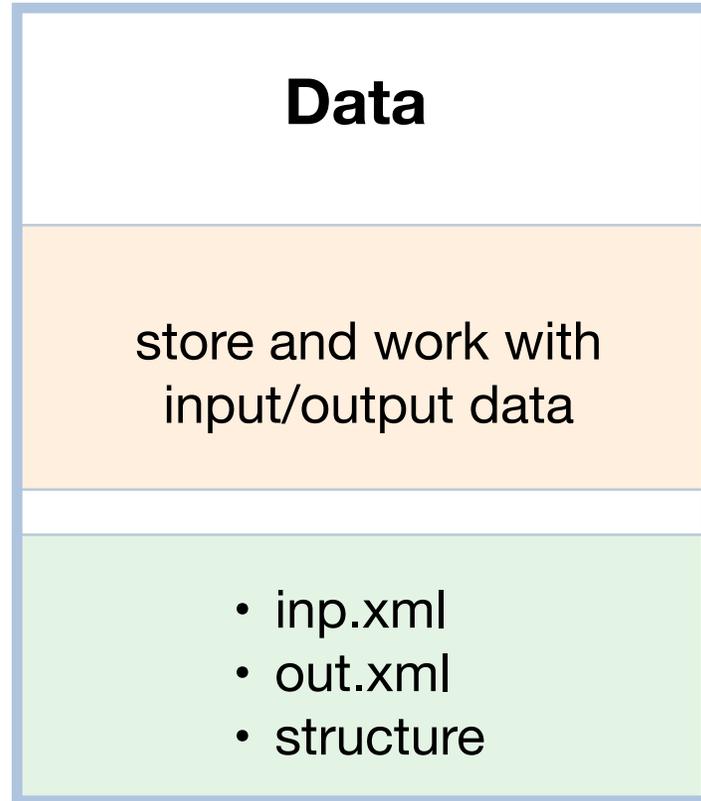
when created?

where executed?

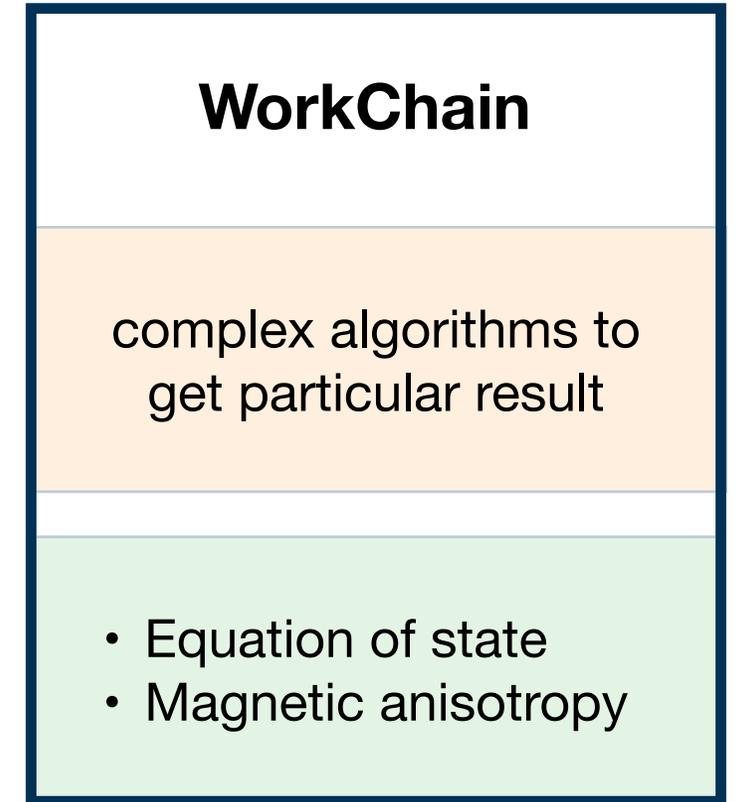
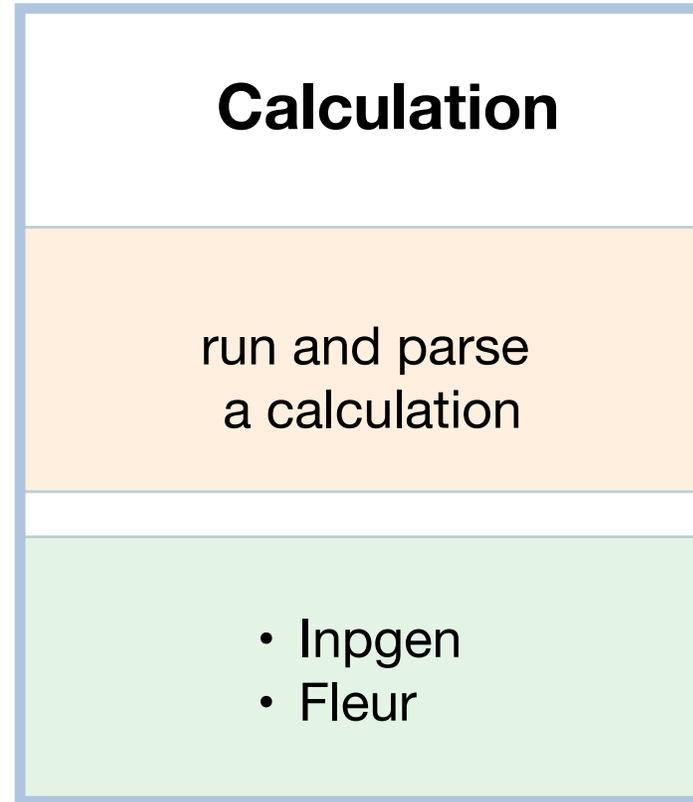
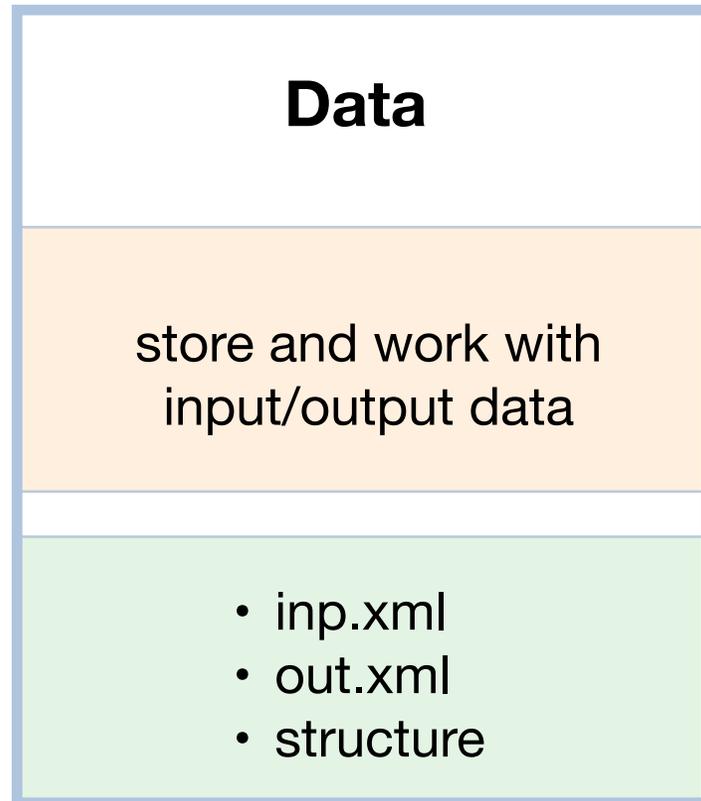
what are the inputs?

what are the outputs?

Plugin Structure



Plugin Structure



AiiDA engine types

CalcJob

Calculation *process*



Runs a single Fleur calculation and parses results

AiiDA engine types

CalcJob

Calculation *process*



Runs a single Fleur calculation and parses results

WorkChain

Chain of processes



Runs a sequence of Fleur calculations

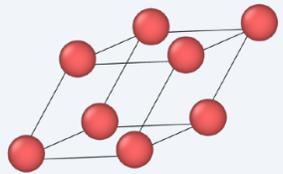
Workchain

Calculation of a property consists of a sequence of calculations

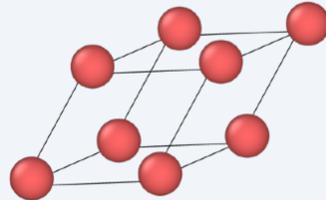
Workchain

Calculation of a property consists of a sequence of calculations

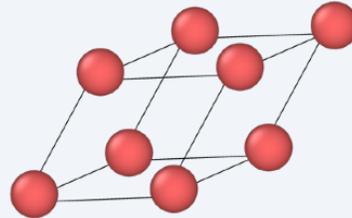
Equation of States:



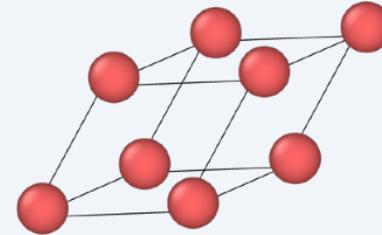
Energy



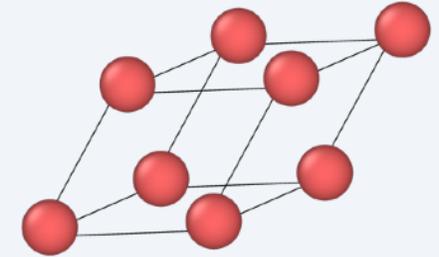
Energy



Energy



Energy

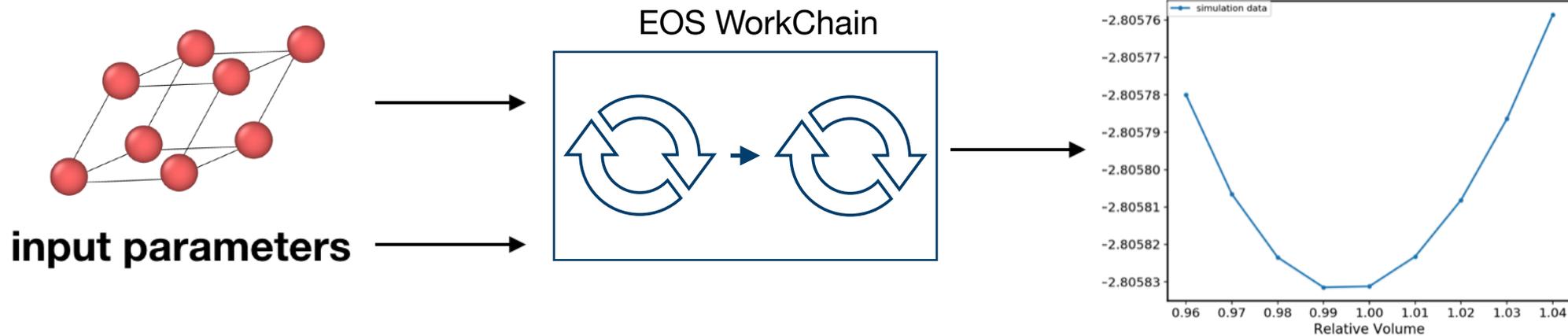
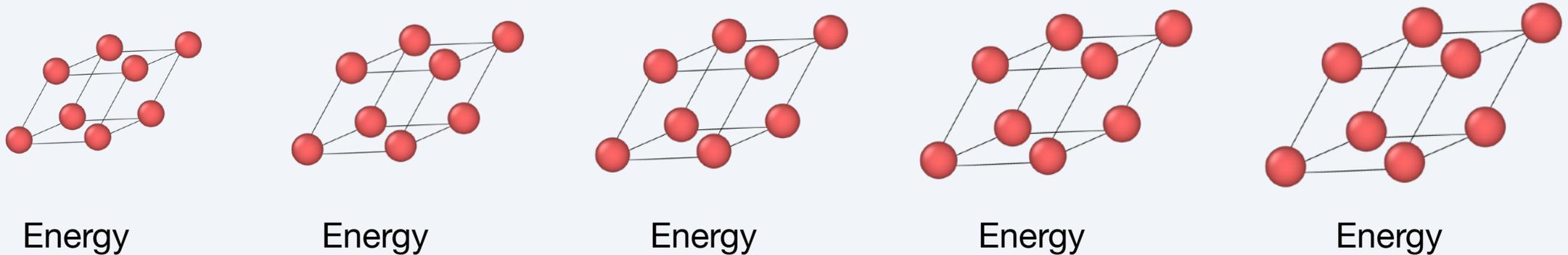


Energy

Workchain

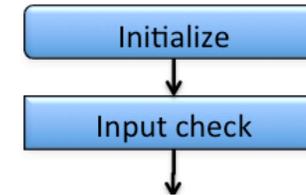
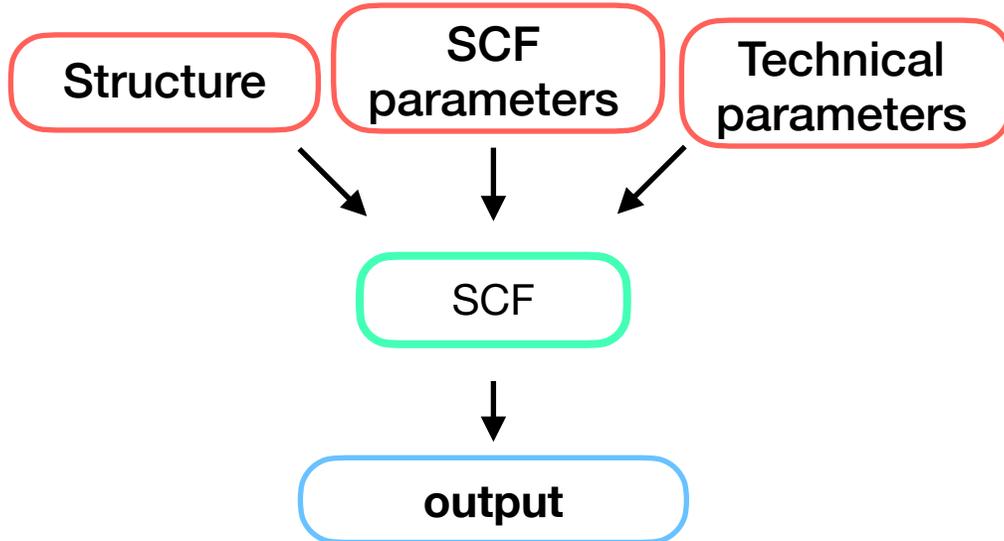
Calculation of a property consists of a sequence of calculations

Equation of States:



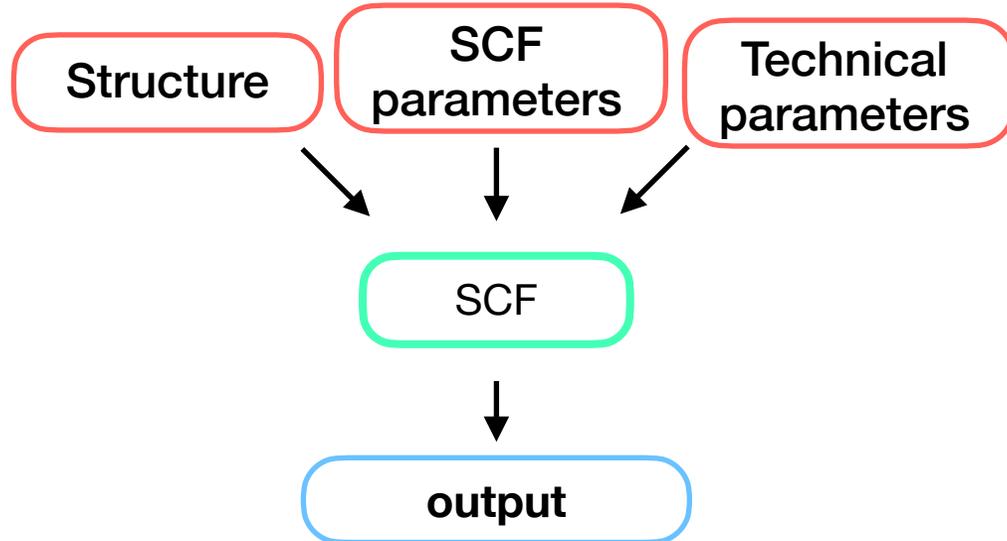
SCF WorkChain

Converges charge density

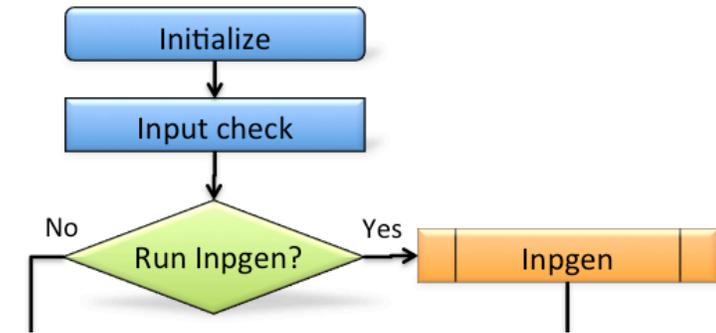


SCF WorkChain

Converges charge density

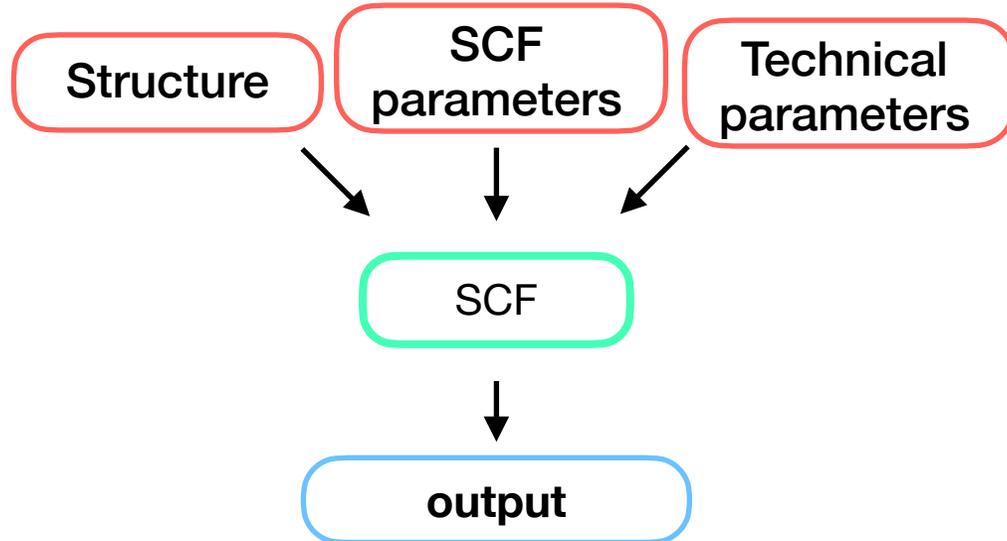


1. Run inpgen

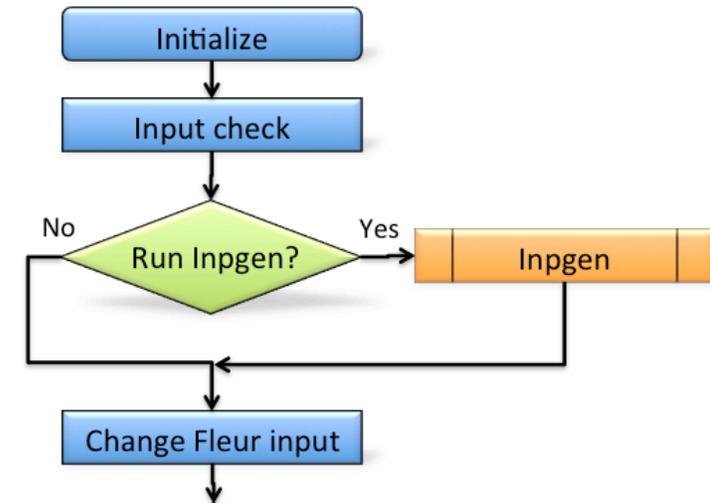


SCF WorkChain

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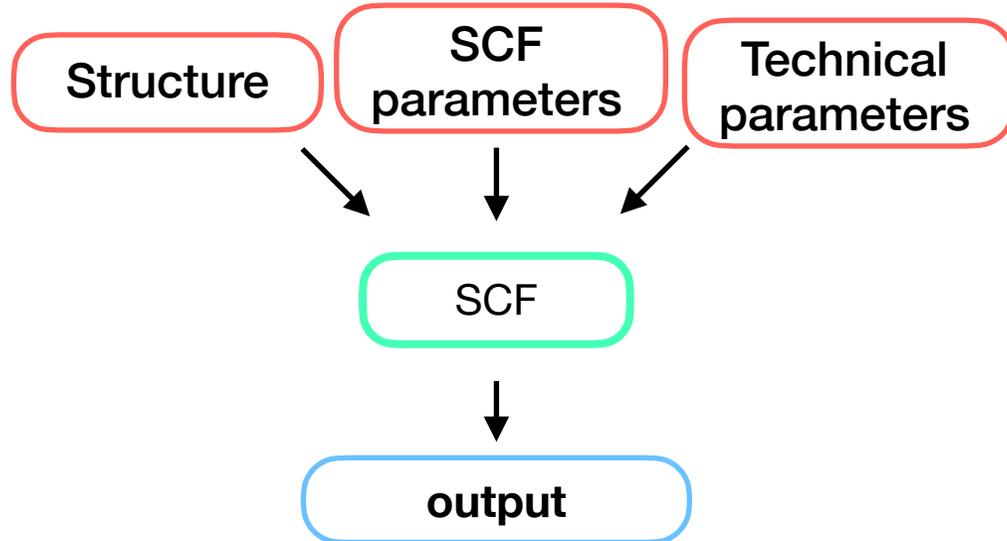


1. Run inpgen
2. Change FleurinpData

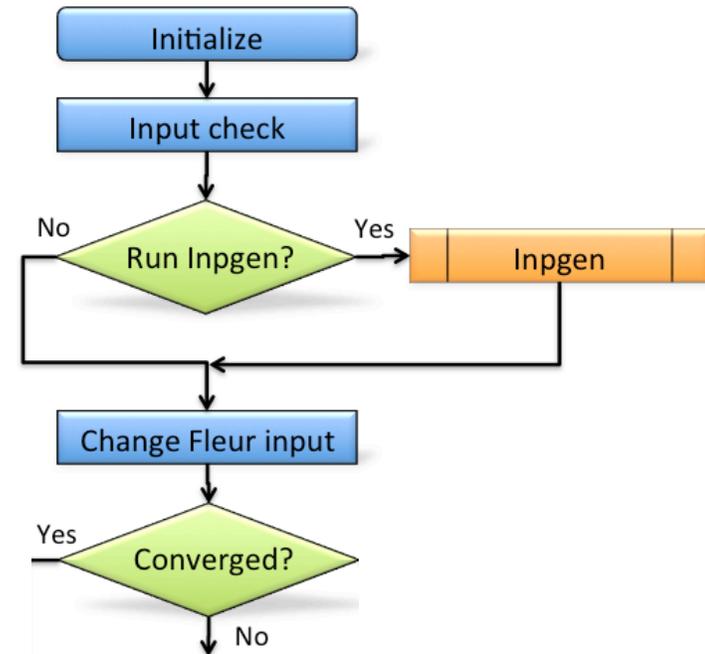


SCF WorkChain

Converges charge density

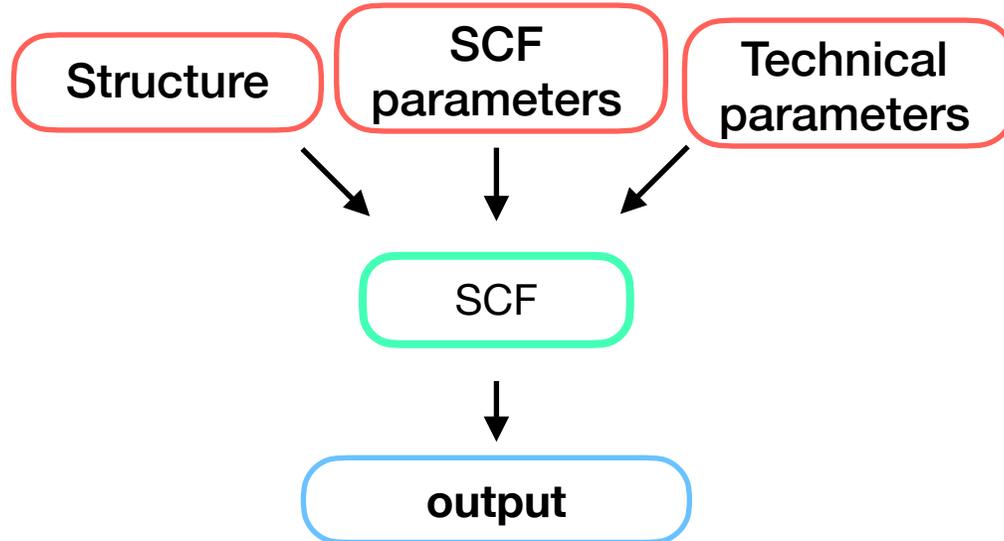


1. Run inpgen
2. Change FleurinpData
3. Check convergence (density, energy or force)

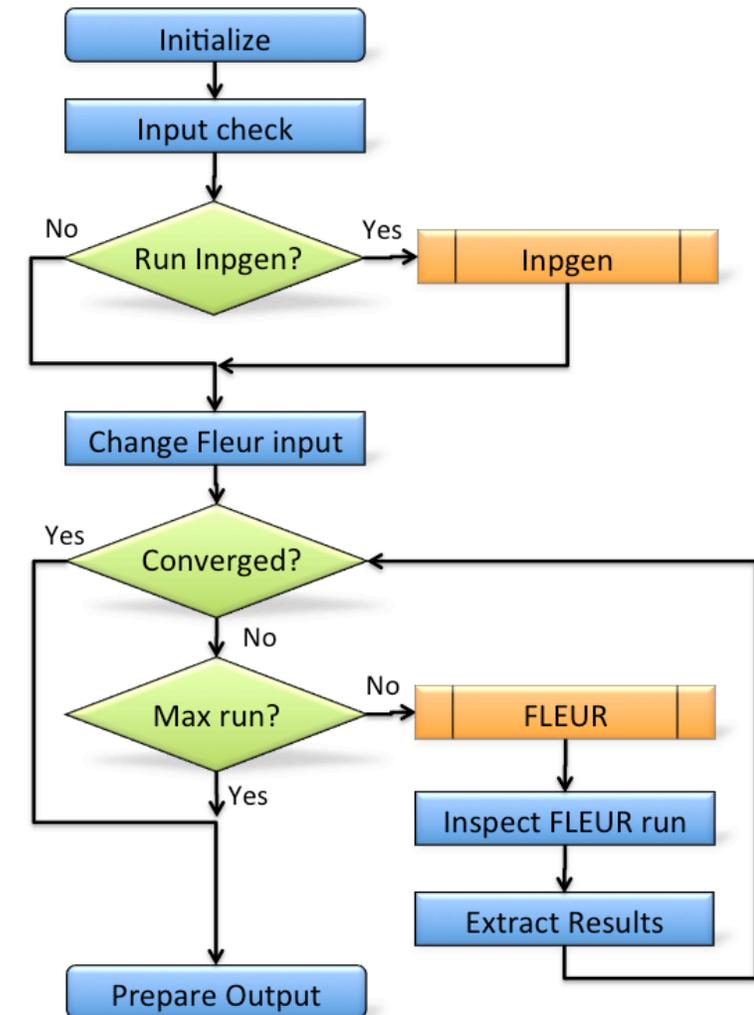


SCF WorkChain

Converges charge density

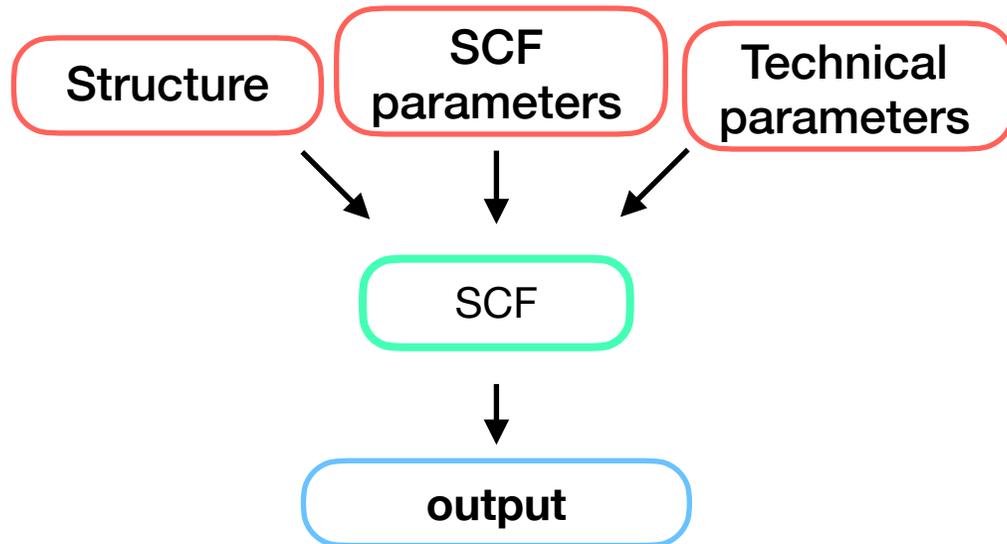


1. Run inpgen
2. Change FleurinpData
3. Check convergence (density, energy or force)
4. Run Fleur

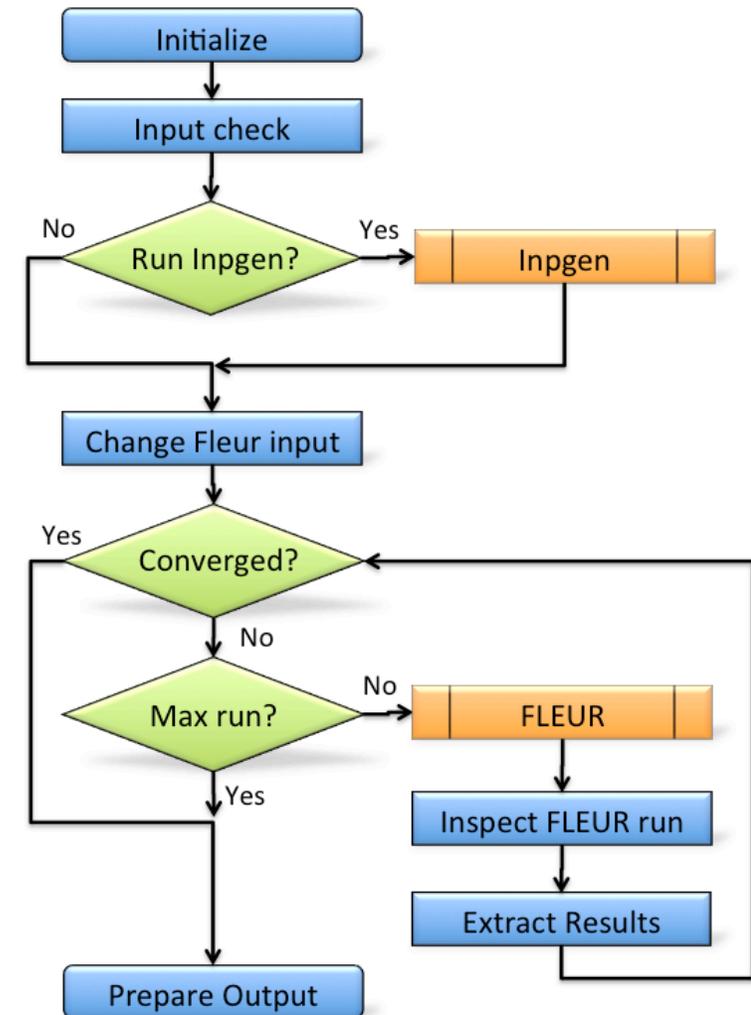


SCF WorkChain

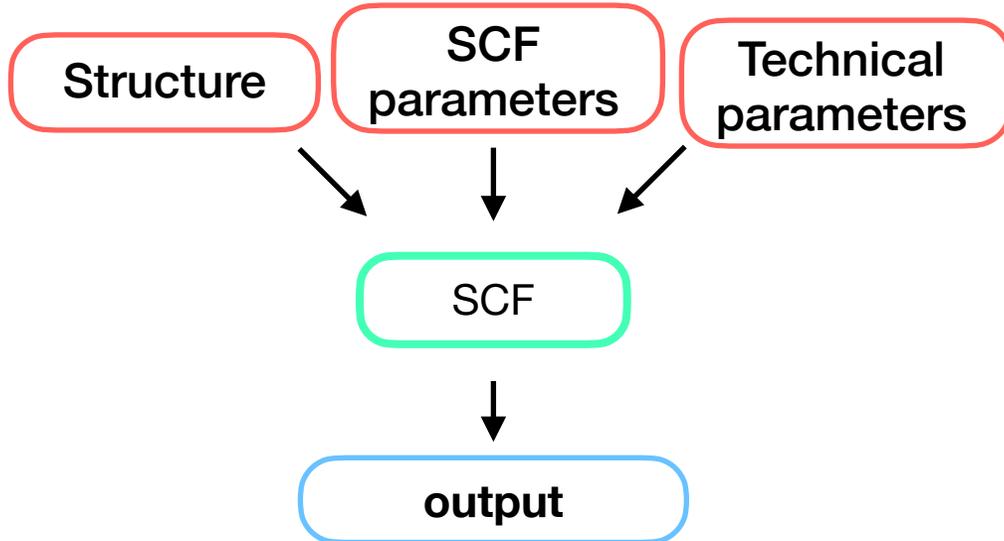
Converges charge density



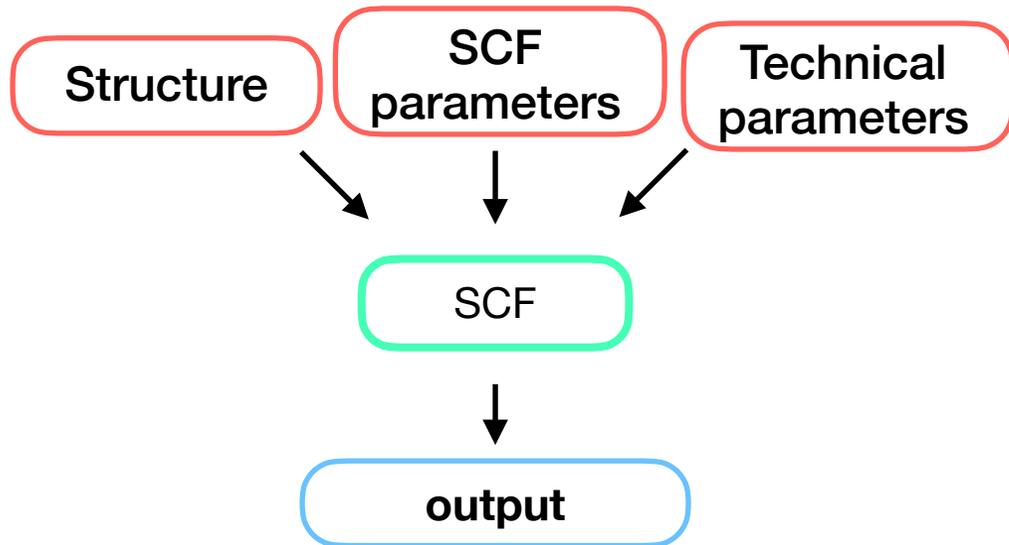
1. Run inpgen
2. Change FleurinpData
3. Check convergence (density, energy or force)
4. Run Fleur



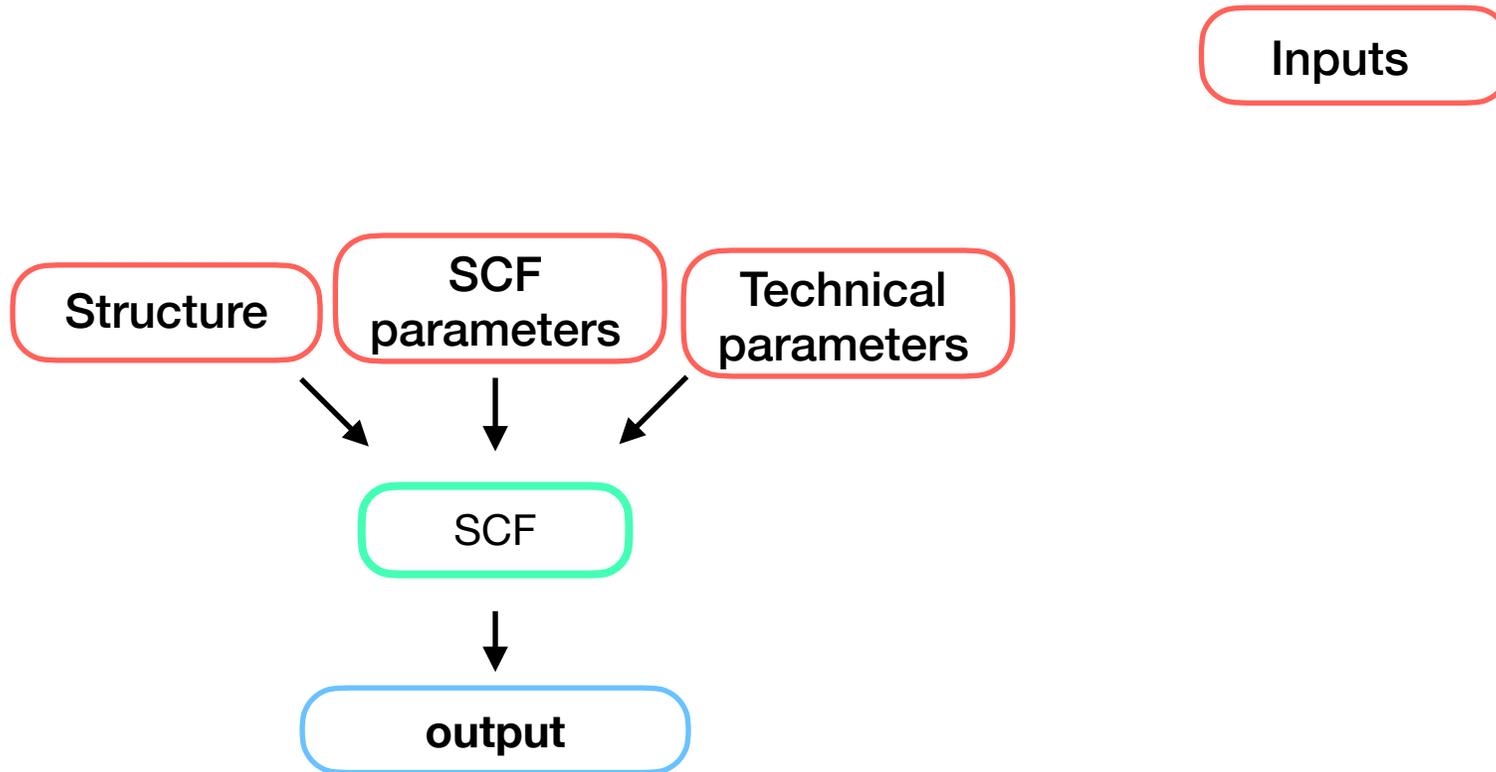
SCF WorkChain



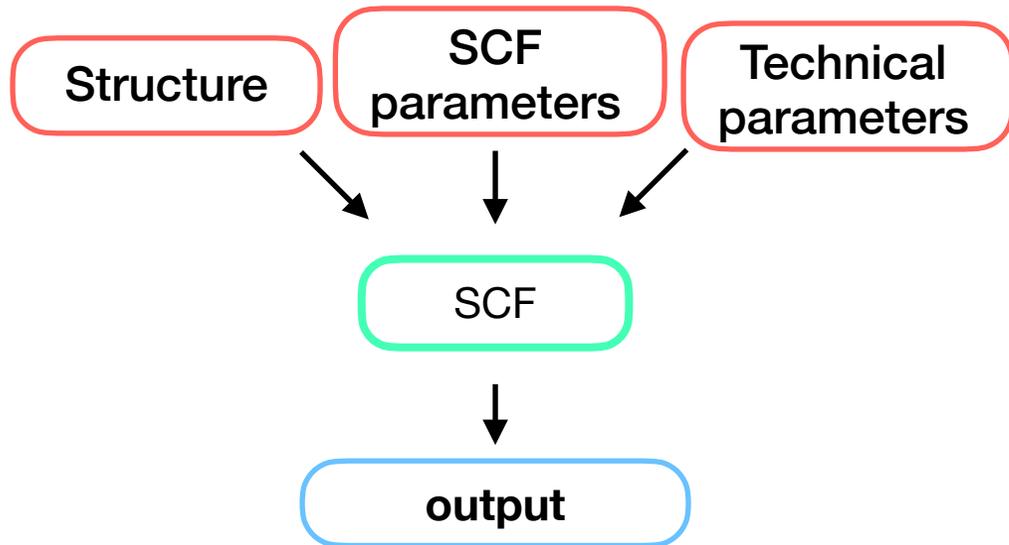
SCF WorkChain



SCF WorkChain



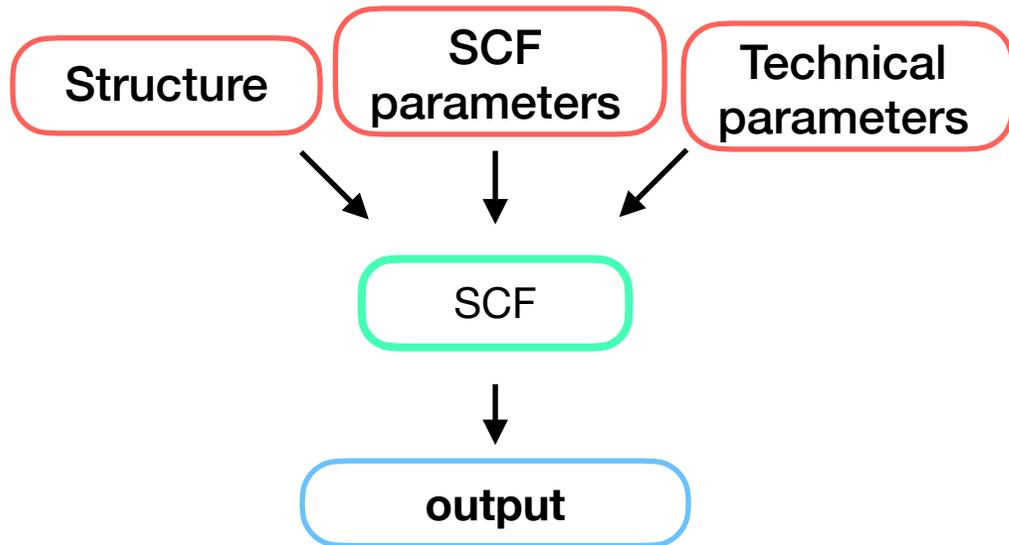
SCF WorkChain



Inputs

'wf_parameters': SCF parameters

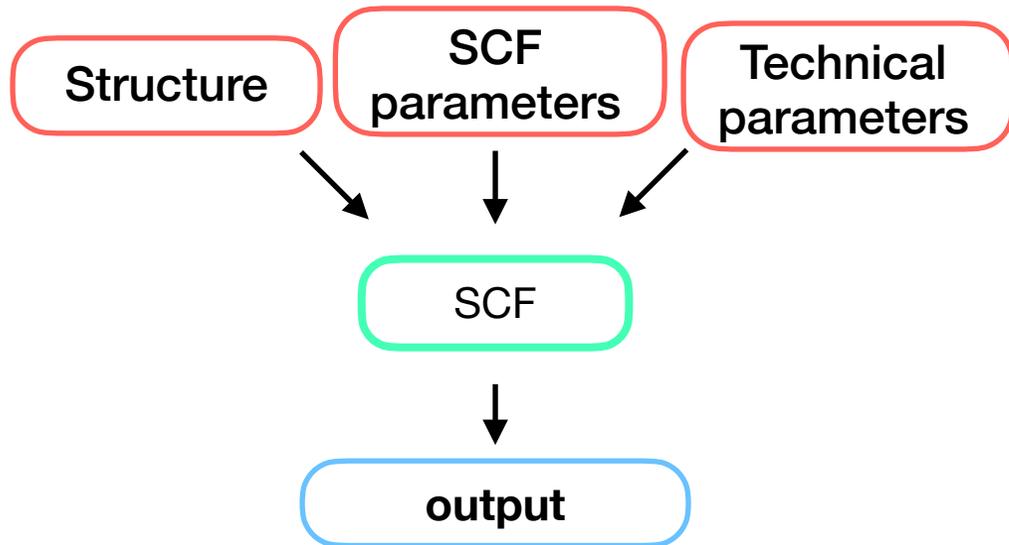
SCF WorkChain



Inputs

'wf_parameters': SCF parameters
'calc_parameters': inpgen parameters

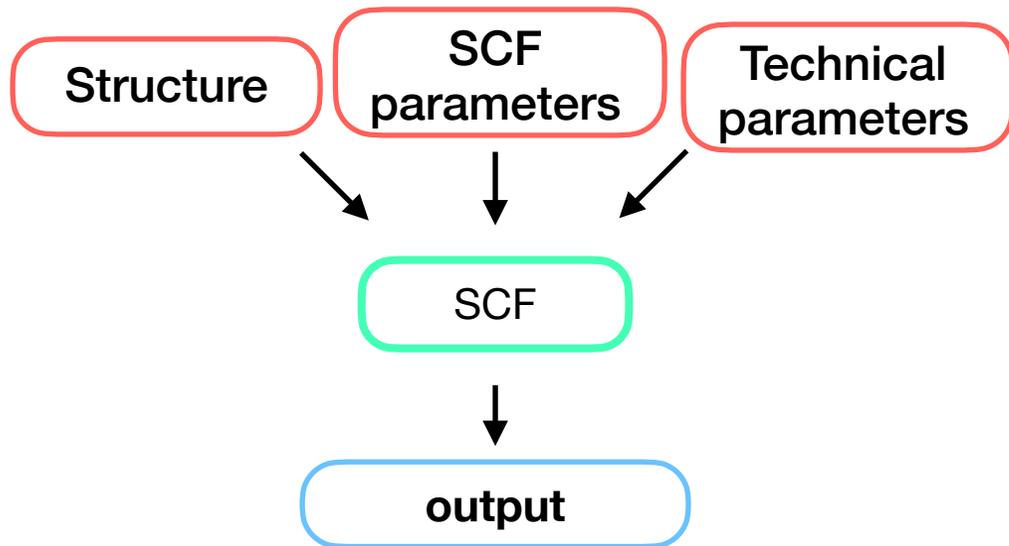
SCF WorkChain



Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure
```

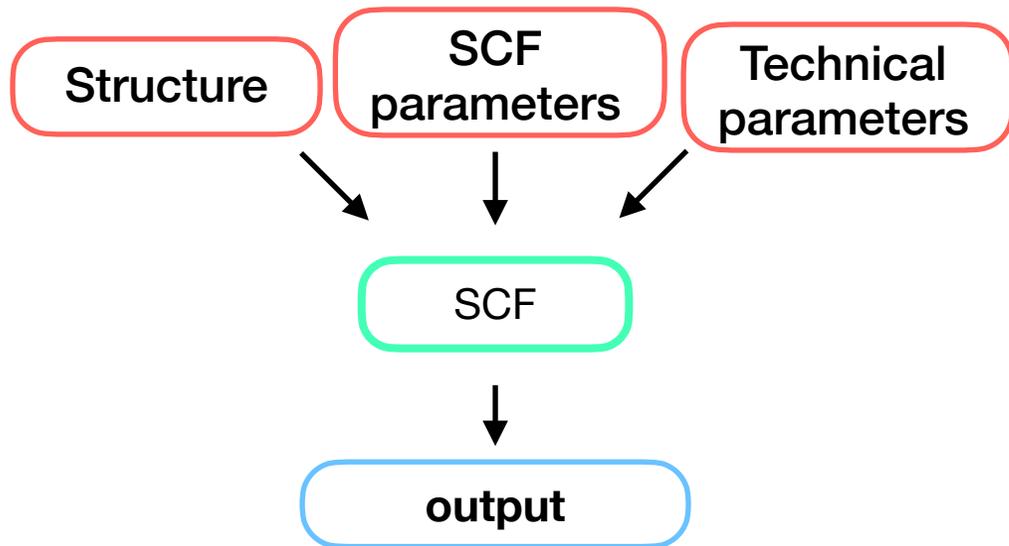
SCF WorkChain



Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation
```

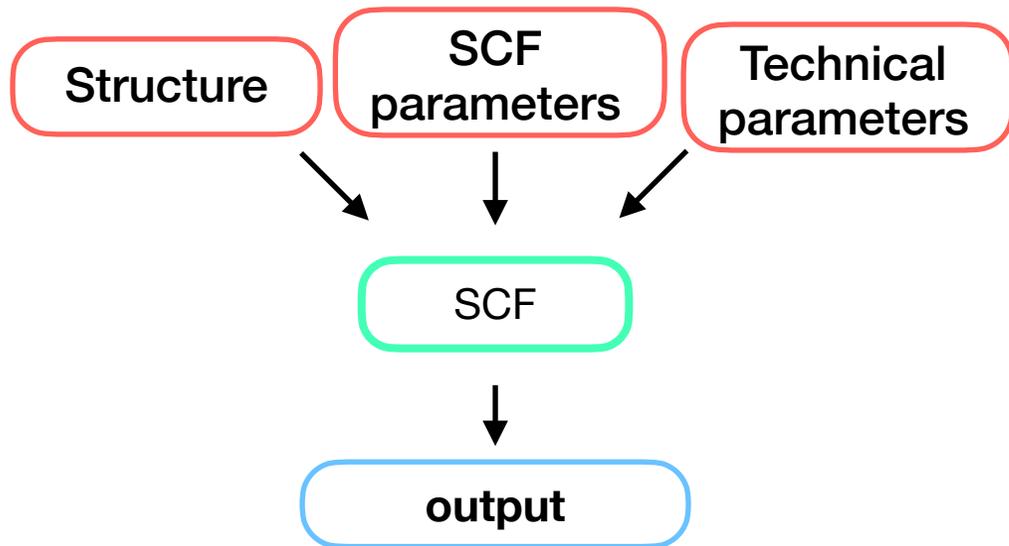
SCF WorkChain



Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code
```

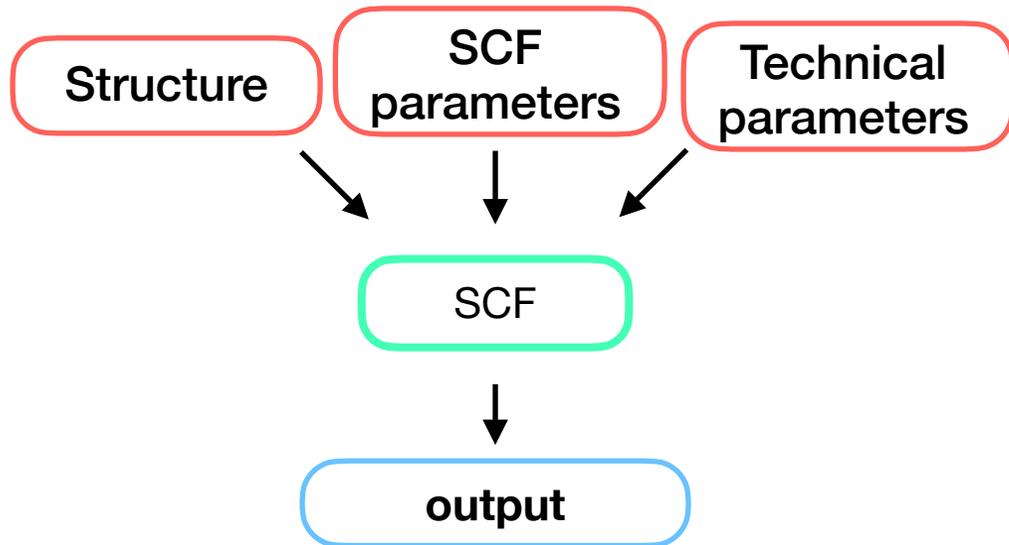
SCF WorkChain



Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code  
'fleur': FLEUR Code
```

SCF WorkChain

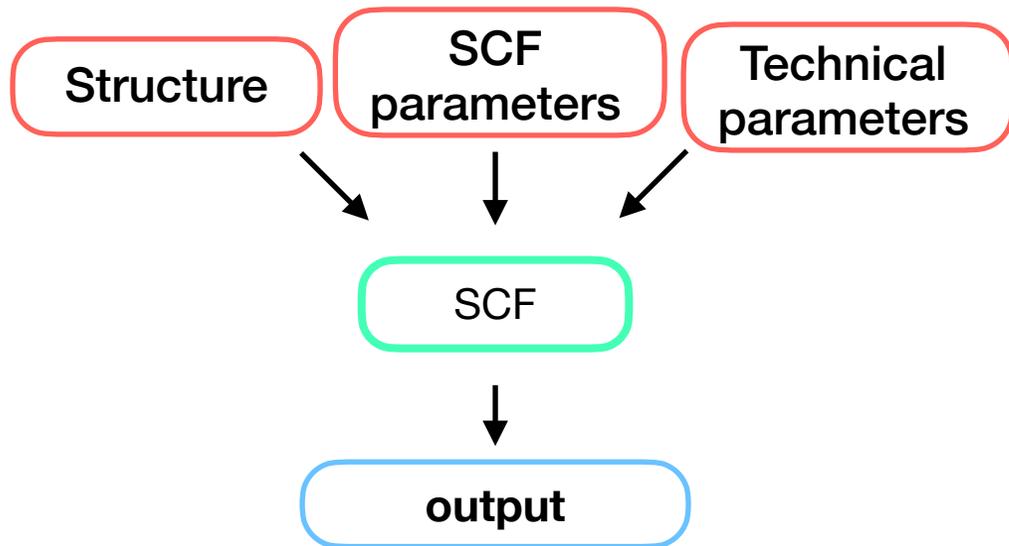


Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code  
'fleur': FLEUR Code
```

SCF parameters

SCF WorkChain



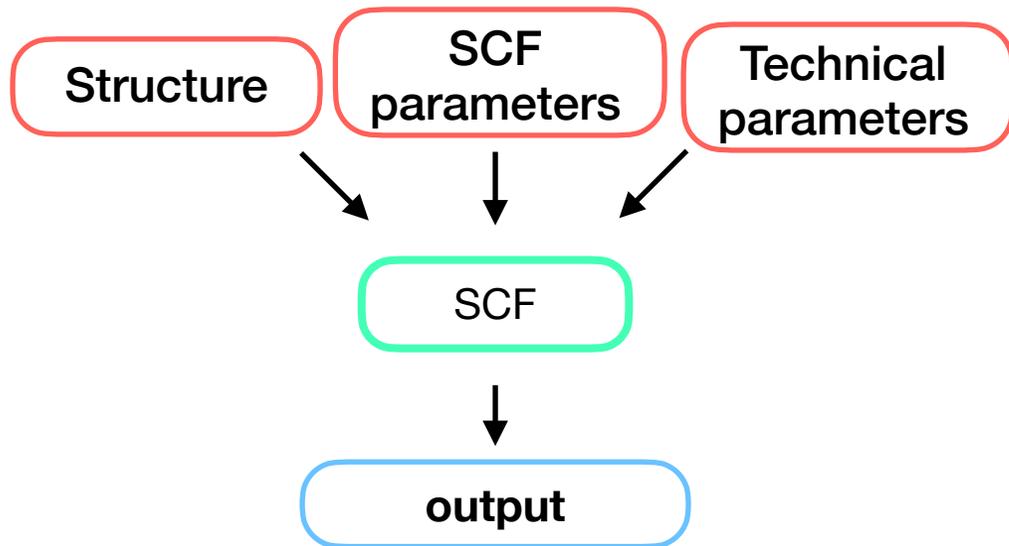
Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code  
'fleur': FLEUR Code
```

SCF parameters

```
'fleur_runmax': 3,
```

SCF WorkChain



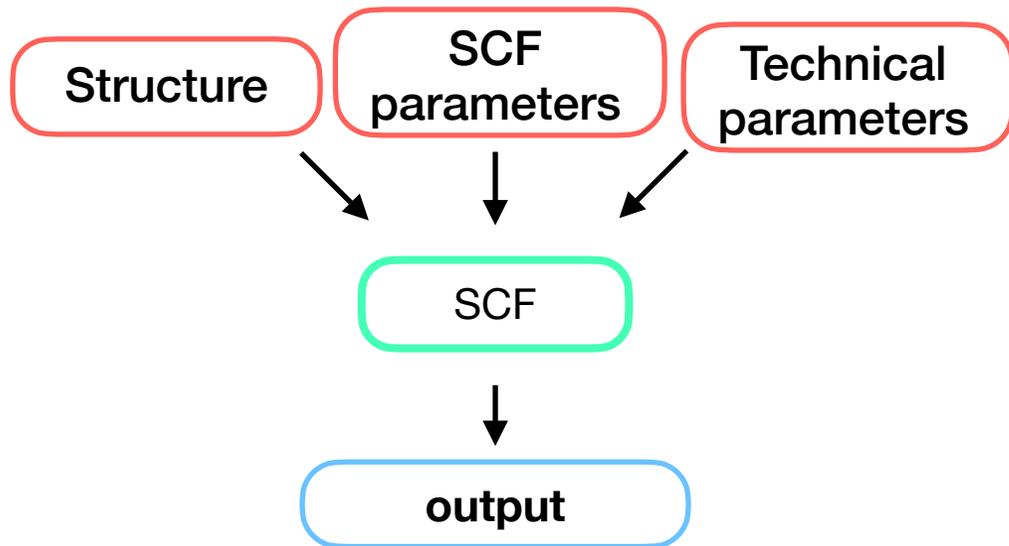
Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code  
'fleur': FLEUR Code
```

SCF parameters

```
'fleur_runmax': 3,  
'itmax_per_run': 10,
```

SCF WorkChain



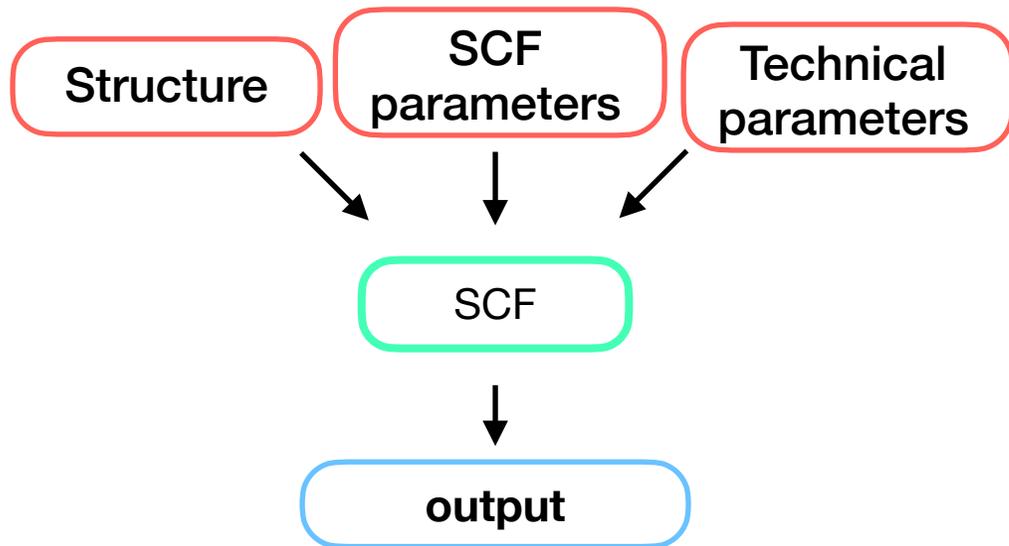
Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code  
'fleur': FLEUR Code
```

SCF parameters

```
'fleur_runmax': 3,  
'itmax_per_run': 10,  
'density_converged': 0.00002,
```

SCF WorkChain



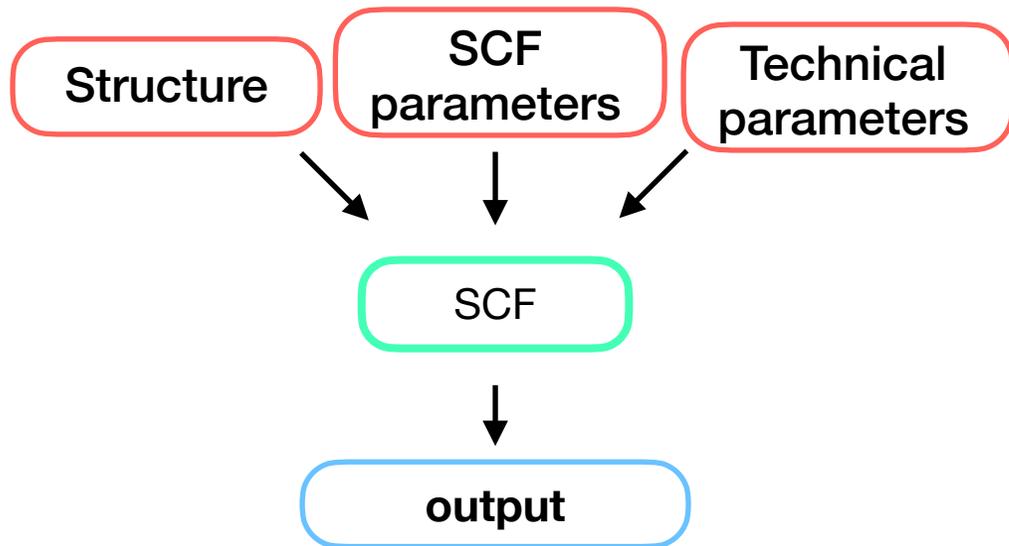
Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code  
'fleur': FLEUR Code
```

SCF parameters

```
'fleur_runmax': 3,  
'itmax_per_run': 10,  
'density_converged': 0.00002,  
'mode': 'density',
```

SCF WorkChain



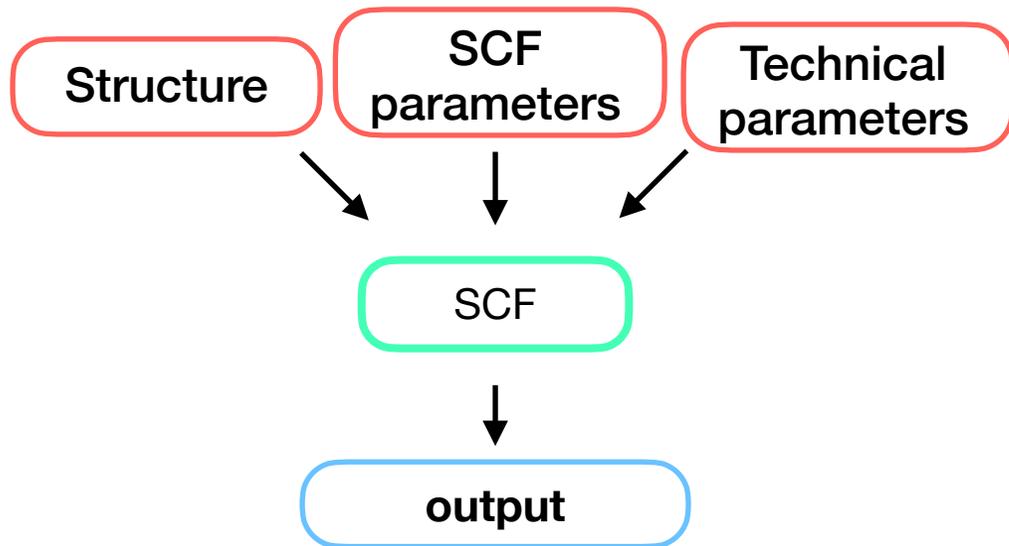
Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code  
'fleur': FLEUR Code
```

SCF parameters

```
'fleur_runmax': 3,  
'itmax_per_run': 10,  
'density_converged': 0.00002,  
'mode': 'density',  
'serial': False,
```

SCF WorkChain



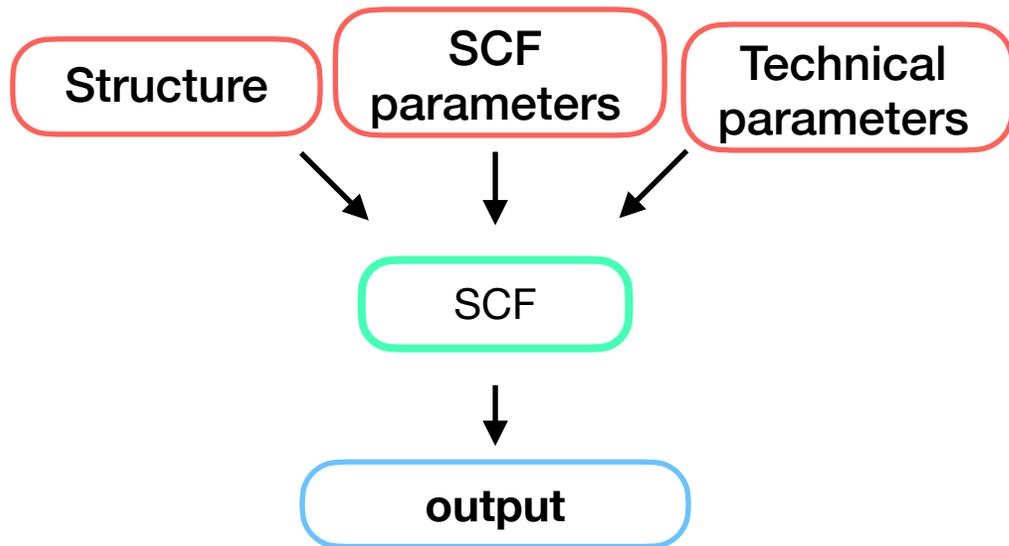
Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code  
'fleur': FLEUR Code
```

SCF parameters

```
'fleur_runmax': 3,  
'itmax_per_run': 10,  
'density_converged': 0.00002,  
'mode': 'density',  
'serial': False,  
'only_even_MPI': False,
```

SCF WorkChain



Inputs

```
'wf_parameters': SCF parameters  
'calc_parameters': inpgen parameters  
'structure': structure  
'options': technical parameters i.e. parallelisation  
'inpgen': inpgen Code  
'fleur': FLEUR Code
```

SCF parameters

```
'fleur_runmax': 3,  
'itmax_per_run': 10,  
'density_converged': 0.00002,  
'mode': 'density',  
'serial': False,  
'only_even_MPI': False,  
'inxml_changes': []
```

SCF WorkChain

output

```
"conv_mode": "density",
"distance_charge": 1.13714e-05,
"distance_charge_all": [
  29.9211648204,
  ~~~
],
"distance_charge_units": "me/bohr^3",
"force_diff_last": "can not be determined",
"force_largest": 0.0,
"iterations_total": 30,
"last_calc_uuid": "4c0a1cf4-932b-4b88-96ea-8ff443bad13c",
"loop_count": 3,
"material": "FePt2",
"total_energy": -38143.906981714,
"total_energy_all": [
  -38144.008129573,
  ~~~
],
"total_energy_units": "Htr",
"total_wall_time": 545,
"total_wall_time_units": "s",
"workflow_name": "FleurScfWorkChain",
"workflow_version": "0.4.0"
```

SCF WorkChain

output

```
"conv_mode": "density",
"distance_charge": 1.13714e-05,
"distance_charge_all": [
  29.9211648204,
  ~~~
],
"distance_charge_units": "me/bohr^3",
"force_diff_last": "can not be determined",
"force_largest": 0.0,
"iterations_total": 30,
"last_calc_uuid": "4c0a1cf4-932b-4b88-96ea-8ff443bad13c",
"loop_count": 3,
"material": "FePt2",
"total_energy": -38143.906981714,
"total_energy_all": [
  -38144.008129573,
  ~~~
],
"total_energy_units": "Htr",
"total_wall_time": 545,
"total_wall_time_units": "s",
"workflow_name": "FleurScfWorkChain",
"workflow_version": "0.4.0"
```

SCF WorkChain

output

```
"conv_mode": "density",  
"distance_charge": 1.13714e-05,  
"distance_charge_all": [  
  29.9211648204,  
  ~~~  
],  
"distance_charge_units": "me/bohr^3",  
"force_diff_last": "can not be determined",  
"force_largest": 0.0,  
"iterations_total": 30,  
"last_calc_uuid": "4c0a1cf4-932b-4b88-96ea-8ff443bad13c",  
"loop_count": 3,  
"material": "FePt2",  
"total_energy": -38143.906981714,  
"total_energy_all": [  
  -38144.008129573,  
  ~~~  
],  
"total_energy_units": "Htr",  
"total_wall_time": 545,  
"total_wall_time_units": "s",  
"workflow_name": "FleurScfWorkChain",  
"workflow_version": "0.4.0"
```

SCF WorkChain

output

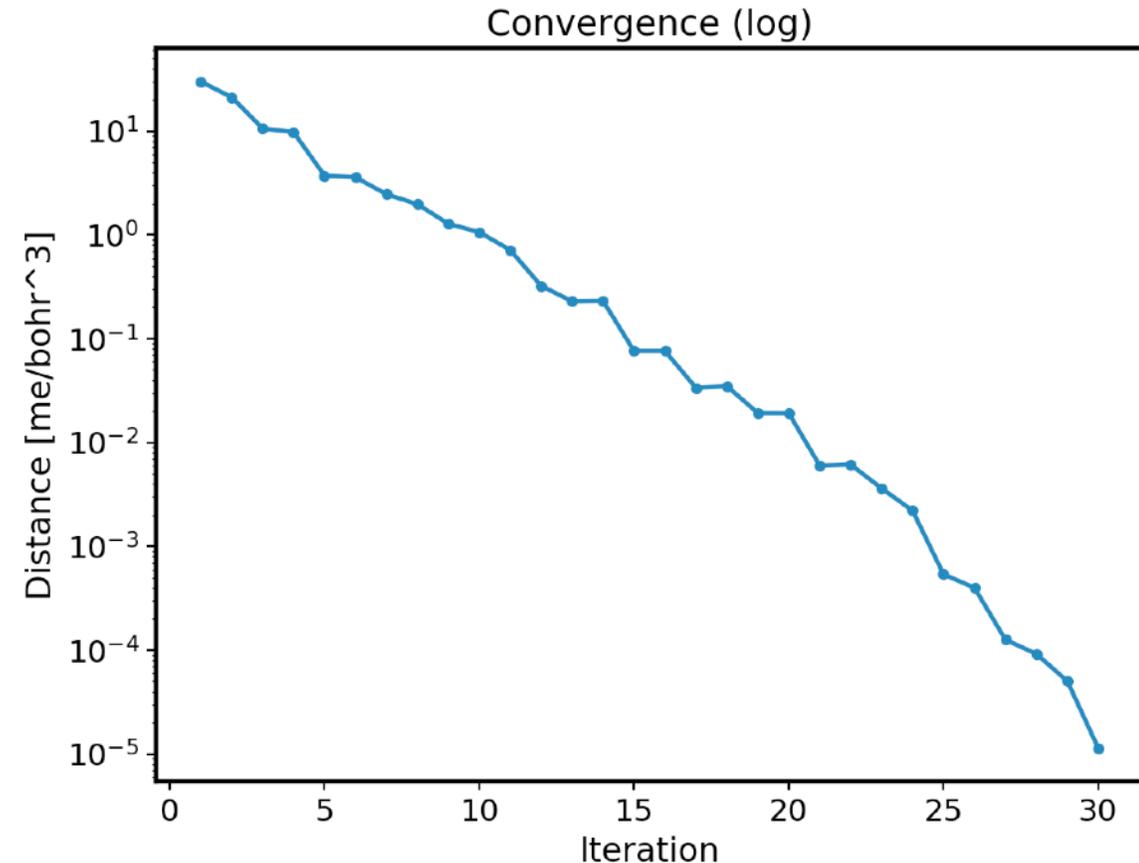
```
"conv_mode": "density",
"distance_charge": 1.13714e-05,
"distance_charge_all": [
  29.9211648204,
  ~~~
],
"distance_charge_units": "me/bohr^3",
"force_diff_last": "can not be determined",
"force_largest": 0.0,
"iterations_total": 30,
"last_calc_uuid": "4c0a1cf4-932b-4b88-96ea-8ff443bad13c",
"loop_count": 3,
"material": "FePt2",
"total_energy": -38143.906981714,
"total_energy_all": [
  -38144.008129573,
  ~~~
],
"total_energy_units": "Htr",
"total_wall_time": 545,
"total_wall_time_units": "s",
"workflow_name": "FleurScfWorkChain",
"workflow_version": "0.4.0"
```

SCF WorkChain

output

```
"conv_mode": "density",  
"distance_charge": 1.13714e-05,  
"distance_charge_all": [  
    29.9211648204,  
    ~~~  
],  
"distance_charge_units": "me/bohr^3",  
"force_diff_last": "can not be determined",  
"force_largest": 0.0,  
"iterations_total": 30,  
"last_calc_uuid": "4c0a1cf4-932b-4b88-96ea-8ff443bad13c",  
"loop_count": 3,  
"material": "FePt2",  
"total_energy": -38143.906981714,  
"total_energy_all": [  
    -38144.008129573,  
    ~~~  
],  
"total_energy_units": "Htr",  
"total_wall_time": 545,  
"total_wall_time_units": "s",  
"workflow_name": "FleurScfWorkChain",  
"workflow_version": "0.4.0"
```

plot_fleur()

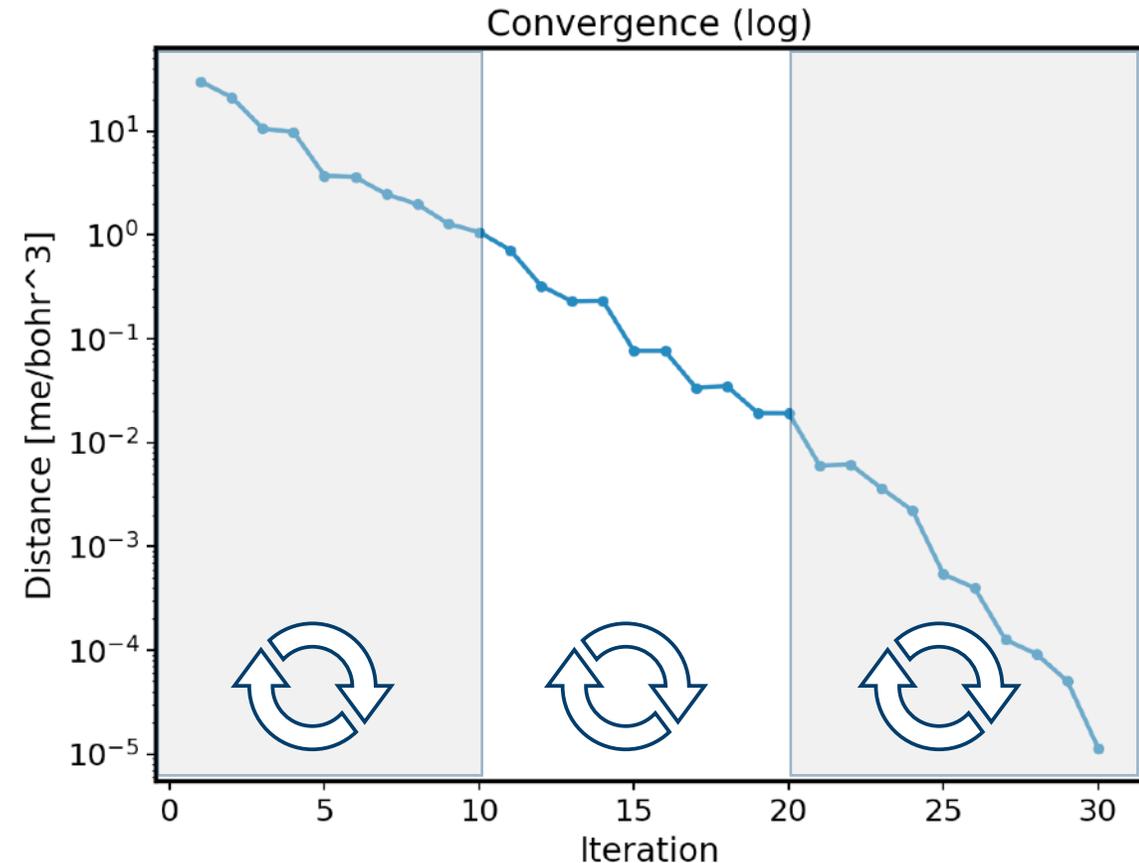


SCF WorkChain

output

```
"conv_mode": "density",
"distance_charge": 1.13714e-05,
"distance_charge_all": [
  29.9211648204,
  ~~~
],
"distance_charge_units": "me/bohr^3",
"force_diff_last": "can not be determined",
"force_largest": 0.0,
"iterations_total": 30,
"last_calc_uuid": "4c0a1cf4-932b-4b88-96ea-8ff443bad13c",
"loop_count": 3,
"material": "FePt2",
"total_energy": -38143.906981714,
"total_energy_all": [
  -38144.008129573,
  ~~~
],
"total_energy_units": "Htr",
"total_wall_time": 545,
"total_wall_time_units": "s",
"workflow_name": "FleurScfWorkChain",
"workflow_version": "0.4.0"
```

plot_fleur()

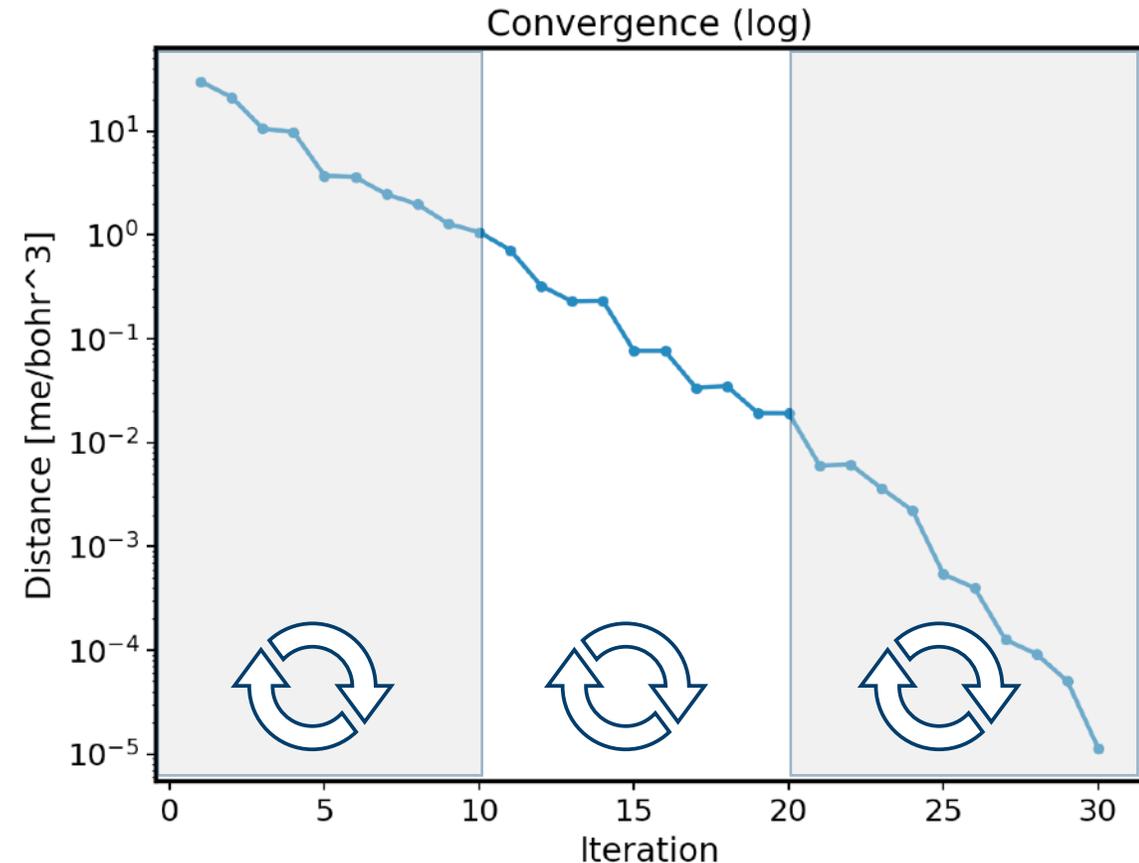


SCF WorkChain

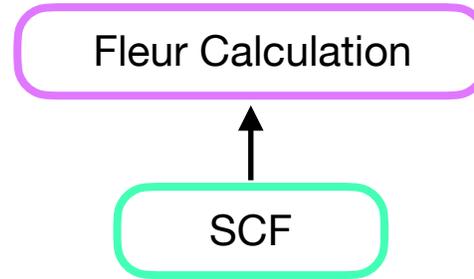
output

```
"conv_mode": "density",
"distance_charge": 1.13714e-05,
"distance_charge_all": [
  29.9211648204,
  ~~~
],
"distance_charge_units": "me/bohr^3",
"force_diff_last": "can not be determined",
"force_largest": 0.0,
"iterations_total": 30,
"last_calc uuid": "4c0a1cf4-932b-4b88-96ea-8ff443bad13c",
"loop_count": 3,
"material": "FePt2",
"total_energy": -38143.906981714,
"total_energy_all": [
  -38144.008129573,
  ~~~
],
"total_energy_units": "Htr",
"total_wall_time": 545,
"total_wall_time_units": "s",
"workflow_name": "FleurScfWorkChain",
"workflow_version": "0.4.0"
```

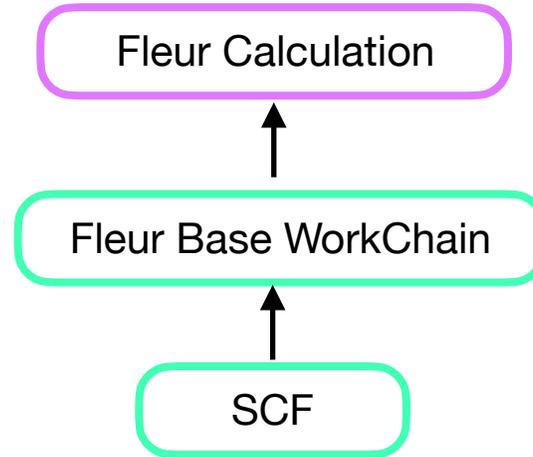
plot_fleur()



Nested WorkChains

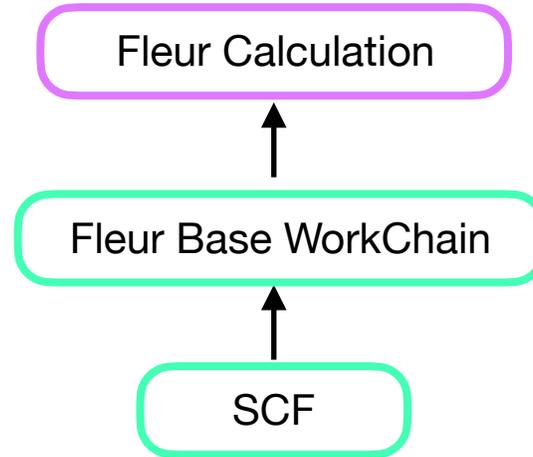


Nested WorkChains

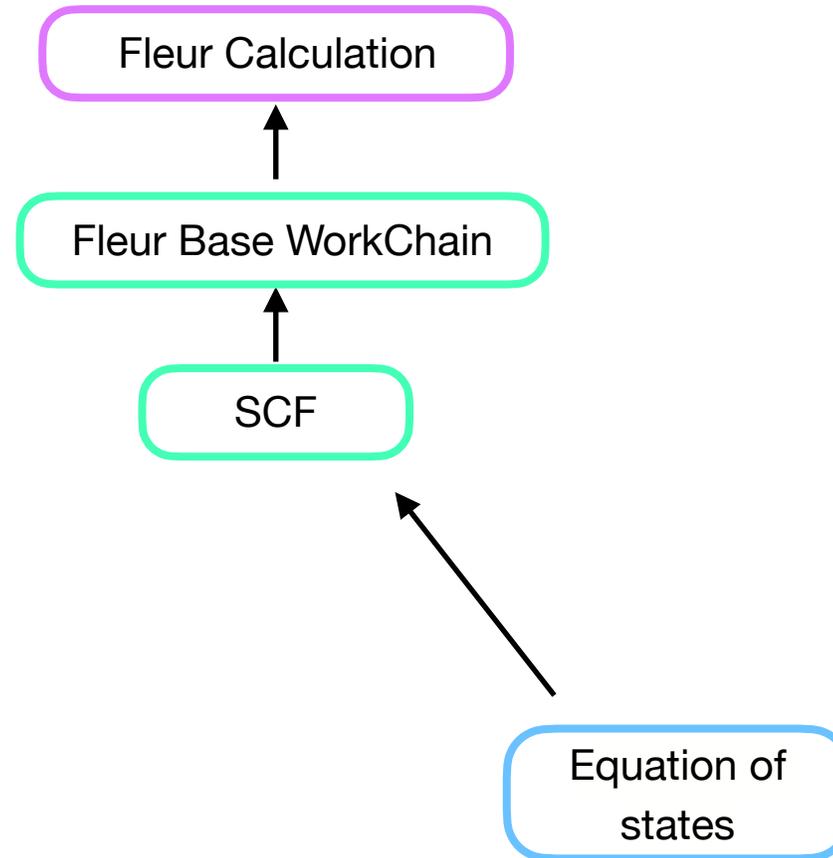


FleurBaseWorkChain wraps FleurCalculation:
tries to automatically resolve failures

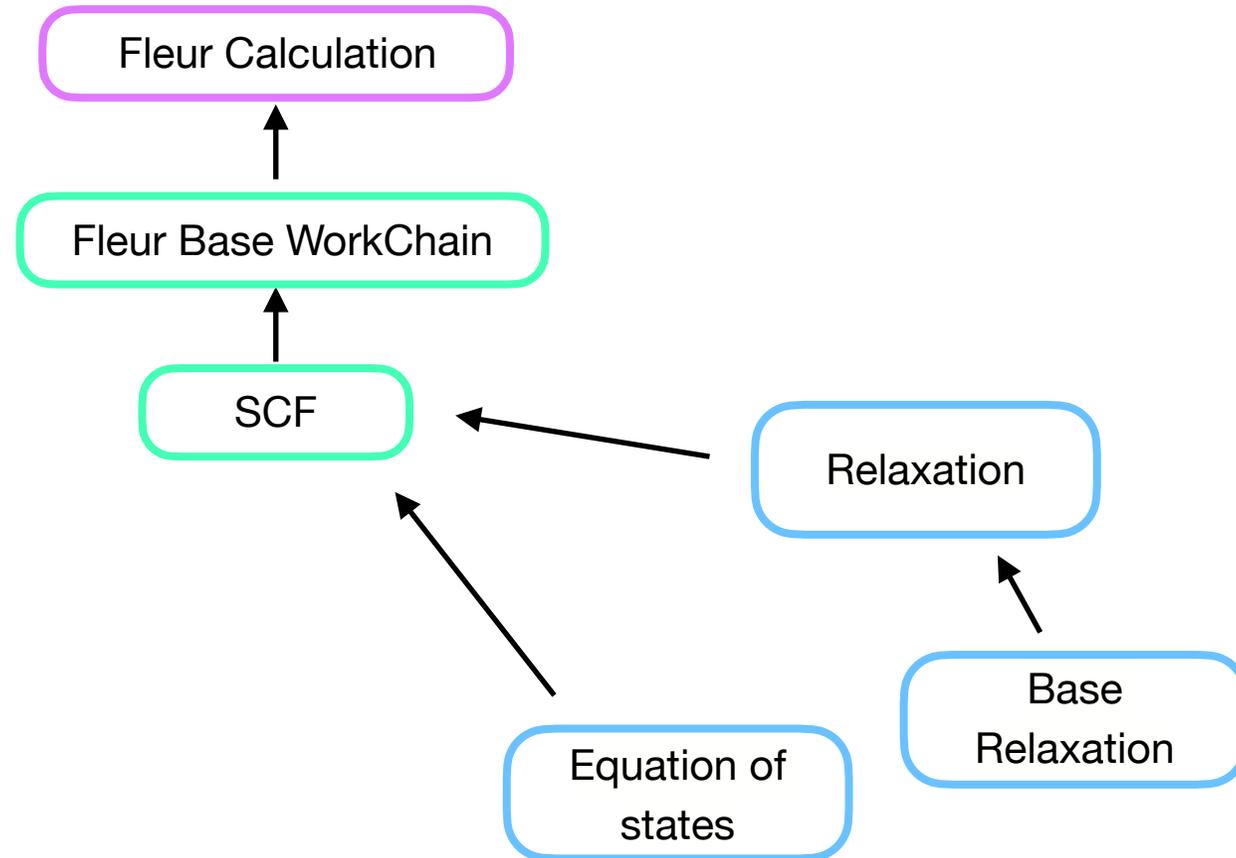
Nested WorkChains



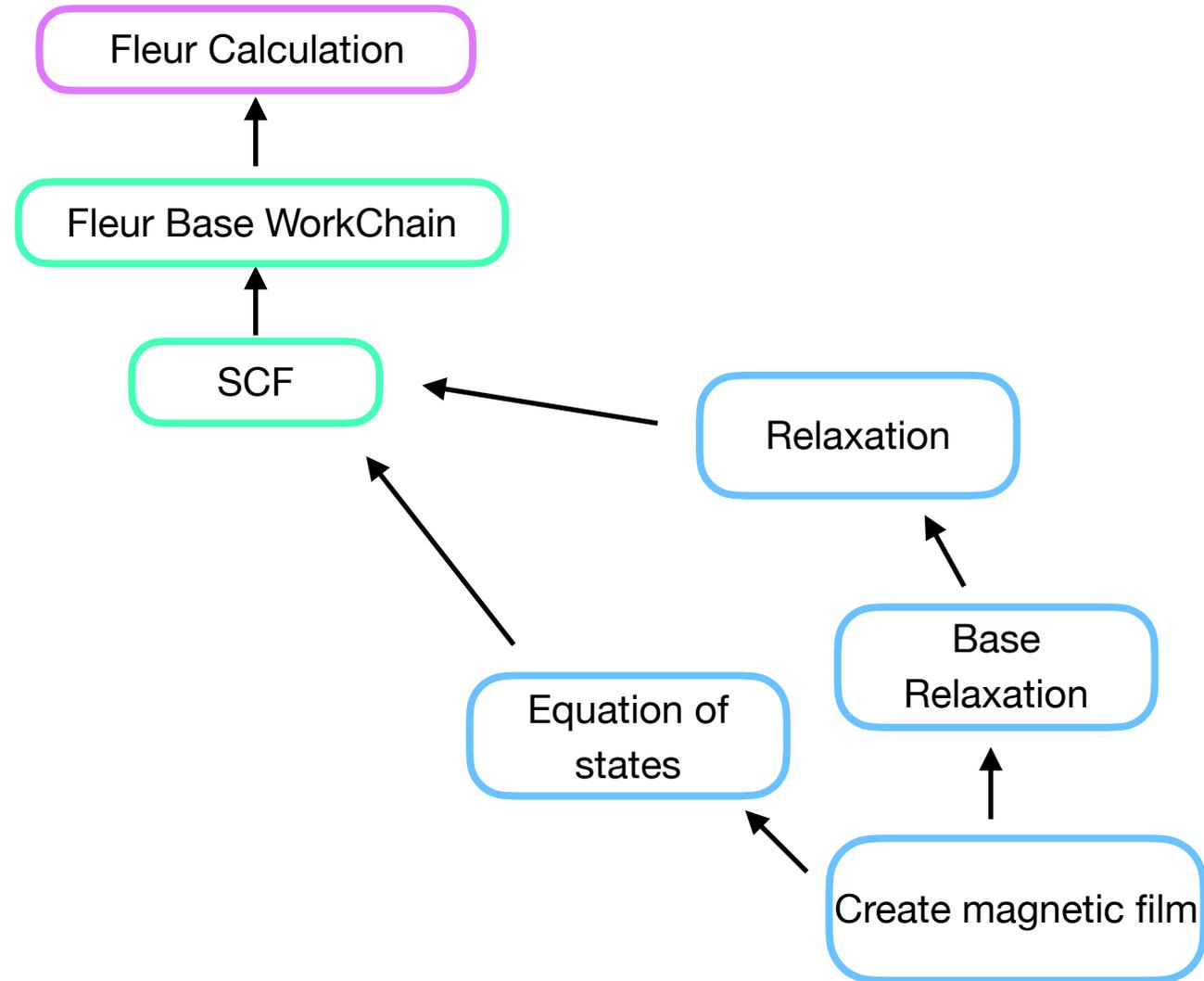
Nested WorkChains



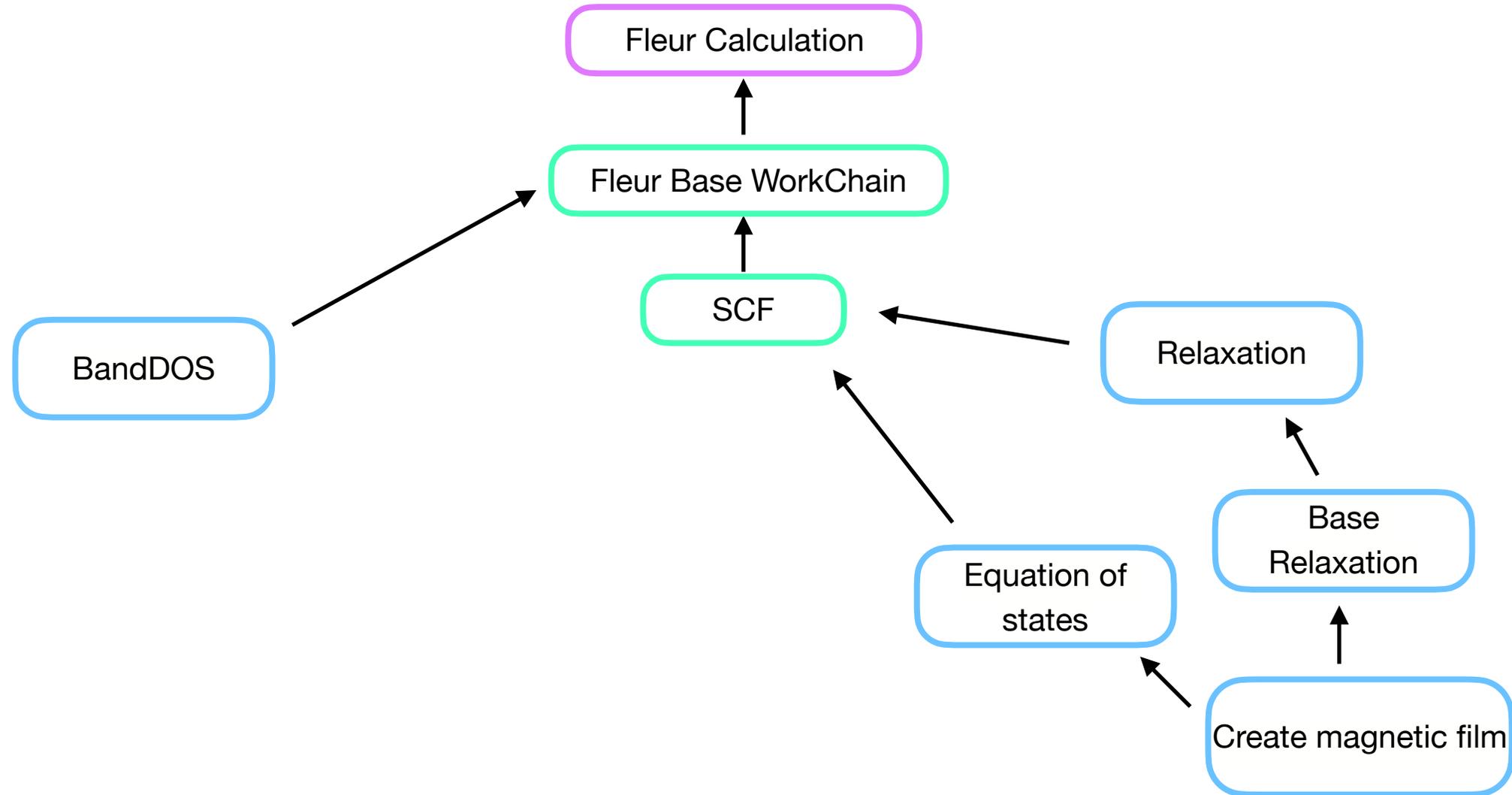
Nested WorkChains



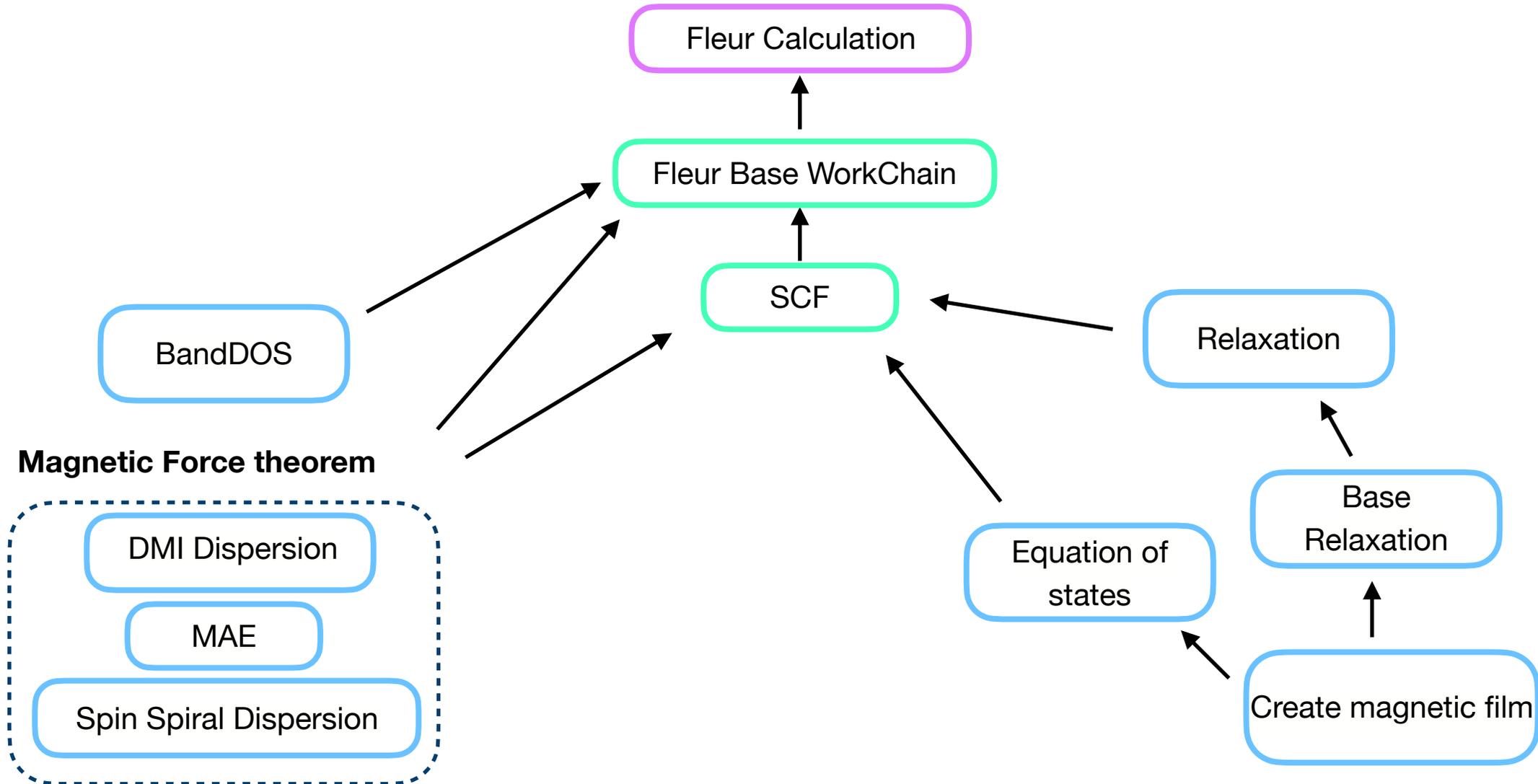
Nested WorkChains



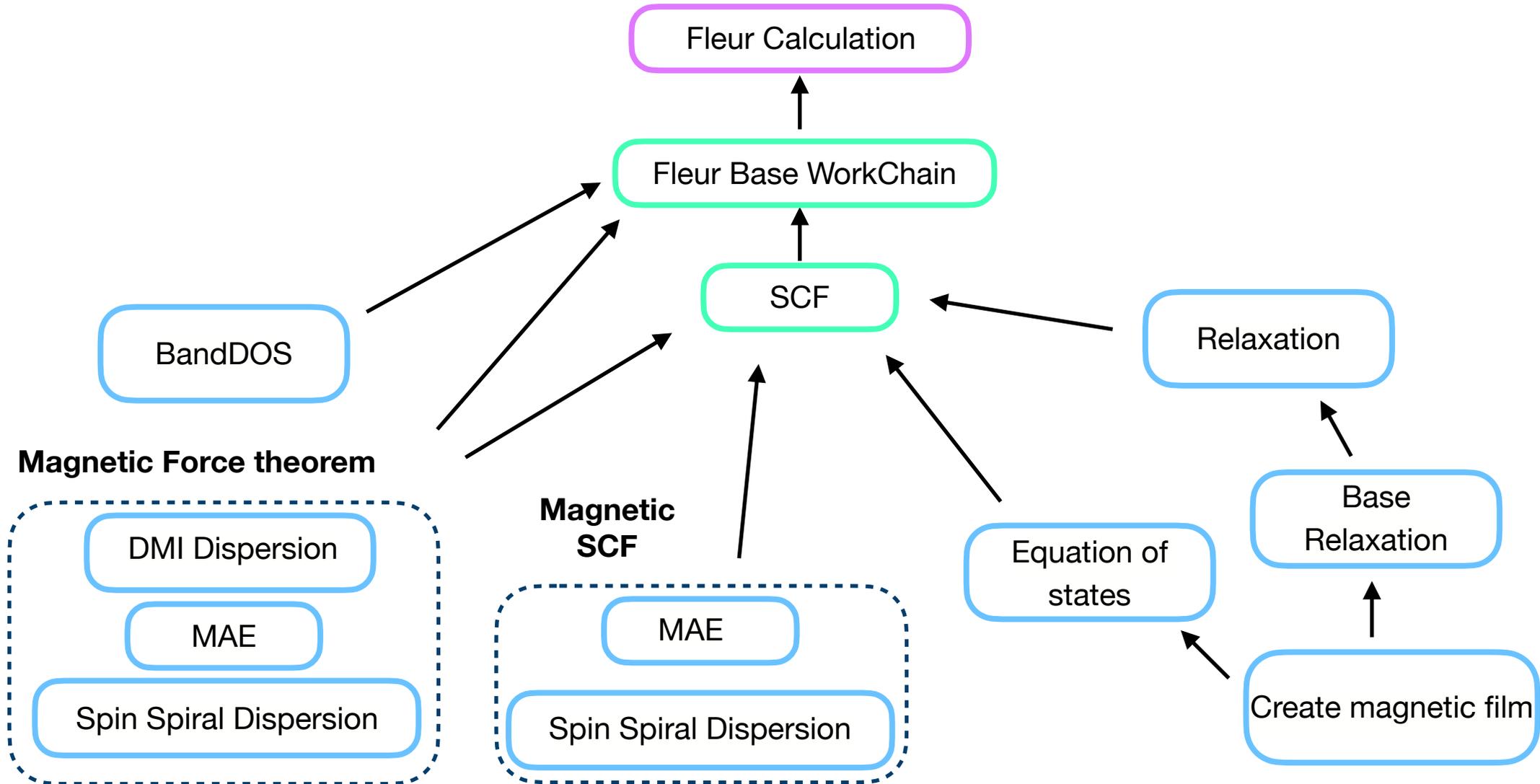
Nested WorkChains



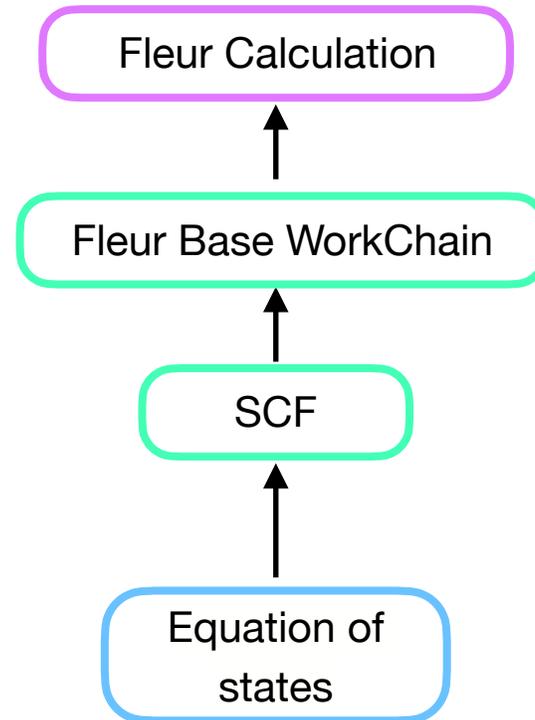
Nested WorkChains



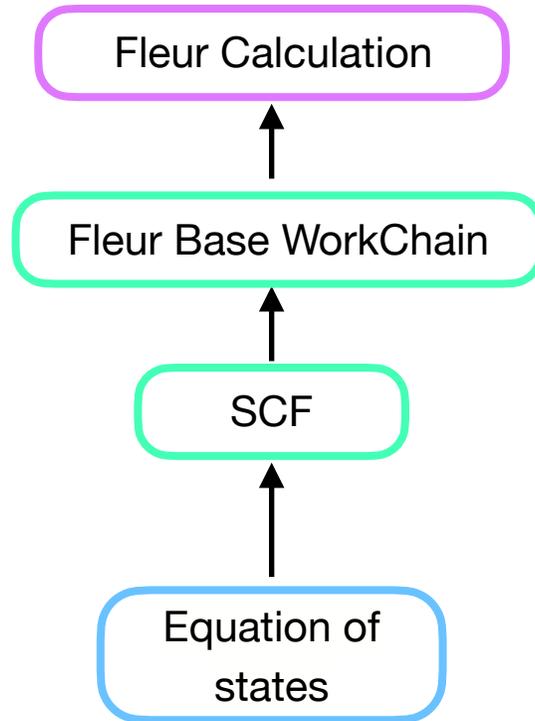
Nested WorkChains



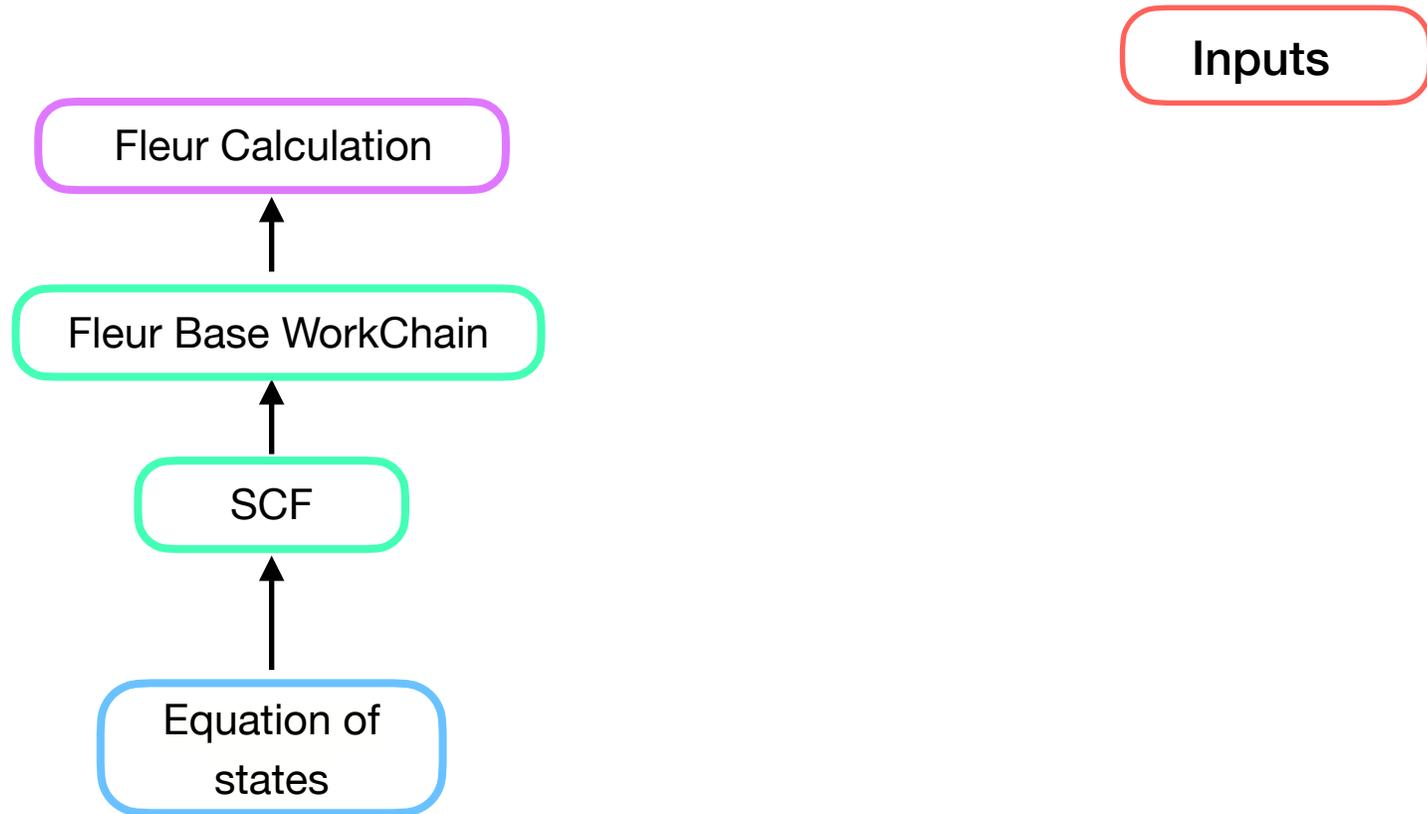
Nested WorkChains: EOS



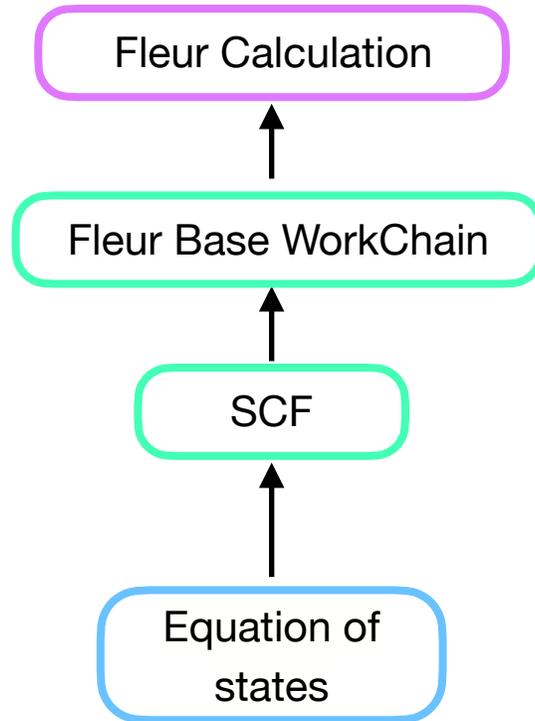
Nested WorkChains: EOS



Nested WorkChains: EOS



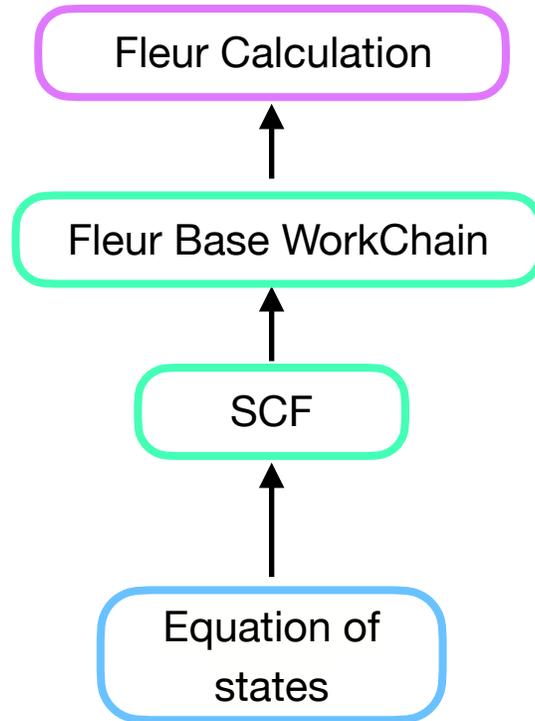
Nested WorkChains: EOS



Inputs

```
'scf': {'wf_parameters': SCF parameters
```

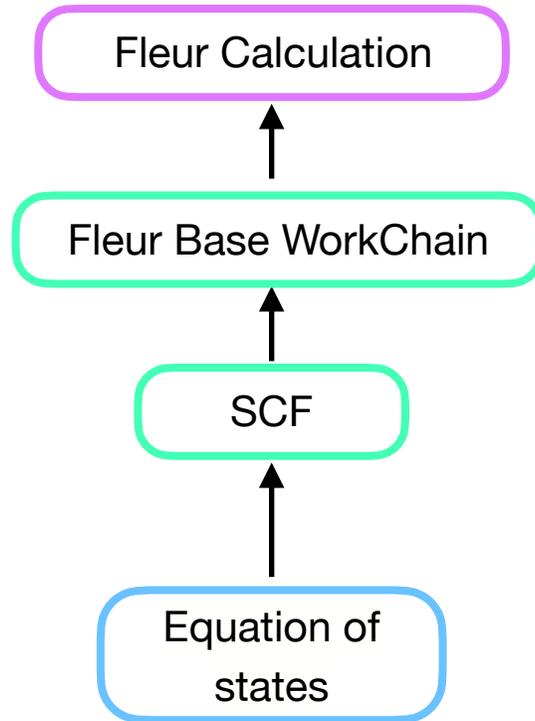
Nested WorkChains: EOS



Inputs

```
'scf': {'wf_parameters': SCF parameters  
       'calc_parameters': inpgen parameters
```

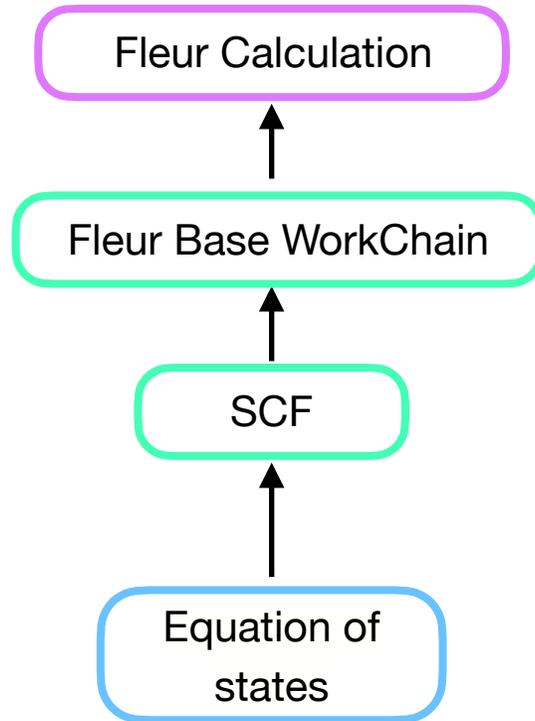
Nested WorkChains: EOS



Inputs

```
'scf': {'wf_parameters': SCF parameters  
       'calc_parameters': inpgen parameters  
       'options': technical parameters i.e. parallelisation
```

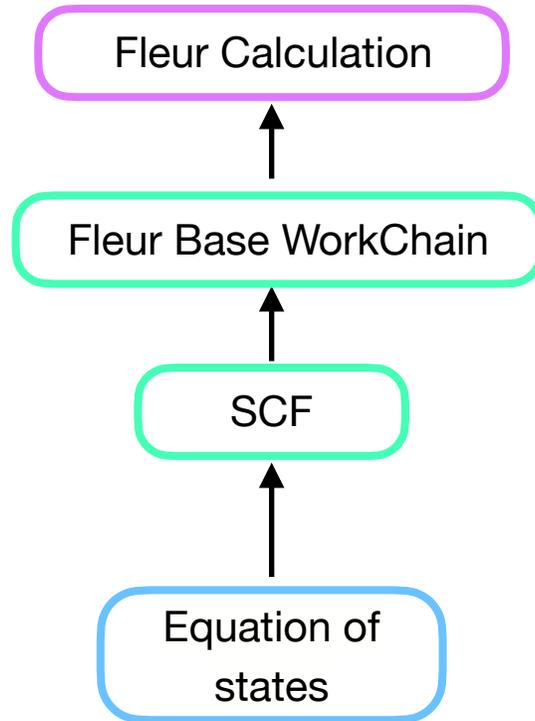
Nested WorkChains: EOS



Inputs

```
'scf': {'wf_parameters': SCF parameters  
       'calc_parameters': inpgen parameters  
       'options': technical parameters i.e. parallelisation  
       'inpgen': inpgen Code
```

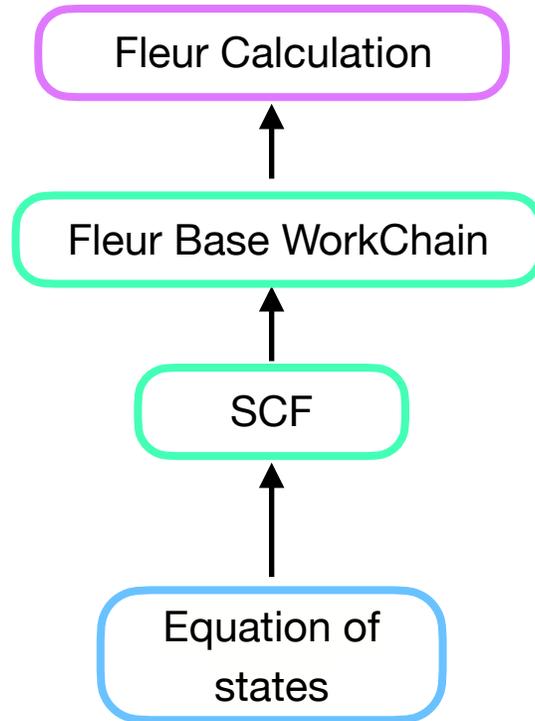
Nested WorkChains: EOS



Inputs

```
'scf': {'wf_parameters': SCF parameters  
        'calc_parameters': inpgen parameters  
        'options': technical parameters i.e. parallelisation  
        'inpgen': inpgen Code  
        'fleur': FLEUR Code
```

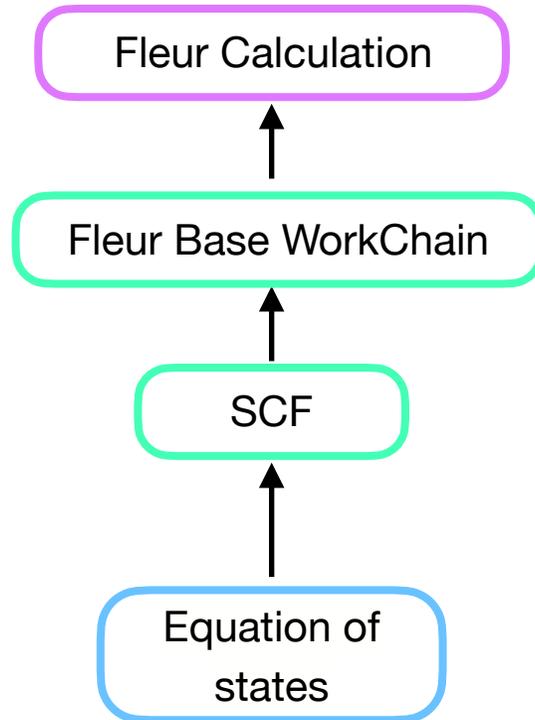
Nested WorkChains: EOS



Inputs

```
'scf': {'wf_parameters': SCF parameters  
       'calc_parameters': inpgen parameters  
       'options': technical parameters i.e. parallelisation  
       'inpgen': inpgen Code  
       'fleur': FLEUR Code  
},
```

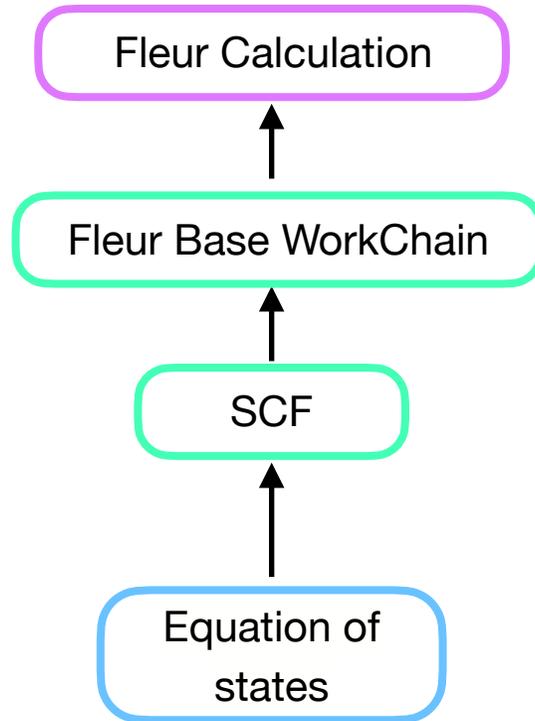
Nested WorkChains: EOS



Inputs

```
'scf': {'wf_parameters': SCF parameters
        'calc_parameters': inpgen parameters
        'options': technical parameters i.e. parallelisation
        'inpgen': inpgen Code
        'fleur': FLEUR Code
      },
'structure': structure,
```

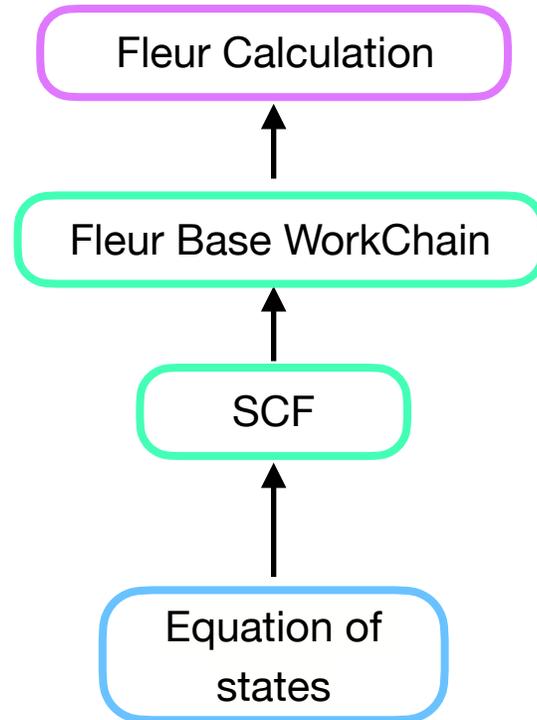
Nested WorkChains: EOS



Inputs

```
'scf': {'wf_parameters': SCF parameters  
       'calc_parameters': inpgen parameters  
       'options': technical parameters i.e. parallelisation  
       'inpgen': inpgen Code  
       'fleur': FLEUR Code  
       },  
'structure': structure,  
'wf_parameters': EOS parameters
```

Nested WorkChains: EOS

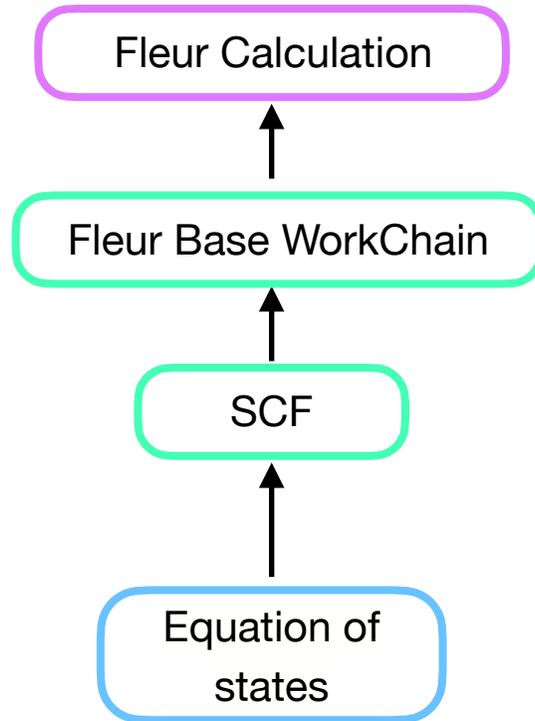


Inputs

```
'scf': {'wf_parameters': SCF parameters  
       'calc_parameters': inpgen parameters  
       'options': technical parameters i.e. parallelisation  
       'inpgen': inpgen Code  
       'fleur': FLEUR Code  
       },  
'structure': structure,  
'wf_parameters': EOS parameters
```

EOS parameters

Nested WorkChains: EOS



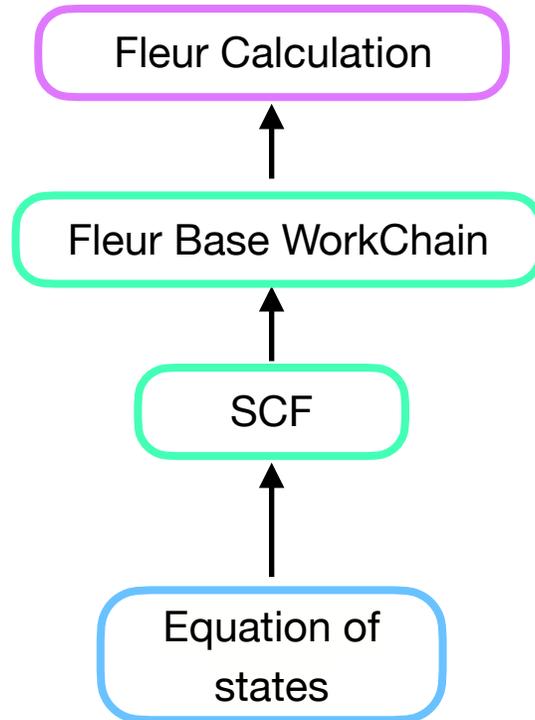
Inputs

```
'scf': {'wf_parameters': SCF parameters
        'calc_parameters': inpgen parameters
        'options': technical parameters i.e. parallelisation
        'inpgen': inpgen Code
        'fleur': FLEUR Code
      },
'structure': structure,
'wf_parameters': EOS parameters
```

EOS parameters

```
'points': 9,
```

Nested WorkChains: EOS



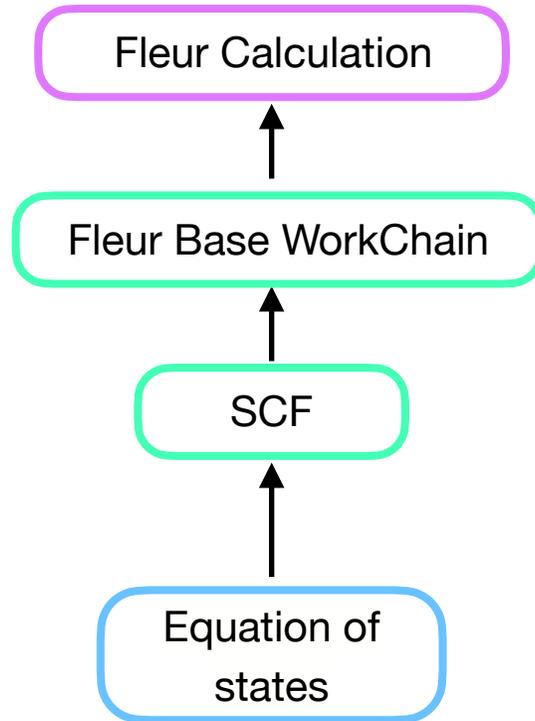
Inputs

```
'scf': {'wf_parameters': SCF parameters
        'calc_parameters': inpgen parameters
        'options': technical parameters i.e. parallelisation
        'inpgen': inpgen Code
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'structure': structure,
'wf_parameters': EOS parameters
```

EOS parameters

```
'points': 9,
'step': 0.002,
```

Nested WorkChains: EOS



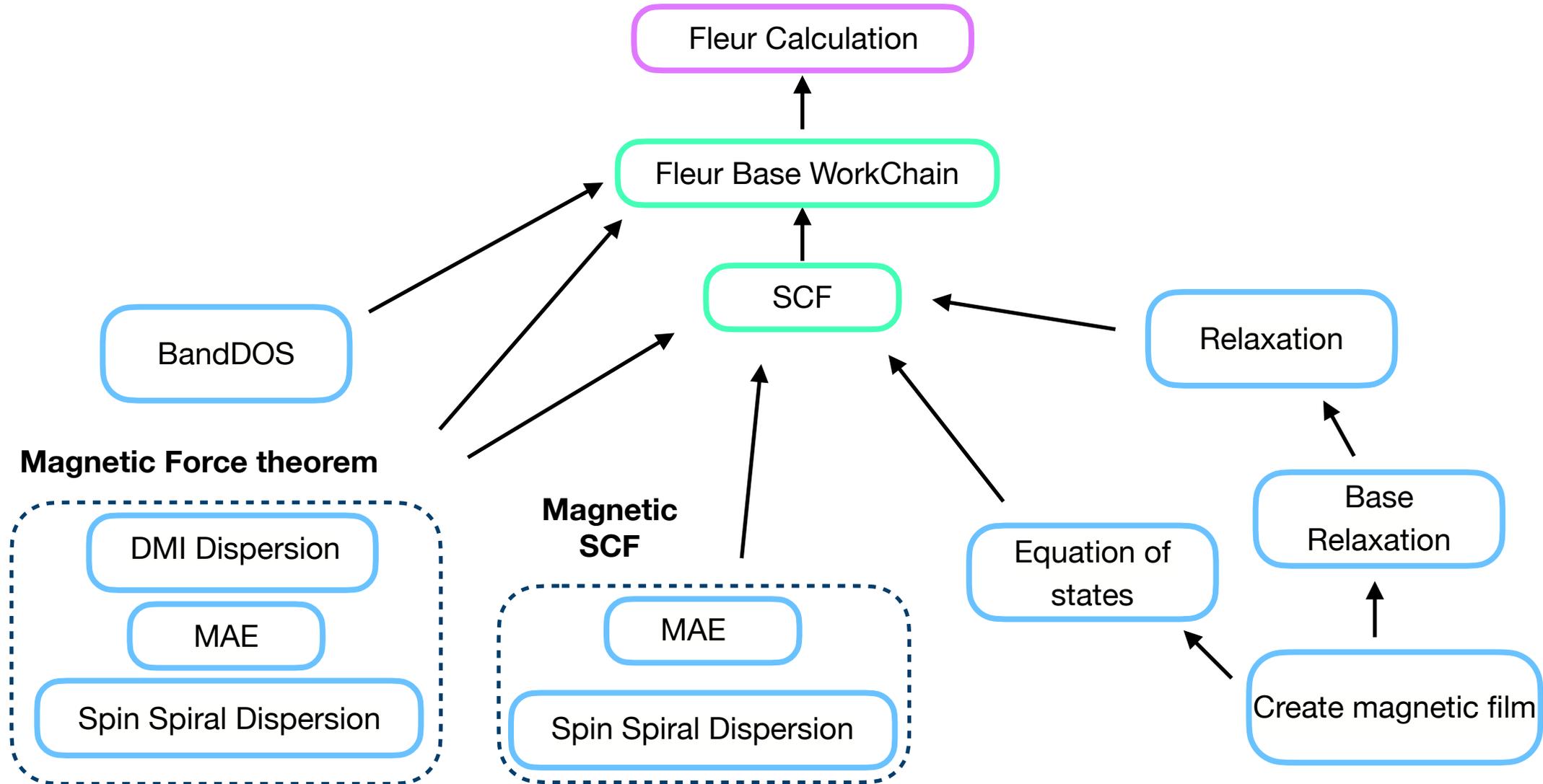
Inputs

```
'scf': {'wf_parameters': SCF parameters
        'calc_parameters': inpgen parameters
        'options': technical parameters i.e. parallelisation
        'inpgen': inpgen Code
        'fleur': FLEUR Code
      },
'structure': structure,
'wf_parameters': EOS parameters
```

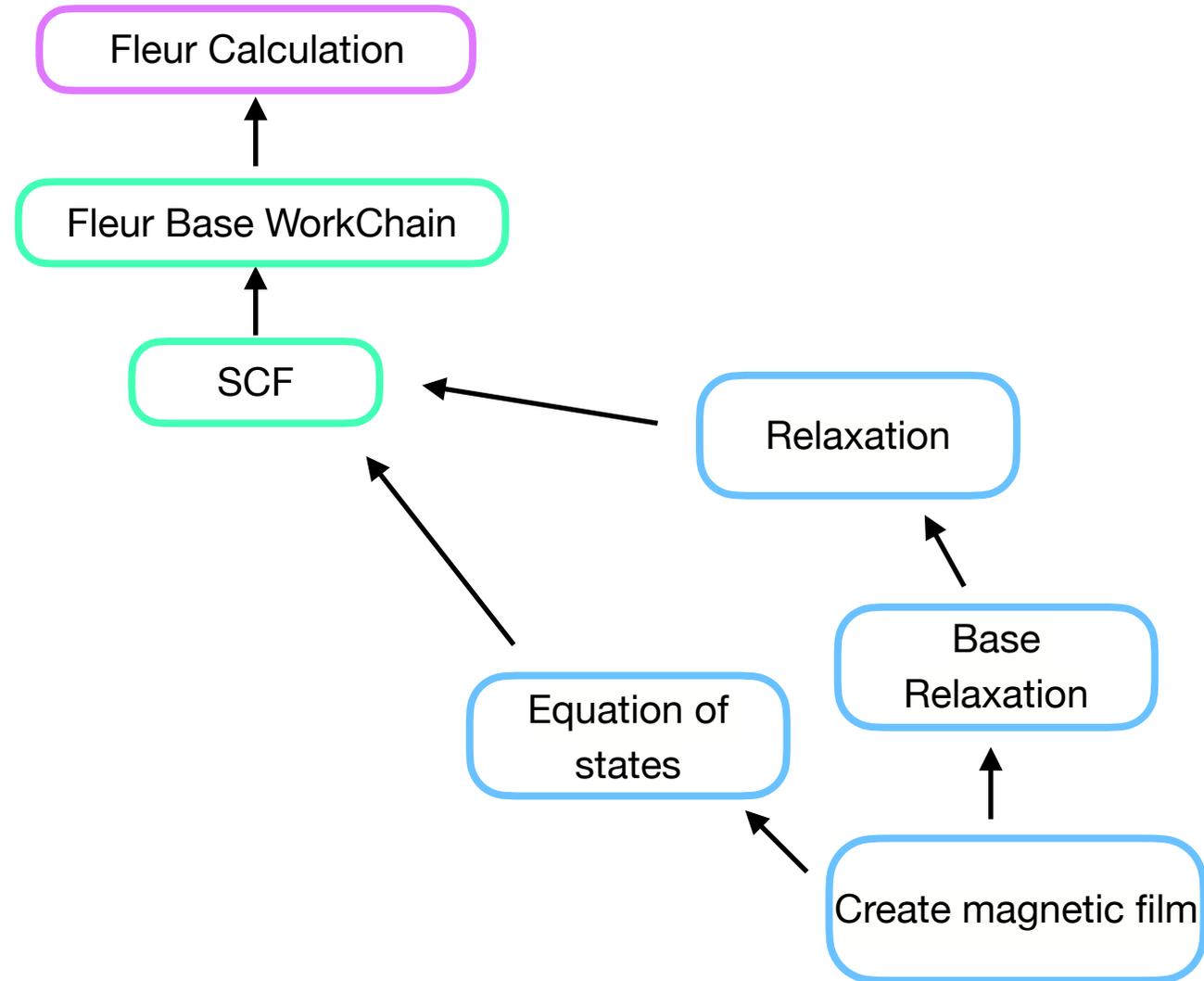
EOS parameters

```
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'step': 0.002,
'guess': 1.00
```

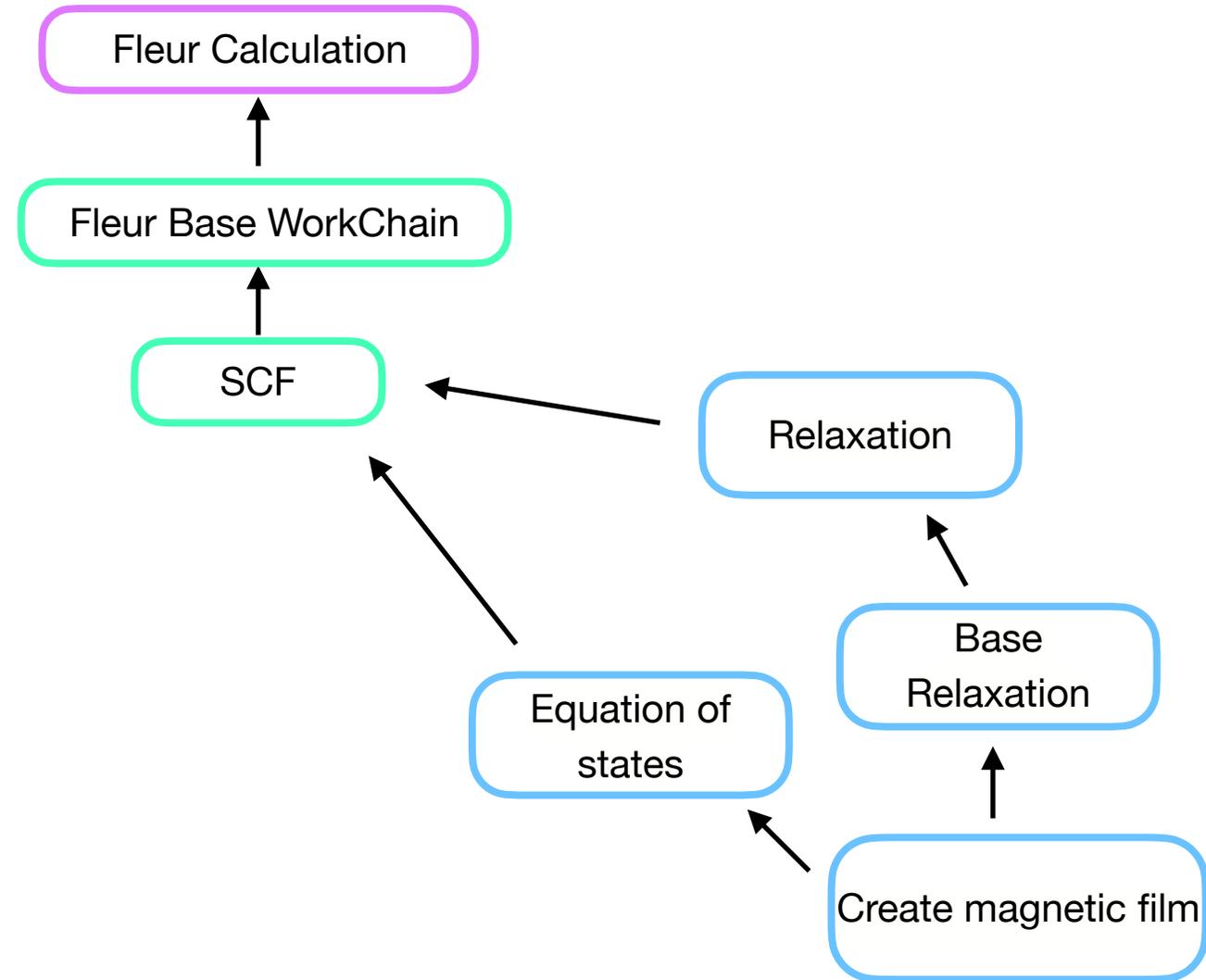
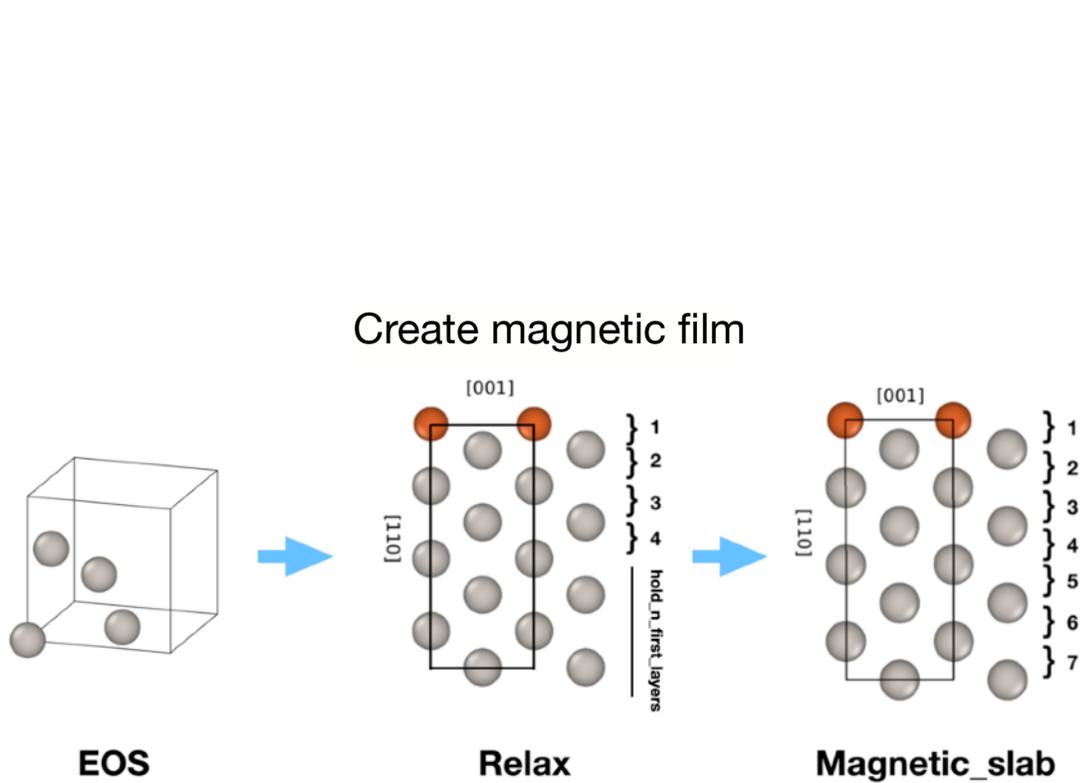
Nested WorkChains



Nested WorkChains: CMF

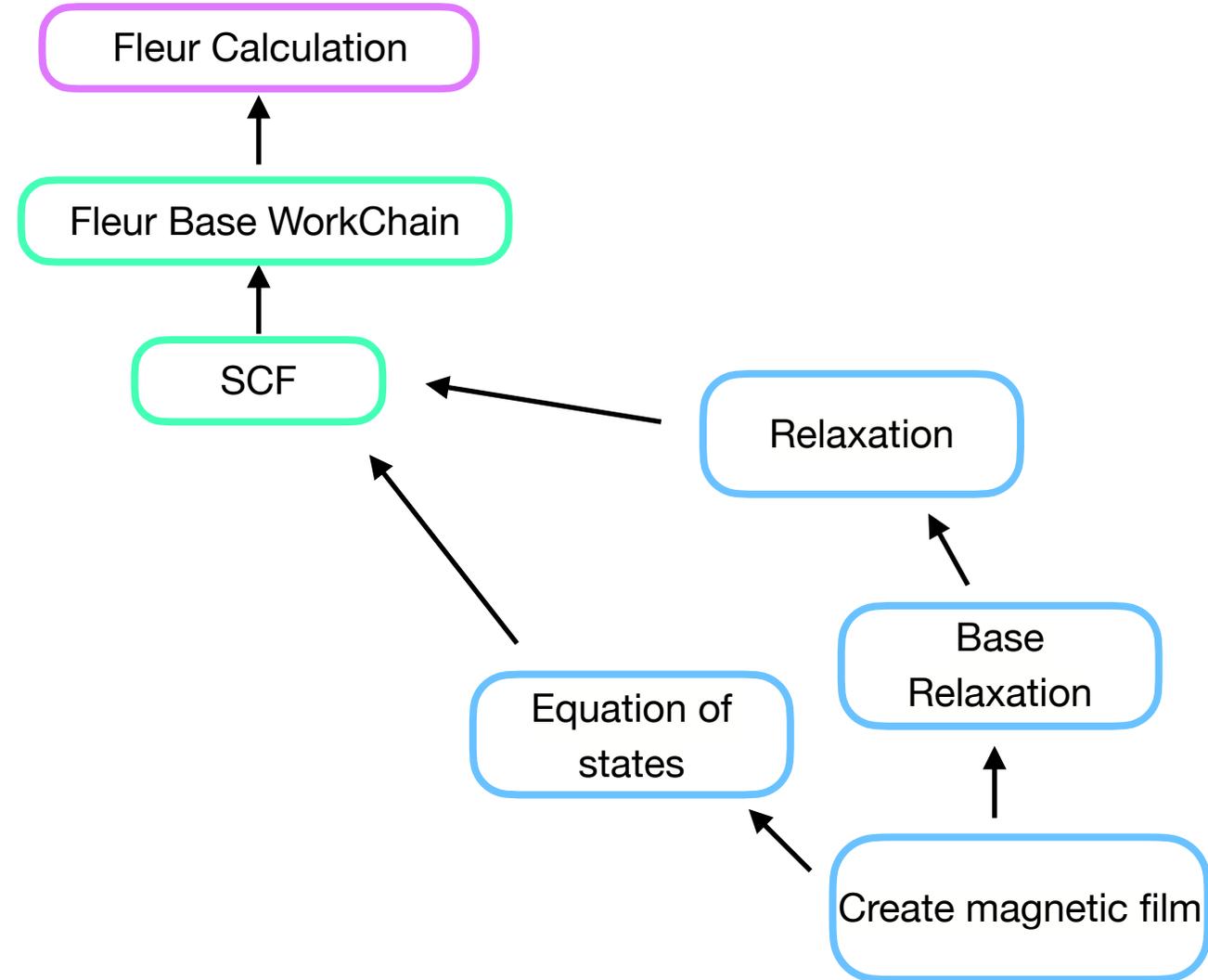


Nested WorkChains: CMF



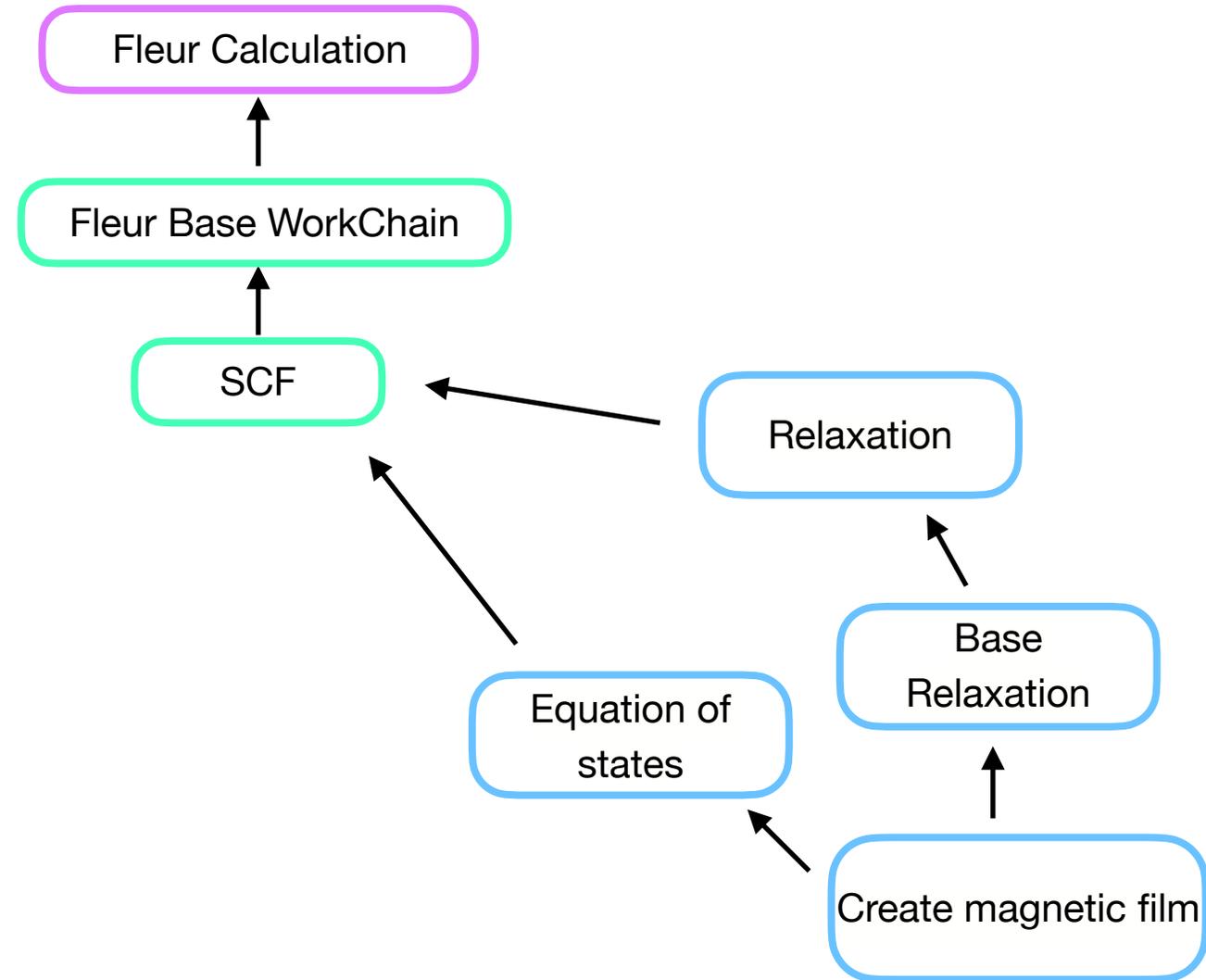
Nested WorkChains: CMF

```
'eos': {  
  'scf': {  
    'wf_parameters': SCF para,  
    'calc_parameters': inpgen para,  
    'options': technical para,  
    'inpgen': inpgen code,  
    'fleur': FLEUR code  
  },  
  'wf_parameters': EOS para  
},
```



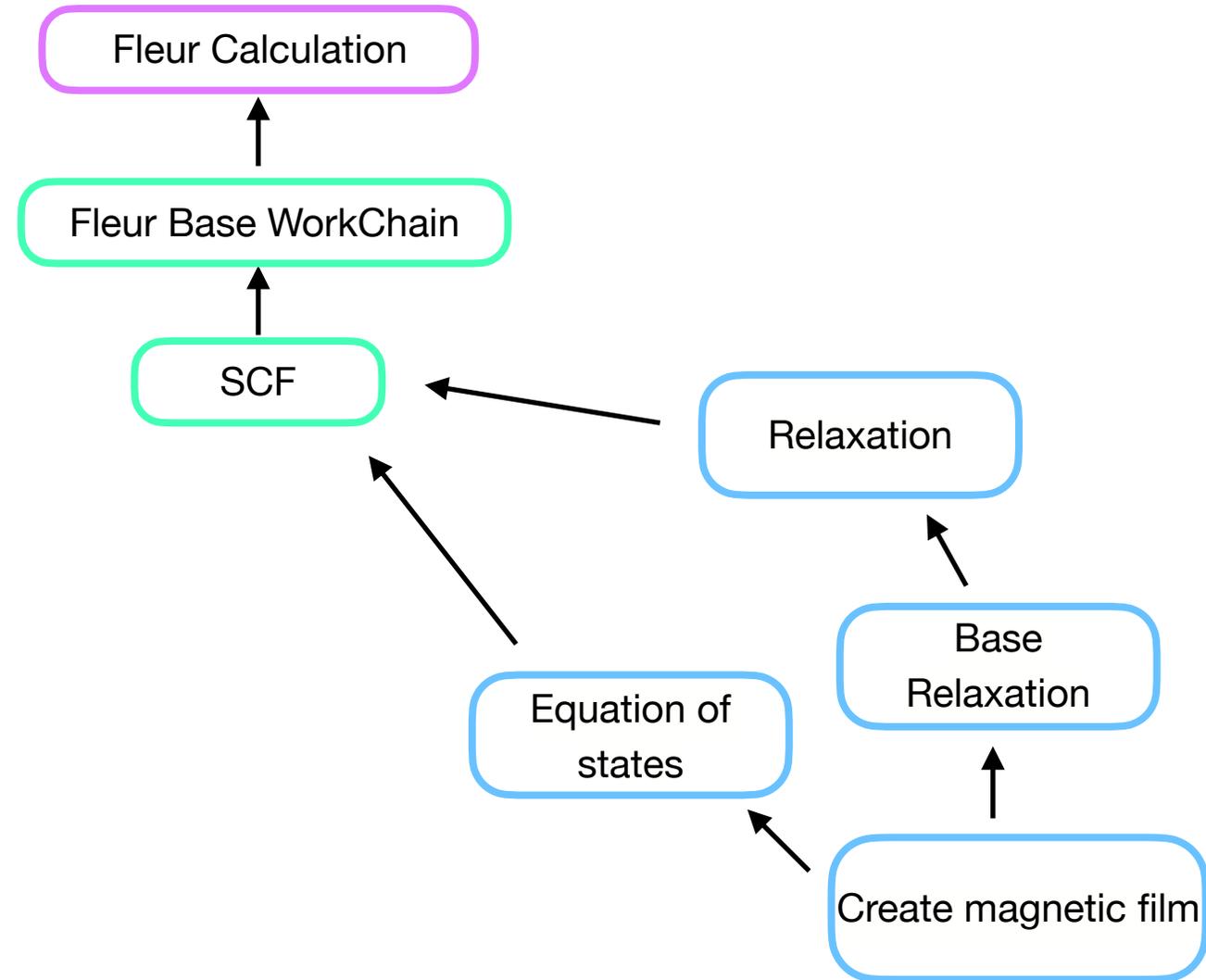
Nested WorkChains: CMF

```
'eos': {  
  'scf': {  
    'wf_parameters': SCF para,  
    'calc_parameters': inpgen para,  
    'options': technical para,  
    'inpgen': inpgen code,  
    'fleur': FLEUR code  
  },  
  'wf_parameters': EOS para  
},  
'relax': {  
  'scf': {  
    'wf_parameters': SCF para 2,  
    'calc_parameters': inpgen para 2,  
    'options': technical para 2,  
    'inpgen': inpgen code 2,  
    'fleur': FLEUR code 2  
  },  
  'wf_parameters': Relax para,  
},
```



Nested WorkChains: CMF

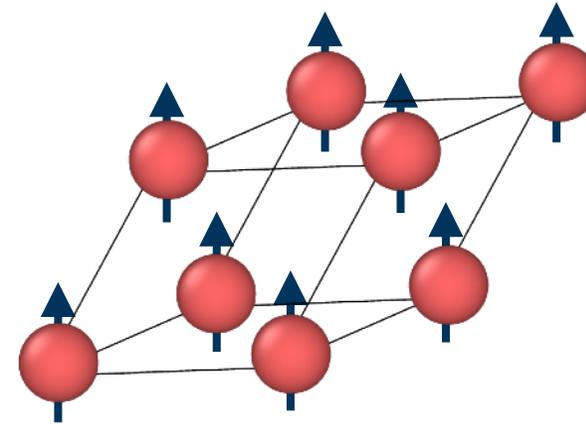
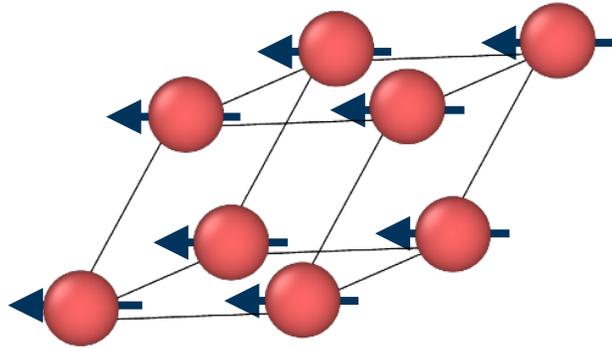
```
'eos': {  
  'scf': {  
    'wf_parameters': SCF para,  
    'calc_parameters': inpgen para,  
    'options': technical para,  
    'inpgen': inpgen code,  
    'fleur': FLEUR code  
  },  
  'wf_parameters': EOS para  
,  
'relax': {  
  'scf': {  
    'wf_parameters': SCF para 2,  
    'calc_parameters': inpgen para 2,  
    'options': technical para 2,  
    'inpgen': inpgen code 2,  
    'fleur': FLEUR code 2  
  },  
  'wf_parameters': Relax para,  
,  
'wf_parameters': Create Magnetic para
```



HIGHER-LEVEL WORKCHAINS

MAE Workchain

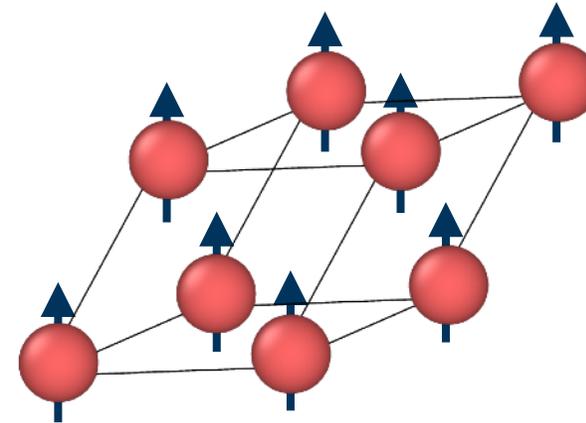
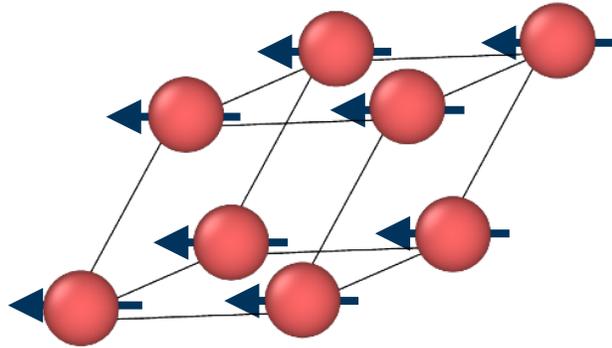
Energies are not the same for:



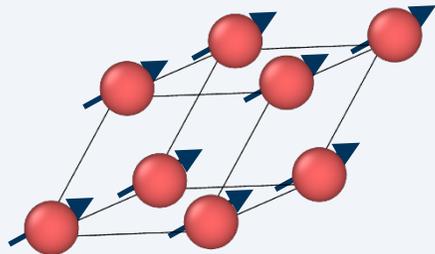
What is a qualitative energy difference?

MAE Workchain

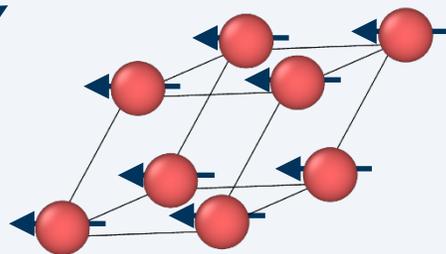
Energies are not the same for:



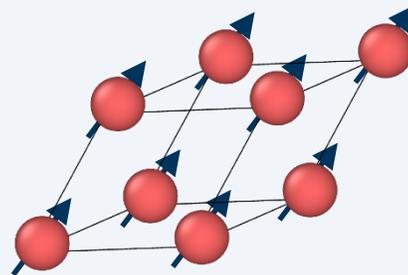
What is a qualitative energy difference?



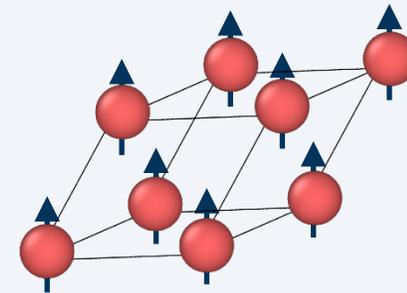
Energy



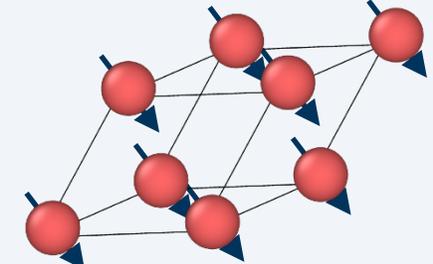
Energy



Energy



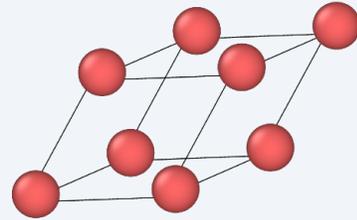
Energy



Energy

MAE SCF Workchain

Inputs

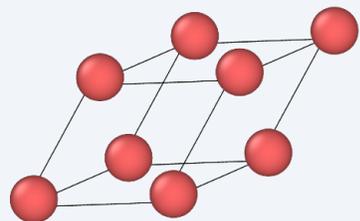


+

WorkChain parameters

MAE SCF Workchain

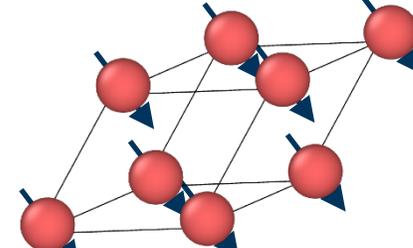
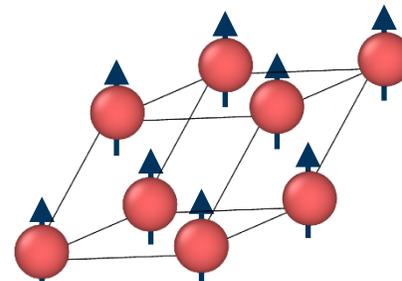
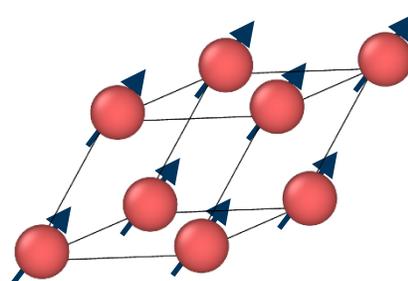
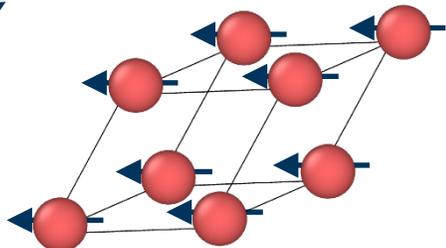
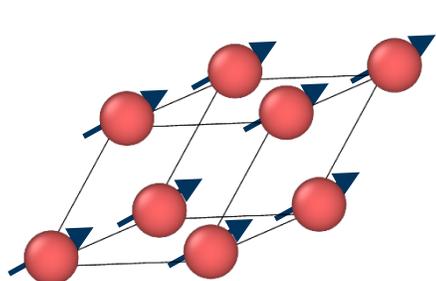
Inputs



+

WorkChain parameters

SCF



SCF

SCF

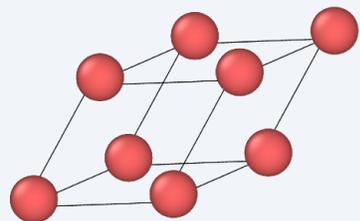
SCF

SCF

SCF

MAE SCF Workchain

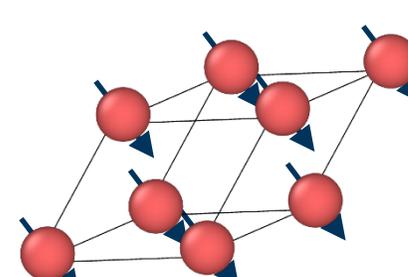
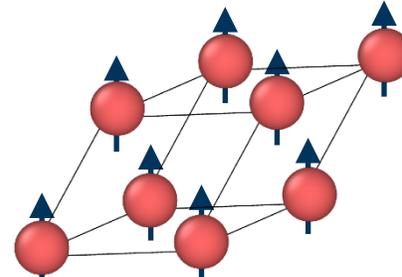
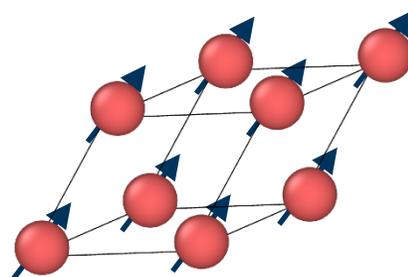
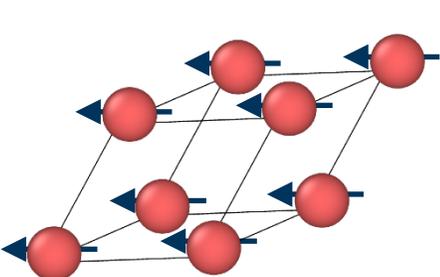
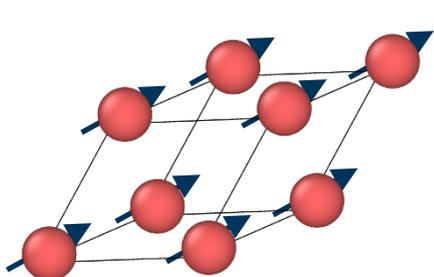
Inputs



+

WorkChain parameters

SCF



SCF

SCF

SCF

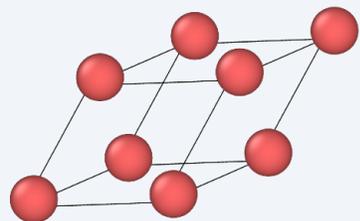
SCF

SCF

~50 iterations
with SOC

MAE SCF Workchain

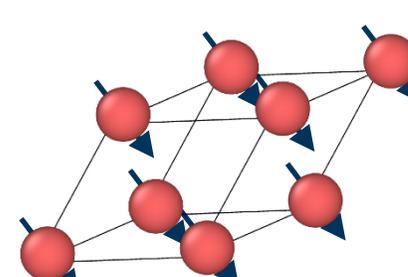
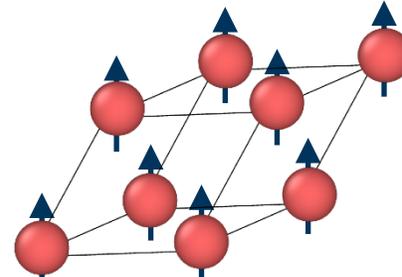
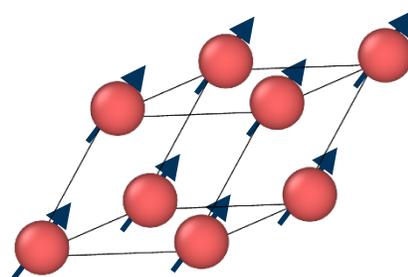
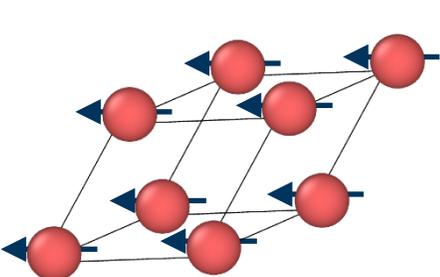
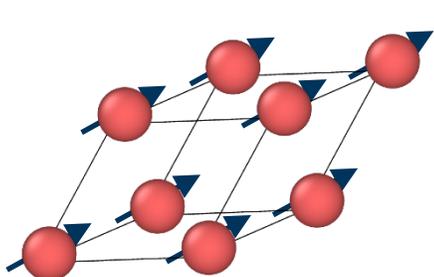
Inputs



+

WorkChain parameters

SCF



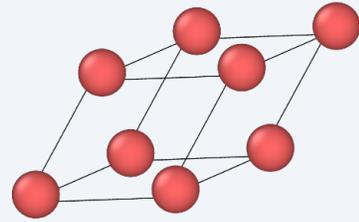
SCF

~50 iterations
with SOC

output

MAE Force theorem Workchain

Initialisation

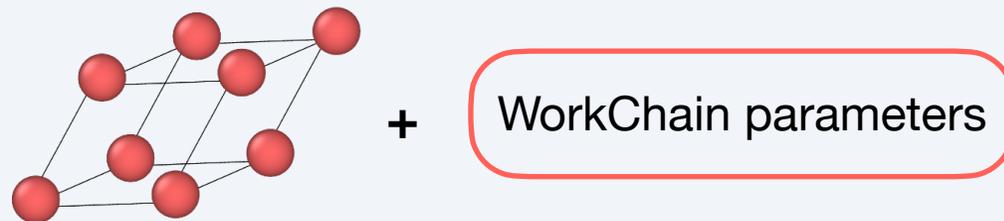


+

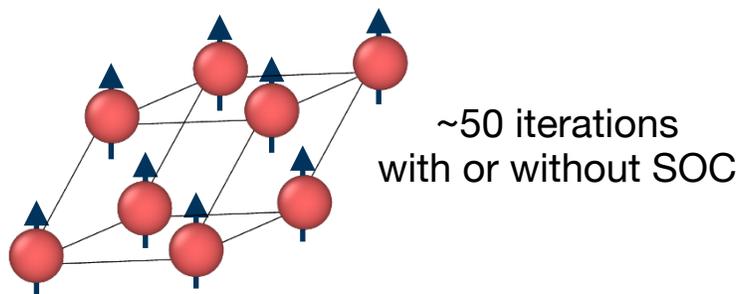
WorkChain parameters

MAE Force theorem Workchain

Initialisation

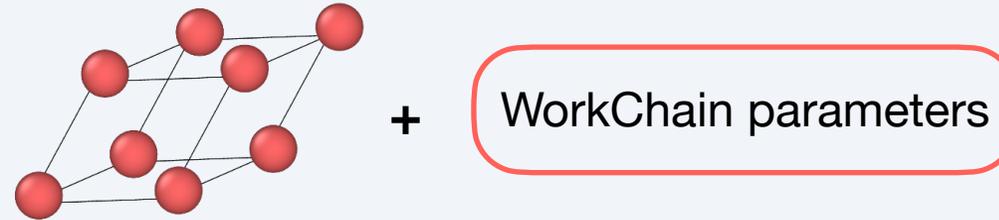


Reference calculation

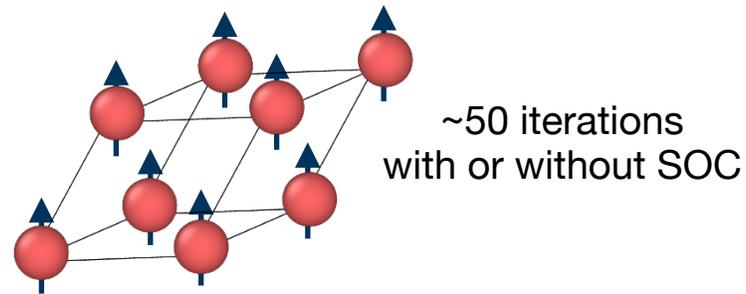


MAE Force theorem Workchain

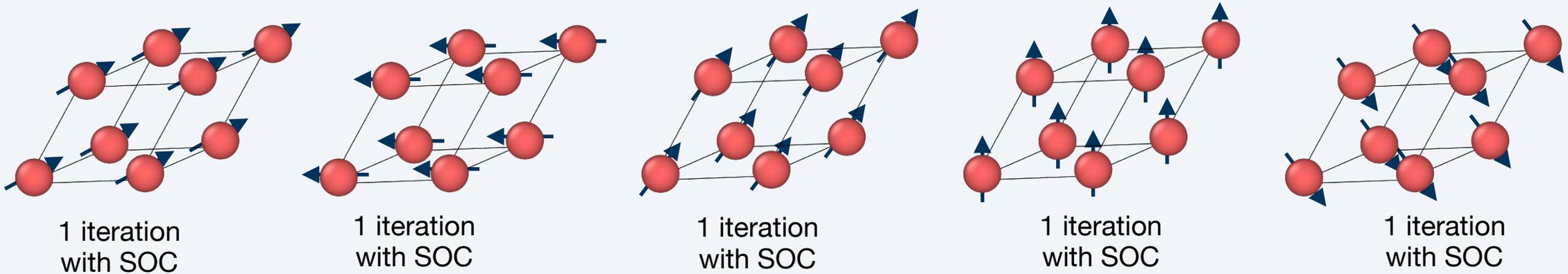
Initialisation



Reference calculation

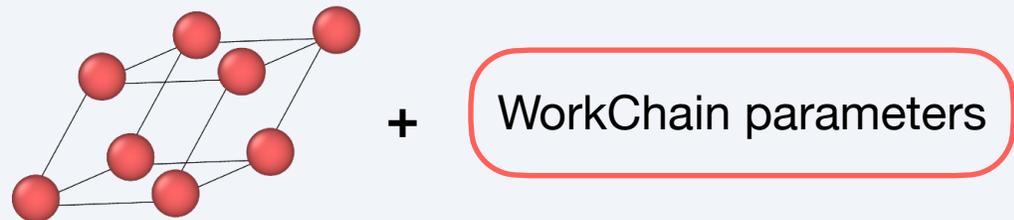


Force theorem

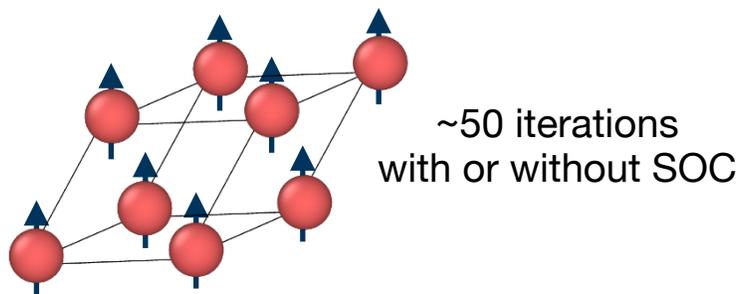


MAE Force theorem Workchain

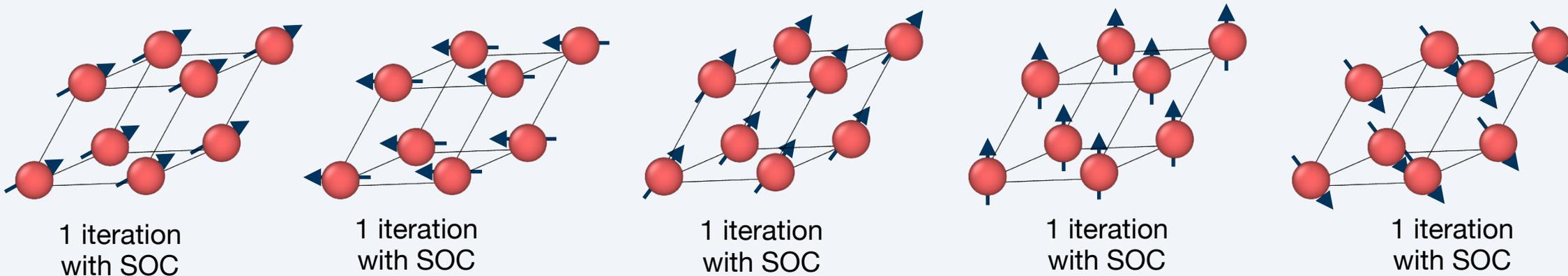
Initialisation



Reference calculation

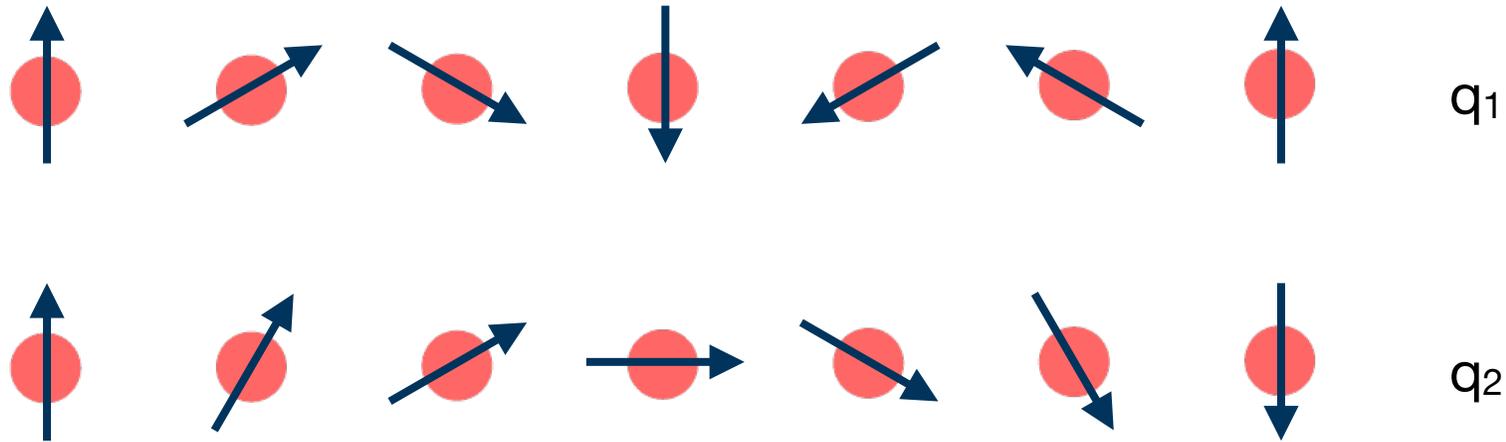


Force theorem



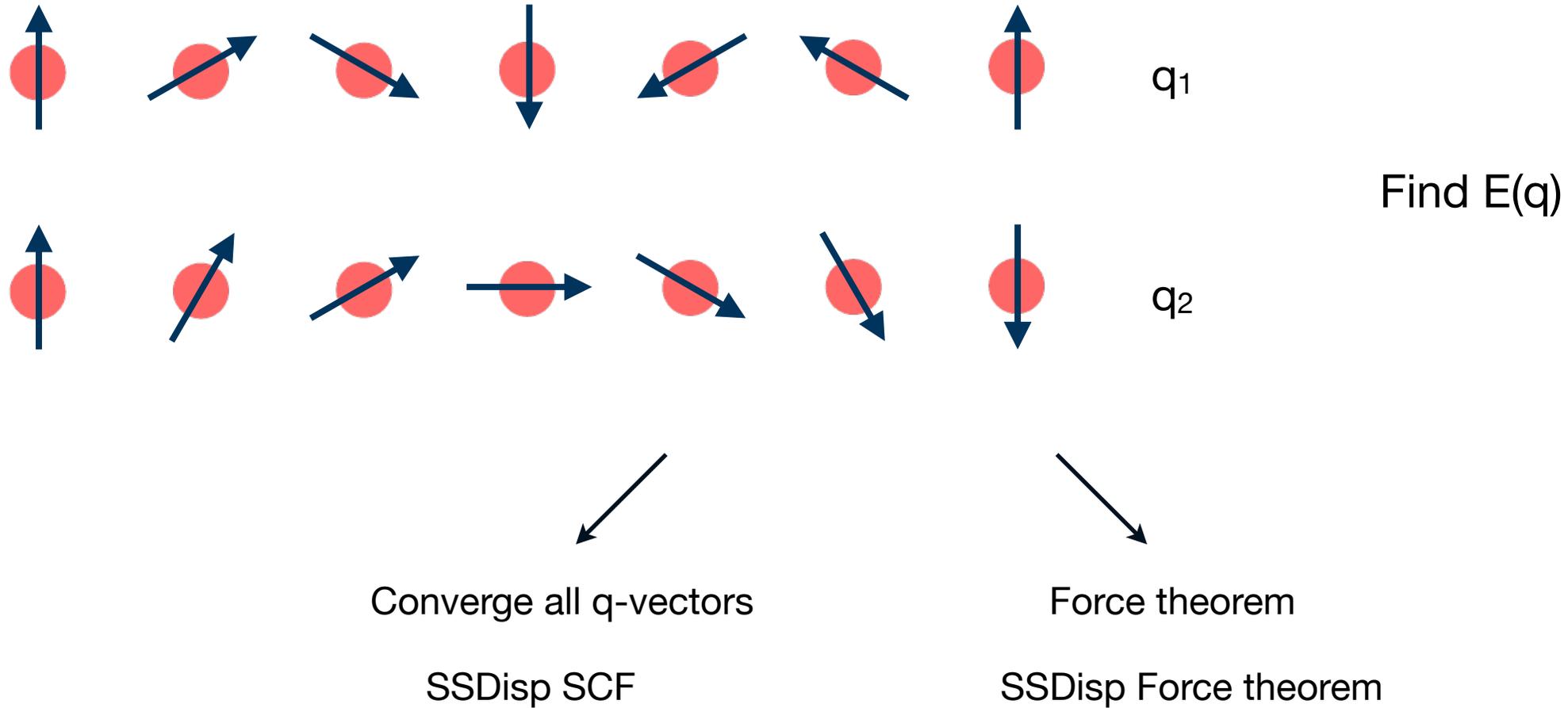
output

Spin spiral dispersion workchain



Find $E(q)$

Spin spiral dispersion workchain



SSDisp SCF Workchain

Initialisation

SCF

SSDisp SCF Workchain

Initialisation



SCF

SSDisp SCF Workchain

Initialisation



SCF

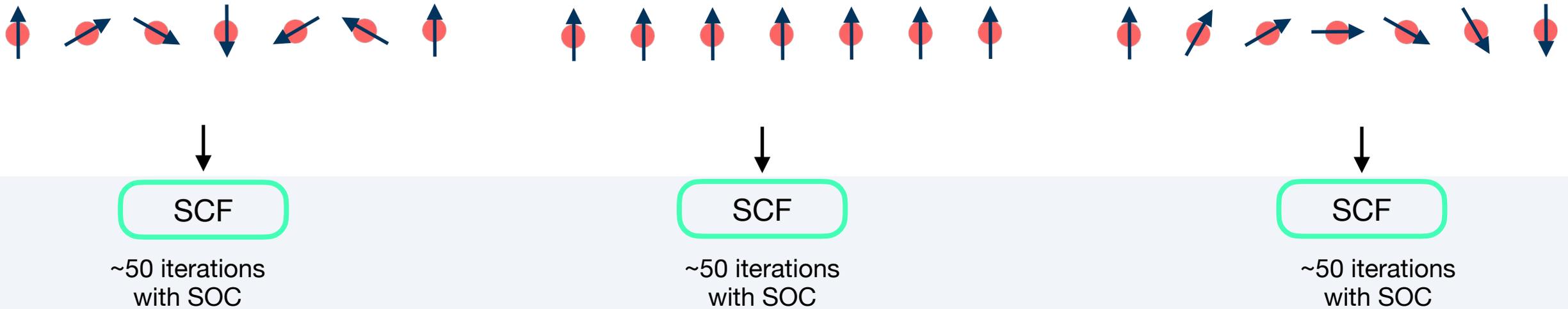


SSDisp SCF Workchain

Initialisation

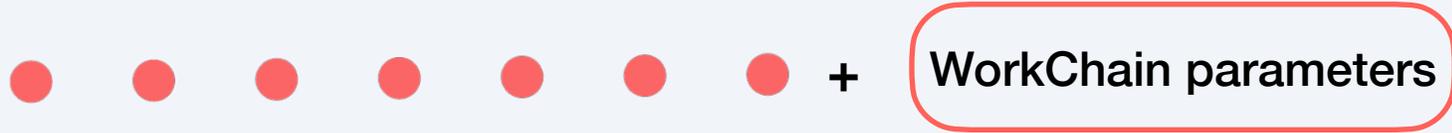


SCF



SSDisp SCF Workchain

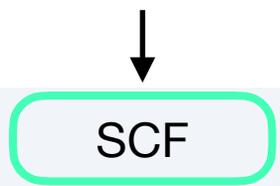
Initialisation



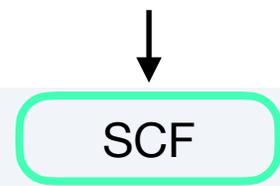
SCF



~50 iterations with SOC



~50 iterations with SOC



~50 iterations with SOC



SSDisp Force theorem Workchain

Initialisation

Reference calculation

Force theorem

SSDisp Force theorem Workchain

Initialisation



Reference calculation

Force theorem

SSDisp Force theorem Workchain

Initialisation



Reference calculation



Force theorem

SSDisp Force theorem Workchain

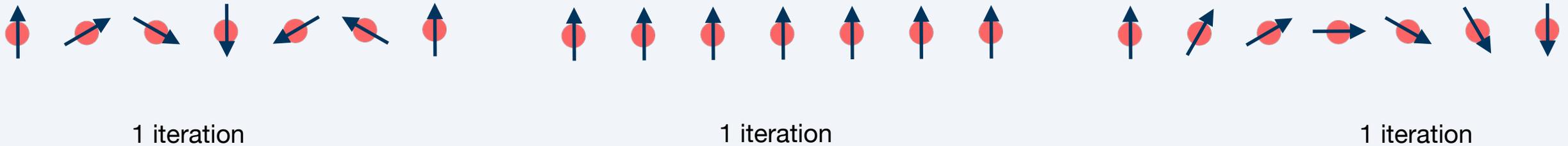
Initialisation



Reference calculation



Force theorem



SSDisp Force theorem Workchain

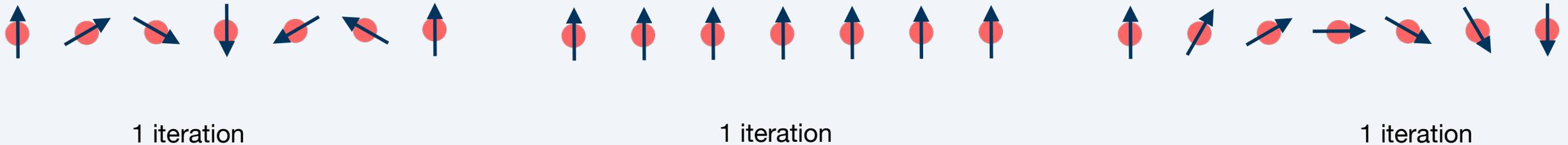
Initialisation



Reference calculation

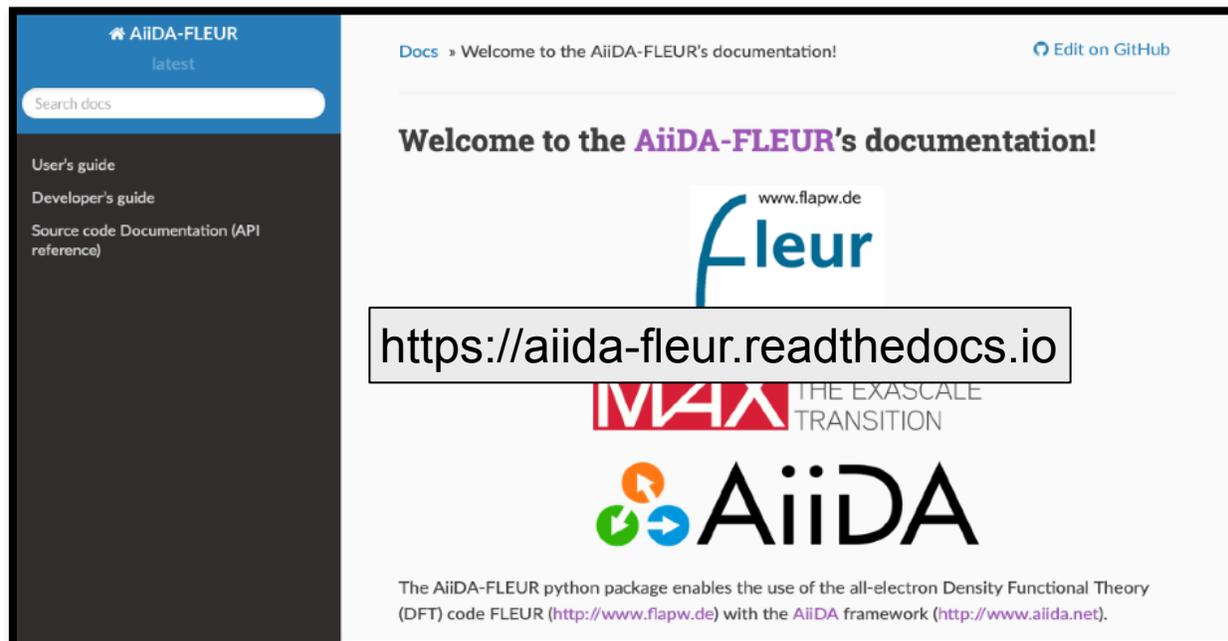


Force theorem



output

Details



AiiDA-FLEUR
latest

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User's guide
Developer's guide
Source code Documentation (API reference)

Docs » Welcome to the AiiDA-FLEUR's documentation! [Edit on GitHub](#)

Welcome to the **AiiDA-FLEUR's** documentation!

www.flapw.de
fleur

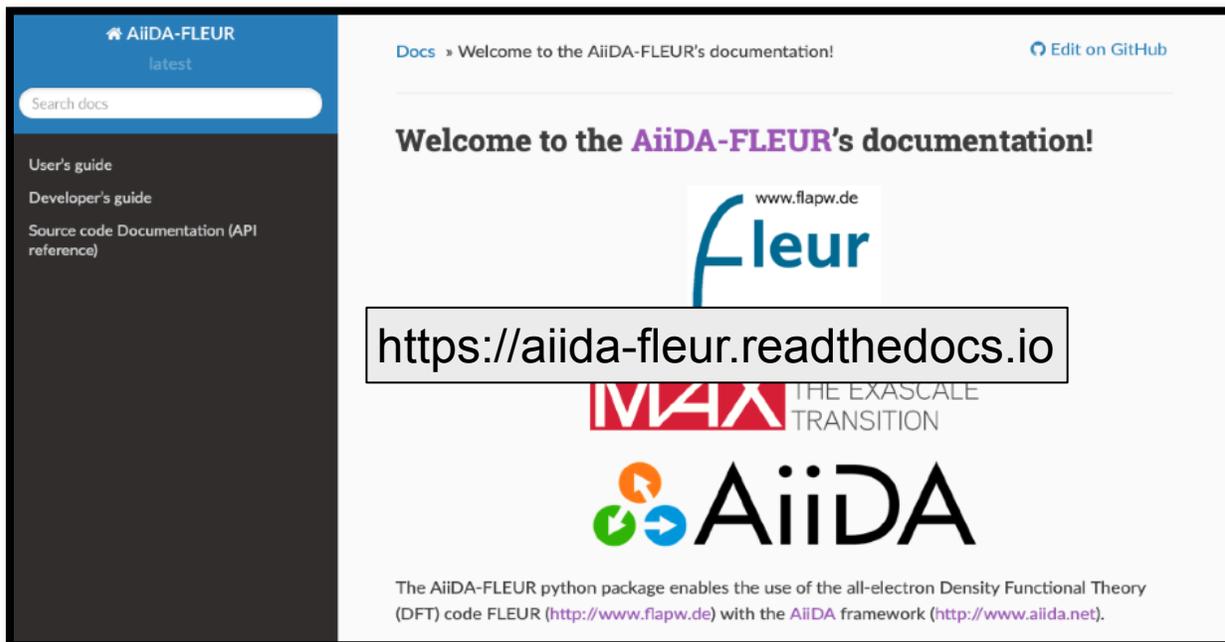
<https://aiida-fleur.readthedocs.io>

MAX THE EXASCALE
TRANSITION

 **AiiDA**

The AiiDA-FLEUR python package enables the use of the all-electron Density Functional Theory (DFT) code FLEUR (<http://www.flapw.de>) with the AiiDA framework (<http://www.aiida.net>).

Details



AiiDA-FLEUR
latest

Search docs

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Welcome to the AiiDA-FLEUR's documentation!

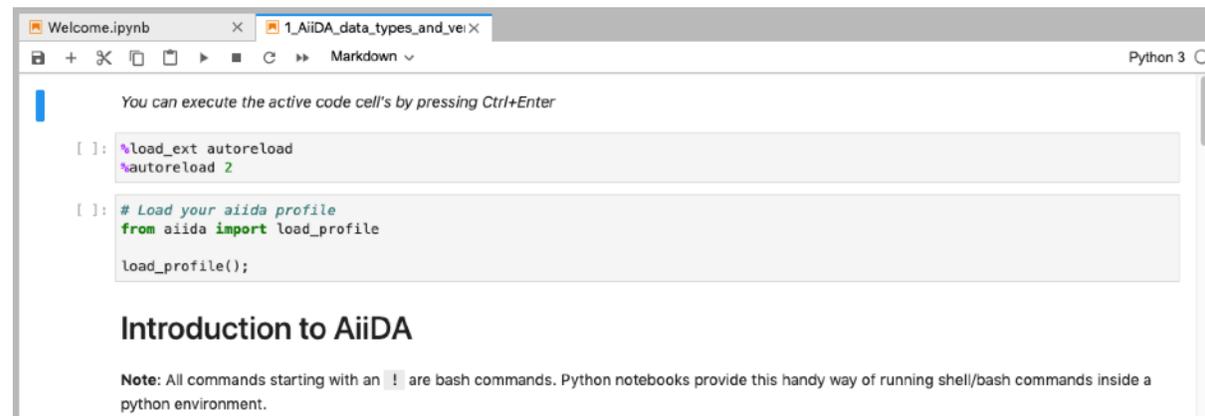
www.flapw.de
fleur

<https://aiida-fleur.readthedocs.io>

MAX THE EXASCALE TRANSITION

AiiDA

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Welcome.ipynb x 1_AiiDA_data_types_and_vei x

Python 3

You can execute the active code cell's by pressing Ctrl+Enter

```
[ ]: %load_ext autoreload
      %autoreload 2

[ ]: # Load your aiida profile
      from aiida import load_profile
      load_profile();
```

Introduction to AiiDA

Note: All commands starting with an `!` are bash commands. Python notebooks provide this handy way of running shell/bash commands inside a python environment.

ACKNOWLEDGEMENTS

ACKNOWLEDGEMENTS

The FLEUR community:

D. Wortmann, G. Michalicek,
U. Alekseeva, G. Bihlmayer,
M. Redies, C. R. Gerhorst,
S. Blügel, ...

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Virtual materials design team:

A. Chandran, R. Kovacik,
P. Rüßmann, J. Bröder, ...

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From the AiiDA community:

G. Pizzi, S. Huber, L. Talirz, M. Uhrin,
L. Kahle, N. Mounet, S. Zoupanos,
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IT: I. Meyer, D. Kaiser

ACKNOWLEDGEMENTS

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