AiiDA-KKR documentation

Release 1.1.9

The AiiDA-KKR team.

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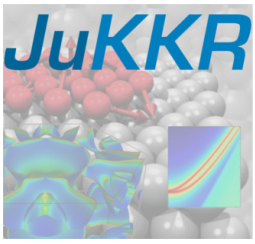
Contents


JuKKR


AiiDA

CHAPTER 1

Welcome to documentation of the AiiDA plugin for the Jülich KKRcode!

The plugin is available at https://github.com/JuDFTteam/aiida-kkr

If you use this plugin for your research, please cite the following work:

> Author Name1, Author Name2, *Paper title*, Jornal Name XXX, YYYY (Year).

Also please cite the original AiiDA paper:

> Giovanni Pizzi, Andrea Cepellotti, Riccardo Sabatini, Nicola Marzari, and Boris Kozinsky, *AiiDA: automated interactive infrastructure and database for computational science*, Comp. Mat. Sci 111, 218-230 (2016); http://dx.doi.org/10.1016/j.commatsci.2015.09.013; http://www.aiida.net.

1.1 Requirements

- Installation of aiida-core
- Installation of KKR codes (*kkrhost*, *kkrimp*, *voronoi*) of the JuKKR package
- Installation of aiida-kkr

Once all requirements are installed you need to set up the computers and codes before you can submit KKR calcutions using the *aiida-kkr* plugin.

1.1.1 User's guide

1.1.1.1 User's guide

Calculations

Here the calculations of the aiida-kkr plugin are presented. It is assumed that the user already has basic knowledge of python, aiida (e.g. database structure, verdi commands, structure nodes) and KKR (e.g. LMAX cutoff, energy contour integration). Also *aiida-kkr* should be installed as well as the Voronoi, KKR and KKRimp codes should already be configured.

In practice, the use of the workflows is more convenient but here the most basic calculations which are used underneath in the workflows are introduced step by step.

In the following the calculation plugins provided by aiida-kkr are introduced at the example of bulk Cu.

Note: If you follow the steps described here please make sure that your python script contains:

```
from aiida import load_profile
load_profile()
```

To ensure that the aiida database is properly integrated.

Voronoi starting potential generator

The Voronoi code creates starting potentials for a KKR calculation and sets up the atom-centered division of space into voronoi cells. Also corresponding shape functions are created, which are needed for full-potential corrections.

The voronoi plugin is called `kkr.voro` and it has the following input and output nodes:

Three input nodes:

- `parameters` KKR parameter set for Voronoi calculation (Dict)
- `structure` structure data node node describing the crystal lattice (StructureData)
- `code` Voronoi code node (code)

Three output nodes:

- `remote_folder` (RemoteData)
- `retrieved` (FolderData)
- `output_parameters` (Dict)

Additional optional input nodes that trigger special behavior of a Voronoi calculation are:

- `parent_KKR` (RemoteData of a KKR Calculation)
- `potential_overwrite` (SingleFileData)

Now the basic usage of the voronoi plugin is demonstrated at the example of Cu bulk for which first the aiida structure node and the parameter node containing KKR specific parameters (LMAX cutoff etc.) are created before a voronoi calculation is set up and submitted.

Input structure node

First we create an aiida structure:

```
# get aiida StructureData class:
from aiida.plugins import DataFactory
StructureData = DataFactory('structure')
```

Then we create the aiida StructureData node (here for bulk Cu):

```
alat = 3.61 # lattice constant in Angstroem
bravais = [[0.5*alat, 0.5*alat, 0], [0.5*alat, 0, 0.5*alat], [0, 0.5*alat, 0.5*alat]]
↪# Bravais matrix in Ang. units
# now create StructureData instance and set Bravais matrix and atom in unit cell
Cu = StructureData(cell=bravais)
Cu.append_atom(position=[0,0,0], symbols='Cu')
```

Input parameter node

Next we create an empty set of KKR parameters (LMAX cutoff etc.) for voronoi code:

```
# load kkrparms class which is a useful tool to create the set of input parameters␣
↪for KKR-family of calculations
from masci_tools.io.kkr_params import kkrparams
params = kkrparams(params_type='voronoi')
```

Note: we can find out which parameters are mandatory to be set using `missing_params = params.get_missing_keys(use_aiida=True)`

and set at least the mandatory parameters:

```
params.set_multiple_values(LMAX=2, NSPIN=1, RCLUSTZ=2.3)
```

finally create an aiida Dict node and fill with the dictionary of parameters:

```
Dict = DataFactory('dict') # use DataFactory to get ParamerterData class
ParaNode = Dict(dict=params.get_dict())
```

Submit calculation

Now we get the voronoi code:

```
from aiida.orm import Code # load aiida 'Code' class

codename = 'voronoi@localhost'
code = Code.get_from_string(codename)
```

Note: Make sure that the voronoi code is installed: `verdi code list` should give you a list of installed codes where *codename* should be in.

and create new process builder for a VoronoiCalculation:

```
builder = code.get_builder()
```

Note: This will already set `builder.code` to the voronoi code which we loaded above.

and set resources that will be used (here serial job) in the options dict of the metadata:

```
builder.metadata.options = {'resources': {'num_machines':1, 'tot_num_mpiprocs':1} }
```

Note: If you use a computer without a default queue you need to set the name of the queue as well: `builder.metadata.options['queue_name'] = 'th1'`)

then set structure and input parameter:

```
builder.structure = Cu
builder.parameters = ParaNode
```

Note: Additionally you could set the `parent_KKR` and `potential_overwrite` input nodes which trigger special run modes of the voronoi code that are discussed below.

Now we are ready to submit the calculation:

```
from aiida.engine import submit
voro_calc = submit(builder)
```

Note: check calculation state (or use verdi calculation list -a -p1) using `voro_calc.process_state`

Voronoi calculation with the `parent_KKR` input node

To come . . .

Voronoi calculation with the `potential_overwrite` input node

To come . . .

KKR calculation for bulk and interfaces

A KKR calculation is provided by the `kkr.kkr` plugin, which has the following input and output nodes.

Three input nodes:

- `parameters` KKR parameter fitting the requirements for a KKR calculation (Dict)
- `parent_folder` parent calulation remote folder node (RemoteFolder)
- `code` KKR code node (code)

Three output nodes:

- `remote_folder` (RemoteData)
- `retrieved` (FolderData)
- `output_parameters` (Dict)

Note: The parent calculation can be one of the following:

1. Voronoi calculation, initial calculation starting from structure
2. previous KKR calculation, e.g. preconverged calculation

The necessary structure information is always extracted from the voronoi parent calculation. In case of a continued calculation the voronoi parent is recuresively searched for.

Special features exist where a fourth input node is persent and which triggers special behavior of the KKR calculation:

- `impurity_info` Node specifying the impurity cluster (*Dict*)
- `kpoints` Node specifying the kpoints for which the bandstructure is supposed to be calculated (*Kpoints-Data*)

The different possible modes to run a kkr calculation (start from Voronoi calculation, continue from previous KKR calculation, *host Greenfunction writeout* feature) are demonstrated in the following.

Start KKR calculation from voronoi parent

Reuse settings from voronoi calculation:

```
voronoi_calc_folder = voro_calc.out.remote_folder
voro_params = voro_calc.inputs.parameters
```

Now we update the KKR parameter set to meet the requirements for a KKR calculation (slightly different than voronoi calculation). Thus, we create a new set of parameters for a KKR calculation and fill the already set values from the previous voronoin calculation:

```
# new kkrparams instance for KKR calculation
params = kkrparams(params_type='kkr', **voro_params.get_dict())

# set the missing values
params.set_multiple_values(RMAX=7., GMAX=65.)

# choose 20 simple mixing iterations first to preconverge potential (here 5% simple␣
↪mixing)
params.set_multiple_values(NSTEPS=20, IMIX=0, STRMIX=0.05)

# create aiida Dict node from the KKR parameters
ParaNode = Dict(dict=params.get_dict())
```

Note: You can find out which parameters are missing for the KKR calculation using `params.get_missing_keys()`

Now we can get the KKR code and create a new calculation instance and set the input nodes accordingly:

```
code = Code.get_from_string('KKRcode@localhost')
builder = code.get_builder()

# set input Parameter, parent calulation (previous voronoi calculation), computer␣
↪resources
builder.parameters = ParaNode
builder.parent_folder = voronoi_calc_folder
builder.metadata.options = {'resources' :{'num_machines': 1, 'num_mpiprocs_per_machine
↪':1}}
```

We can then run the KKR calculation:

```
kkr_calc = submit(builder)
```

Continue KKR calculation from KKR parent calculation

First we create a new KKR calculation instance to continue KKR ontop of a previous KKR calclation:

```
builder = code.get_builder()
```

Next we reuse the old KKR parameters and update scf settings (default is NSTEPS=1, IMIX=0):

```
params.set_multiple_values(NSTEPS=50, IMIX=5)
```

and create the aiida Dict node:

```
ParaNode = Dict(dict=params.get_dict())
```

Then we set the input nodes for calculation:

```
builder.parameters = ParaNode
kkr_calc_parent_folder = kkr_calc.outputs.remote_folder # parent remote folder of␣
↪previous calculation
builder.parent_folder = kkr_calc_parent_folder
builder.metadata.options = {'resources': {'num_machines': 1, 'num_mpiprocs_per_machine
↪':1}}
```

store input nodes and submit calculation:

```
kkr_calc_continued = submit(builder)
```

The finished calculation should have this output node that can be access within python using `kkr_calc_continued.outputs.output_parameters.get_dict()`. An excerpt of the ouput dictionary may look like this:

```
{u'alat_internal': 4.82381975,
 u'alat_internal_unit': u'a_Bohr',
 u'convergence_group': {
     u'calculation_converged': True,
     u'charge_neutrality': -1.1e-05,
     u'nsteps_exhausted': False,
     u'number_of_iterations': 47,
     u'rms': 6.4012e-08,
     ...},
u'energy': -44965.5181266111,
u'energy_unit': u'eV',
u'fermi_energy': 0.6285993399,
u'fermi_energy_units': u'Ry',
u'nspin': 1,
u'number_of_atoms_in_unit_cell': 1,
u'parser_errors': [],
...
u'warnings_group': {u'number_of_warnings': 0, u'warnings_list': []}}
```

Special run modes: host GF writeout (for KKRimp)

Here we take the remote folder of the converged calculation to reuse settings and write out Green function and tmat of the crystalline host system:

```
kkr_converged_parent_folder = kkr_calc_continued.outputs.remote_folder
```

Now we extract the parameters of the kkr calculation and add the `KKRFLEX` run-option:

```
kkrcalc_converged = kkr_converged_parent_folder.get_incoming().first().node
kkr_params_dict = kkrcalc_converged.inputs.parameters.get_dict()
kkr_params_dict['RUNOPT'] = ['KKRFLEX']
```

The parameters dictionary is not passed to the aiida Dict node:

```
ParaNode = Dict(dict=kkr_params_dict)
```

Now we create a new KKR calculation and set input nodes:

```
code = kkrcalc_converged.inputs.code # take the same code as in the calculation before
builder= code.get_builder()
resources = kkrcalc_converged.attributes['resources']
builder.metadata.options = {'resources': resources}
builder.parameters = ParaNode
builder.parent_folder = kkr_converged_parent_folder
# prepare impurity_info node containing the information about the impurity cluster
imp_info = Dict(dict={'Rcut':1.01, 'ilayer_center': 0, 'Zimp':[79.]})
# set impurity info node to calculation
builder.impurity_info = imp_info
```

Note: The `impurity_info` node should be a Dict node and its dictionary should describe the impurity cluster using the following parameters:

- `ilayer_center` (int) layer index of position in the unit cell that describes the center of the impurity cluster
- `Rcut` (float) cluster radius of impurity cluster in units of the lattice constant
- `hcut` (float, *optional*) height of a cylindrical cluster with radius `Rcut`, if not given spherical cluster is taken
- `cylinder_orient` (list of 3 float values, *optional*)
- `Zimp` (list of *Nimp* float entries) atomic charges of the substitutional impurities on positions defined by `Rimp_rel`
- `Rimp_rel` (list of *Nimp* [float, float, float] entries, *optional*, defaults to [0,0,0] for single impurity) cartesian positions of all *Nimp* impurities, relative to the center of cluster (i.e. position defined by `ilayer_center`)
- `imp_cls` (list of [float, float, float, int] entries, *optional*) full list of impurity cluster positions and layer indices *(x, y, z, ilayer)*, overwrites auto generation using `Rcut` and `hcut` settings

> **Warning:** `imp_cls` functionality not implemented yet

The calculation can then be submitted:

```
# submit calculation
GF_host_calc = submit(builder)
```

Once the calculation has finished the retrieve folder should contain the `kkrflex_*` files needed for the impurity calculation.

Special run modes: bandstructure

Here we take the remote folder of the converged calculation and compute the bandstructure of the Cu bulk system. We reuse the DOS settings for the energy interval in which the bandstructure is computed from a previous calculation:

```
from aiida.orm import load_node
kkr_calc_converged = load_node(<-id-of-previous-calc>)
kkr_dos_calc = load_node(<-id-of-previous-DOS-calc>)
```

Now we need to generate the kpoints node for bandstructure calculation. This is done using aiida's `get_explicit_kpoints_path` function that extracts the kpoints along high symmetry lines from a structure:

```
# first extract the structure node from the KKR parent calculation
from aiida_kkr.calculations.voro import VoronoiCalculation
struc, voro_parent = VoronoiCalculation.find_parent_structure(kkr_calc_converged.
↪outputs.remote_folder)
# then create KpointsData node
from aiida.tools.data.array.kpoints import get_explicit_kpoints_path
kpts = get_explicit_kpoints_path(struc).get('explicit_kpoints')
```

Warning: Note that the `get_explicit_kpoints_path` function returns kpoints for the primitive structure. In this example the input structure is already the primitive cell however in general this may not always be the case.

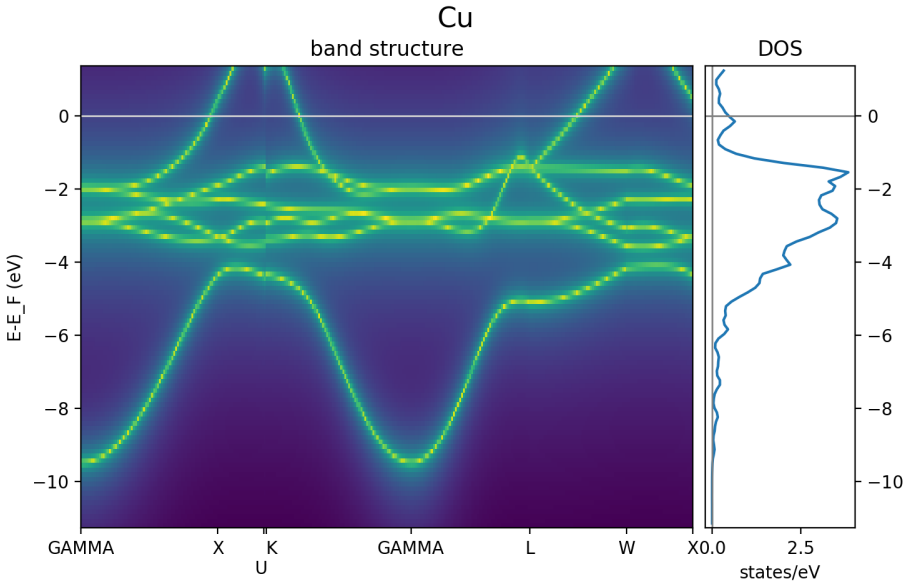
Then we set the `kpoints` input node to a new KKR calculation and change some settings of the input parameters accordingly (i.e. energy contour like in DOS run):

```
# create bandstructure calculation reusing old settings (including same computer and␣
↪resources in this example)
kkrcode = kkr_calc_converged.inputs.code
builder = kkrcode.get_builder()
builder.kpoints = kpts # pass kpoints as input
builder.parent_folder = kkr_calc_converged.outputs.remote_folder
builder.metadata.options = {'resources': kkr_calc_converged.attributes['resources']}
# change parameters to qdos settings (E range and number of points)
from masci_tools.io.kkr_params import kkrparams
qdos_params = kkrparams(**kkr_calc_converged.inputs.parameters.get_dict()) # reuse␣
↪old settings
# reuse the same emin/emax settings as in DOS run (extracted from input parameter␣
↪node)
qdos_params.set_multiple_values(EMIN=host_dos_calc.inputs.parameters.get_dict().get(
↪'EMIN'),
                                EMAX=host_dos_calc.inputs.parameters.get_dict().get(
↪'EMAX'),
                                NPT2=100)
builder.parameters = Dict(dict=qdos_params.get_dict())
```

The calculation is then ready to be submitted:

```
# submit calculation
kkrcalc = submit(builder)
```

The result of the calculation will then contain the `qdos.aa.s.dat` files in the retrieved node, where `aa` is the atom index and `s` the spin index of all atoms in the unit cell. The resulting bandstructure (for the Cu bulk test system considered here) should look like this (see *here for the plotting script*):



Special run modes: Jij extraction

The extraction of exchange coupling parameters is triggered with the `XCPL` run option and needs at lest the `JIJRAD` paramter to be set. Here we take the remote folder of the converged calculation and compute the exchange parameters:

```
from aiida.orm import load_node
kkr_calc_converged = load_node(<-id-of-previous-calc>)
```

Then we set the `XCLP` run option and the `JIJRAD` parameter (the `JIJRADXY`, `JIJSITEI` and `JIJSITEJ` parameters are not mandatory and are ommitted in this example) in the input node to a new KKR calculation:

```
# create bandstructure calculation reusing old settings (including same computer and␣
↪resources in this example)
kkrcode = kkr_calc_converged.inputs.code
builder = kkrcode.get_builder()
builder.parent_folder = kkr_calc_converged.outputs.remote_folder
builder.metadata.options = {'resources': kkr_calc_converged.attributes['resources']}
# change parameters to Jij settings ('XCPL' runopt and JIJRAD parameter)
from aiida_kkr.tools.kkr_params import kkrparams
Jij_params = kkrparams(**kkr_calc_converged.inputs.parameters.get_dict()) # reuse old␣
↪settings
# add JIJRAD (remember: in alat units)
Jij_params.set_value('JIJRAD', 1.5)
# add 'XCPL' runopt to list of runopts
runopts = Jij_params.get_value('RUNOPT')
runopts.append('XCPL    ')
Jij_params.set_value('RUNOPT', runopts)
```

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```
# now use updated parameters
builder.parameters = Dict(dict=qdos_params.get_dict())
```

The calculation is then ready to be submitted:

```
# submit calculation
kkrcalc = submit(builder)
```

The result of the calculation will then contain the `Jijatom.*` files in the retrieved node and the `shells.dat` files which allows to map the values of the exchange interaction to equivalent positions in the different shells.

KKR impurity calculation

Plugin: `kkr.kkrimp`

Four input nodes:

- `parameters`, optional: KKR parameter fitting the requirements for a KKRimp calculation (Dict)
- Only one of
  1. `impurity_potential`: starting potential for the impurity run (SingleFileData)
  2. `parent_folder`: previous KKRimp parent calulation folder (RemoteFolder)
- `code`: KKRimp code node (code)
- `host_Greenfunction_folder`: KKR parent calulation folder containing the writeout of the *host's Green function files* (RemoteFolder)

Note: If no `parameters` node is given then the default values are extracted from the `host_Greenfunction` calculation.

Three output nodes:

- `remote_folder` (RemoteData)
- `retrieved` (FolderData)
- `output_parameters` (Dict)

Note: The parent calculation can be one of the following:

1. Voronoi calculation, initial calculation starting from structure
2. previous KKR calculation, e.g. preconverged calculation

The necessary structure information is always extracted from the voronoi parent calculation. In case of a continued calculation the voronoi parent is recuresively searched for.

Create impurity potential

Now the starting potential for the impurity calculation needs to be generated. This means that we need to create an auxiliary structure which contians the impurity in the system where we want to embed it. Then we run a Voronoi calculation to create the starting potential. Here we use the example of a Au impurity embedded into bulk Cu.

The impurity code expects an aiida SingleFileData object that contains the impurity potential. This is finally constructed using the neworder_potential_wf workfunction from aiida_kkr.tools.common_workfunctions.

We start with the creation of the auxiliary styructure:

```
# use an aiida workfunction to keep track of the provenance
from aiida.work import workfunction as wf
@wf
def change_struc_imp_aux_wf(struc, imp_info): # Note: works for single imp at center␣
↪only!
    from aiida.common.constants import elements as PeriodicTableElements
    _atomic_numbers = {data['symbol']: num for num, data in PeriodicTableElements.
↪iteritems()}

    new_struc = StructureData(cell=struc.cell)
    isite = 0
    for site in struc.sites:
        sname = site.kind_name
        kind = struc.get_kind(sname)
        pos = site.position
        zatom = _atomic_numbers[kind.get_symbols_string()]
        if isite == imp_info.get_dict().get('ilayer_center'):
            zatom = imp_info.get_dict().get('Zimp')[0]
        symbol = PeriodicTableElements.get(zatom).get('symbol')
        new_struc.append_atom(position=pos, symbols=symbol)
        isite += 1

    return new_struc

new_struc = change_struc_imp_aux_wf(voro_calc.inputs.structure, imp_info)
```

Note: This functionality is alreadyincorporated in the kkr_imp_wc workflow.

Then we run the Voronoi calculation for auxiliary structure to create the impurity starting potential:

```
codename = 'voronoi@localhost'
code = Code.get_from_string(codename)

builder = code.get_builder()
builder.metadata.options = {'resources': {'num_machines':1, 'tot_num_mpiprocs':1}}
builder.structure = new_struc
builder.parameters = kkrcalc_converged.inputs.parameters

voro_calc_aux = submit(builder)
```

Now we create the impurity starting potential using the converged host potential for the surrounding of the impurity and the new Au impurity startpot:

```
from aiida_kkr.tools.common_workfunctions import neworder_potential_wf

potname_converged = kkrcalc_converged._POTENTIAL
potname_imp = 'potential_imp'
neworder_pot1 = [int(i) for i in loadtxt(GF_host_calc.outputs.retrieved.get_abs_path(
↪'scoef'), skiprows=1)[:,3]-1]
potname_impvorostart = voro_calc_aux._OUT_POTENTIAL_voronoi
```

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```
replacelist_pot2 = [[0,0]]

settings_dict = {'pot1': potname_converged,  'out_pot': potname_imp, 'neworder':␣
↪neworder_pot1,
                 'pot2': potname_impvorostart, 'replace_newpos': replacelist_pot2,
↪'label': 'startpot_KKRimp',
                 'description': 'starting potential for Au impurity in bulk Cu'}
settings = Dict(dict=settings_dict)

startpot_Au_imp_sfd = neworder_potential_wf(settings_node=settings,
                                            parent_calc_folder=kkrcalc_converged.
↪outputs.remote_folder,
                                            parent_calc_folder2=voro_calc_aux.outputs.
↪remote_folder)
```

Create and submit initial KKRimp calculation

Now we create a new impurity calculation, set all input nodes and submit the calculation to preconverge the impurity potential (Au embedded into Cu ulk host as described in the `impurity_info` node):

```
# needed to link to host GF writeout calculation
GF_host_output_folder = GF_host_calc.outputs.remote_folder

# create new KKRimp calculation
from aiida_kkr.calculations.kkrimp import KkrimpCalculation
kkrimp_calc = KkrimpCalculation()

builder = Code.get_from_string('KKRimp@my_mac')

builder.code(kkrimp_code)
builder.host_Greenfunction_folder = GF_host_output_folder
builder.impurity_potential = startpot_Au_imp_sfd
builder.resources = resources

# first set 20 simple mixing steps
kkrimp_params = kkrparams(params_type='kkrimp')
kkrimp_params.set_multiple_values(SCFSTEPS=20, IMIX=0, MIXFAC=0.05)
ParamsKKRimp = Dict(dict=kkrimp_params.get_dict())
bilder.parameters = ParamsKKRimp

# submit calculation
kkrimp_calc = submit(builder)
```

Restart KKRimp calculation from KKRimp parent

Here we demonstrate how to restart a KKRimp calculation from a parent calculation from which the starting potential is extracted autimatically. This is used to compute the converged impurity potential starting from the previous preconvergence step:

```
builder = kkrimp_code.get_builder()
builder.parent_calc_folder = kkrimp_calc.outputs.remote_folder
builder.metadata.options = {'resources': resources}
builder.host_Greenfunction_folder = kkrimp_calc.inputs.GFhost_folder
```

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```
kkrimp_params = kkrparams(params_type='kkrimp', **kkrimp_calc.inputs.parameters.get_
↪dict())
kkrimp_params.set_multiple_values(SCFSTEPS=99, IMIX=5, MIXFAC=0.05)
ParamsKKRimp = Dict(dict=kkrimp_params.get_dict())
builder.parameters = ParamsKKRimp

# submit
kkrimp_calc_converge = submit(builder)
```

Impurity DOS

create final imp DOS (new host GF for DOS contour, then KKRimp calc using converged potential)

first prepare host GF with DOS contour:

```
params = kkrparams(**GF_host_calc.inputs.parameters.get_dict())
params.set_multiple_values(EMIN=-0.2, EMAX=GF_host_calc.res.fermi_energy+0.1, NPOL=0,␣
↪NPT1=0, NPT2=101, NPT3=0)
ParaNode = Dict(dict=params.get_dict())

code = GF_host_calc.inputs.code # take the same code as in the calculation before
builder= code.new_calc()
resources = GF_host_calc.get_resources()
builder.resources = resources
builder.parameters = ParaNode
builder.parent_folder = kkr_converged_parent_folder
builder.impurity_info = GF_host_calc.inputs.impurity_info

GF_host_doscalc = submit(builder)
```

Then we run the KKRimp step using the converged potential (via the `parent_calc_folder` node) and the host GF which contains the DOS contour information (via `host_Greenfunction_folder`):

```
builder = kkrimp_calc_converge.inputs.code.get_builder()
builder.host_Greenfunction_folder(GF_host_doscalc.outputs.remote_folder)
builder.parent_calc_folder(kkrimp_calc_converge.outputs.remote_folder)
builder.resources(kkrimp_calc_converge.get_resources())

params = kkrparams(params_type='kkrimp', **kkrimp_calc_converge.inputs.parameters.get_
↪dict())
params.set_multiple_values(RUNFLAG=['lmdos'], SCFSTEPS=1)
ParaNode = Dict(dict=params.get_dict())

builder.parameters(ParaNode)

kkrimp_doscalc = submit(builder)
```

Finally we plot the DOS:

```
# get interpolated DOS from GF_host_doscalc calculation:
from masci_tools.io.common_functions import interpolate_dos
dospath_host = GF_host_doscalc.outputs.retrieved.get_abs_path('')
ef, dos, dos_interpol = interpolate_dos(dospath_host, return_original=True)
dos, dos_interpol = dos[0], dos_interpol[0]
```

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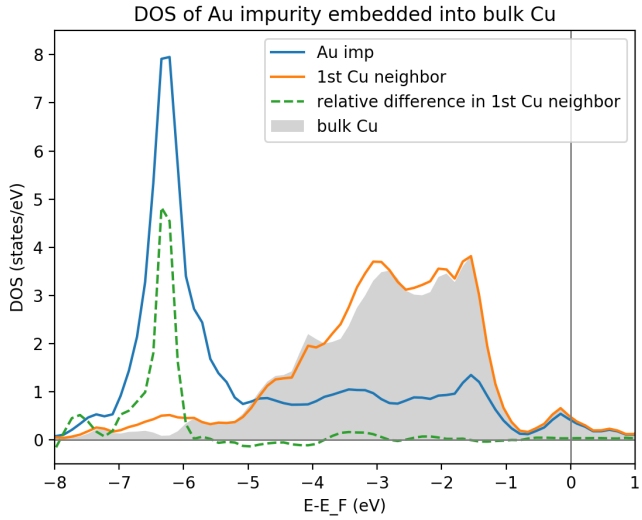
```
# read in impurity DOS
from numpy import loadtxt
impdos0 = loadtxt(kkrimp_doscalc.outputs.retrieved.get_abs_path('out_lmdos.interpol.
↪atom=01_spin1.dat'))
impdos1 = loadtxt(kkrimp_doscalc.outputs.retrieved.get_abs_path('out_lmdos.interpol.
↪atom=13_spin1.dat'))
# sum over spins:
impdos0[:,1:] = impdos0[:,1:]*2
impdos1[:,1:] = impdos1[:,1:]*2

# plot bulk and impurity DOS
from matplotlib.pyplot import figure, fill_between, plot, legend, title, axhline,␣
↪axvline, xlim, ylim, ylabel, xlabel, title, show
figure()
fill_between((dos_interpol[:,0]-ef)*13.6, dos_interpol[:,1]/13.6, color='lightgrey',␣
↪lw=0, label='bulk Cu')
plot((impdos0[:,0]-ef)*13.6, impdos0[:,1]/13.6, label='Au imp')
plot((impdos0[:,0]-ef)*13.6, impdos1[:,1]/13.6, label='1st Cu neighbor')
plot((impdos0[:,0]-ef)*13.6, (impdos1[:,1]-dos_interpol[:,1])/dos_interpol[:,1], '--',
↪ label='relative difference in 1st Cu neighbor')
legend()
title('DOS of Au impurity embedded into bulk Cu')
axhline(0, lw=1, color='grey')
axvline(0, lw=1, color='grey')
xlim(-8, 1)
ylim(-0.5,8.5)
xlabel('E-E_F (eV)')
ylabel('DOS (states/eV)')
show()
```

Which should look like this:



KKR calculation importer

Only functional in version below 1.0

Plugin `kkr.kkrimporter`

The calculation importer can be used to import a already finished KKR calculation to the aiida dbatabase. The KKRimporterCalculation takes the inputs

- `code`: KKR code installation on the computer from which the calculation is imported
- `computer`: computer on which the calulation has been performed
- `resources`: resources used in the calculation
- `remote_workdir`: remote abolute path on `computer` to the path where the calculation has been performed
- `input_file_names`: dictionary of input file names
- `output_file_names`, optional: dictionary of output file names

and mimicks a KKR calculation (i.e. stores KKR parameter set in node `parameters` and the extracted aiida StructureData node `structure` as inputs and creates `remote_folder`, `retrieved` and `output_parameters` output nodes). A KKRimporter calculation can then be used like a KKR claculation to continue calculations with correct provenance tracking in the database.

Note:

- At least `input_file` and `potential_file` need to be given in `input_file_names`.
- Works also if output was a Jij calculation, then `Jijatom.*` and `shells.dat` files are retreived as well.

Example on how to use the calculation importer:

```
# Load the KKRimporter class
from aiida.orm import CalculationFactory
KkrImporter = CalculationFactory('kkr.kkrimporter')

# Load the Code node representative of the one used to perform the calculations
from aiida.orm.code import Code
code = Code.get_from_string('KKRcode@my_mac')

# Get the Computer node representative of the one the calculations were run on
computer = code.get_remote_computer()

# Define the computation resources used for the calculations
resources = {'num_machines': 1, 'num_mpiprocs_per_machine': 1}

# Create calculation
calc1 = KkrImporter(computer=computer,
                    resources=resources,
                    remote_workdir='<absolute-remote-path-to-calculation>',
                    input_file_names={'input_file':'inputcard', 'potential_file':
↪'potential', 'shapefun_file':'shapefun'},
                    output_file_names={'out_potential_file':'potential'})

# Link the code that was used to run the calculations.
calc1.use_code(code)

# Get the computer's transport and create an instance.
from aiida.backends.utils import get_authinfo, get_automatic_user
authinfo = get_authinfo(computer=computer, aiidauser=get_automatic_user())
transport = authinfo.get_transport()
```

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```
# Open the transport for the duration of the immigrations, so it's not
# reopened for each one. This is best performed using the transport's
# context guard through the ``with`` statement.
with transport as open_transport:
    # Parse the calculations' input files to automatically generate and link the
    # calculations' input nodes.
    calc1.create_input_nodes(open_transport)

    # Store the calculations and their input nodes and tell the daeomon the output
    # is ready to be retrieved and parsed.
    calc1.prepare_for_retrieval_and_parsing(open_transport)
```

After the calculation has finished the following nodes should appear in the aiida database:

```
$ verdi calculation show <pk-to-imported-calculation>
-----------  ------------------------------------
type         KkrImporterCalculation
pk           22121
uuid         848c2185-8c82-44cd-ab67-213c20aaa414
label
description
ctime        2018-04-24 15:29:42.136154+00:00
mtime        2018-04-24 15:29:48.496421+00:00
computer     [1] my_mac
code         KKRcode
-----------  ------------------------------------
##### INPUTS:
Link label       PK  Type
------------  -----  -------------
parameters    22120  Dict
structure     22119  StructureData
##### OUTPUTS:
Link label            PK  Type
-----------------  -----  -------------
remote_folder      22122  RemoteData
retrieved          22123  FolderData
output_parameters  22124  Dict
##### LOGS:
There are 1 log messages for this calculation
Run 'verdi calculation logshow 22121' to see them
```

Example scripts

Here is a small collection of example scripts.

Scripts need to be updated for new version (>1.0)

Full example Voronoi-KKR-KKRimp

Compact script starting with structure setup, then voronoi calculation, followed by initial KKR claculation which is then continued for convergence. The converged calculation is then used to write out the host GF and a simple inmpurity calculation is performed.

Download: `this example script`

```
#!/usr/bin/env python

# connect to aiida db
from aiida import load_profile
load_profile()
# load essential aiida classes
from aiida.orm import Code
from aiida.orm import DataFactory
StructureData = DataFactory('structure')
Dict = DataFactory('parameter')

# load kkrparms class which is a useful tool to create the set of input parameters␣
↪for KKR-family of calculations
from aiida_kkr.tools.kkr_params import kkrparams

# load some python modules
from numpy import array

# helper function
def wait_for_it(calc, maxwait=300):
    from time import sleep
    N = 0
    print 'start waiting for calculation to finish'
    while not calc.has_finished() and N<(maxwait/2.):
        N += 1
        if N%5==0:
            print('.')
        sleep(2.)
    print('waiting done after {} seconds: {} {}'.format(N*2, calc.has_finished(),␣
↪calc.has_finished_ok()))


#####################################################
# initial structure
#####################################################

# create Copper bulk aiida Structure
alat = 3.61 # lattice constant in Angstroem
bravais = alat*array([[0.5, 0.5, 0], [0.5, 0, 0.5], [0, 0.5, 0.5]]) # Bravais matrix␣
↪in Ang. units
Cu = StructureData(cell=bravais)
Cu.append_atom(position=[0,0,0], symbols='Cu')


#####################################################
# Voronoi step (preparation of starting potential)
#####################################################

# create empty set of KKR parameters (LMAX cutoff etc. ) for voronoi code
params = kkrparams(params_type='voronoi')

# and set at least the mandatory parameters
params.set_multiple_values(LMAX=2, NSPIN=1, RCLUSTZ=2.3)

# finally create an aiida Dict node and fill with the dictionary of parameters
ParaNode = Dict(dict=params.get_dict())
```

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```
# choose a valid installation of the voronoi code
### !!! adapt to your code name !!! ###
codename = 'voronoi@my_mac'
code = Code.get_from_string(codename)

# create new instance of a VoronoiCalculation
voro_calc = code.new_calc()

# and set resources that will be used (here serial job)
voro_calc.set_resources({'num_machines':1, 'tot_num_mpiprocs':1})

### !!! use queue name if necessary !!! ###
# voro_calc.set_queue_name('<quene_name>')

# then set structure and input parameter
voro_calc.use_structure(Cu)
voro_calc.use_parameters(ParaNode)

# store all nodes and submit the calculation
voro_calc.store_all()
voro_calc.submit()

wait_for_it(voro_calc)

# for future reference
voronoi_calc_folder = voro_calc.outputs.remote_folder
voro_params = voro_calc.inputs.parameters


##################################################
# KKR step (20 iterations simple mixing)
##################################################

# create new set of parameters for a KKR calculation and fill with values from␣
↪previous voronoin calculation
params = kkrparams(params_type='kkr', **voro_params.get_dict())

# and set the missing values
params.set_multiple_values(RMAX=7., GMAX=65.)

# choose 20 simple mixing iterations first to preconverge potential (here 5% simple␣
↪mixing)
params.set_multiple_values(NSTEPS=20, IMIX=0, STRMIX=0.05)

# create aiida Dict node from the KKR parameters
ParaNode = Dict(dict=params.get_dict())

# get KKR code and create new calculation instance
### !!! use your code name !!! ###
code = Code.get_from_string('KKRcode@my_mac')
kkr_calc = code.new_calc()

# set input Parameter, parent calulation (previous voronoi calculation), computer␣
↪resources
kkr_calc.use_parameters(ParaNode)
kkr_calc.use_parent_folder(voronoi_calc_folder)
kkr_calc.set_resources({'num_machines': 1, 'num_mpiprocs_per_machine':1})
```

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```
### !!! use queue name if necessary !!! ###
# kkr_calc.set_queue_name('<quene_name>')

# store nodes and submit calculation
kkr_calc.store_all()
kkr_calc.submit()

# wait for calculation to finish
wait_for_it(kkr_calc)


##################################################
# 2nd KKR step (continued from previous KKR calc)
##################################################

# create new KKR calculation instance to continue KKR ontop of a previous KKR␣
↪calclation
kkr_calc_continued = code.new_calc()

# reuse old KKR parameters and update scf settings (default is NSTEPS=1, IMIX=0)
params.set_multiple_values(NSTEPS=50, IMIX=5)
# and create aiida Dict node
ParaNode = Dict(dict=params.get_dict())

# then set input nodes for calculation
kkr_calc_continued.use_code(code)
kkr_calc_continued.use_parameters(ParaNode)
kkr_calc_parent_folder = kkr_calc.outputs.remote_folder # parent remote folder of␣
↪previous calculation
kkr_calc_continued.use_parent_folder(kkr_calc_parent_folder)
kkr_calc_continued.set_resources({'num_machines': 1, 'num_mpiprocs_per_machine':1})

### !!! use queue name if necessary !!! ###
# kkr_calc_continued.set_queue_name('<quene_name>')

# store input nodes and submit calculation
kkr_calc_continued.store_all()
kkr_calc_continued.submit()

# wait for calculation to finish
wait_for_it(kkr_calc_continued)


##################################################
# writeout host GF (using converged calculation)
##################################################

# take remote folder of converged calculation to reuse setting and write out Green␣
↪function and tmat of the crystalline host system
kkr_converged_parent_folder = kkr_calc_continued.outputs.remote_folder

# extreact kkr calculation from parent calculation folder
kkrcalc_converged = kkr_converged_parent_folder.get_inputs()[0]

# extract parameters from parent calculation and update RUNOPT for KKRFLEX option
kkr_params_dict = kkrcalc_converged.inputs.parameters.get_dict()
```

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```
kkr_params_dict['RUNOPT'] = ['KKRFLEX']

# create aiida Dict node with set parameters that are updated compared to converged␣
↪parent kkr calculation
ParaNode = Dict(dict=kkr_params_dict)

# create new KKR calculation
code = kkrcalc_converged.get_code() # take the same code as in the calculation before
GF_host_calc= code.new_calc()

# set resources, Parameter Node and parent calculation
resources = kkrcalc_converged.get_resources()
GF_host_calc.set_resources(resources)
GF_host_calc.use_parameters(ParaNode)
GF_host_calc.use_parent_folder(kkr_converged_parent_folder)

### !!! use queue name if necessary !!! ###
# GF_host_calc.set_queue_name('<quene_name>')

# prepare impurity_info node containing the information about the impurity cluster
imp_info = Dict(dict={'Rcut':1.01, 'ilayer_center':0, 'Zimp':[79.]})
# set impurity info node to calculation
GF_host_calc.use_impurity_info(imp_info)

# store input nodes and submit calculation
GF_host_calc.store_all()
GF_host_calc.submit()

# wait for calculation to finish
wait_for_it(GF_host_calc)


#######################################################################
# KKRimp calculation (20 simple mixing iterations  for preconvergence)
#######################################################################

# first create impurity start pot using auxiliary voronoi calculation

# creation of the auxiliary styructure:
# use an aiida workfunction to keep track of the provenance
from aiida.work import workfunction as wf
@wf
def change_struc_imp_aux_wf(struc, imp_info): # Note: works for single imp at center␣
↪only!
    from aiida.common.constants import elements as PeriodicTableElements
    _atomic_numbers = {data['symbol']: num for num, data in PeriodicTableElements.
↪iteritems()}

    new_struc = StructureData(cell=struc.cell)
    isite = 0
    for site in struc.sites:
        sname = site.kind_name
        kind = struc.get_kind(sname)
        pos = site.position
        zatom = _atomic_numbers[kind.get_symbols_string()]
        if isite == imp_info.get_dict().get('ilayer_center'):
            zatom = imp_info.get_dict().get('Zimp')[0]
```

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```
        symbol = PeriodicTableElements.get(zatom).get('symbol')
        new_struc.append_atom(position=pos, symbols=symbol)
        isite += 1

    return new_struc

new_struc = change_struc_imp_aux_wf(voro_calc.inputs.structure, imp_info)

# then Voronoi calculation for auxiliary structure
### !!! use your code name !!! ###
codename = 'voronoi@my_mac'
code = Code.get_from_string(codename)
voro_calc_aux = code.new_calc()
voro_calc_aux.set_resources({'num_machines':1, 'tot_num_mpiprocs':1})
voro_calc_aux.use_structure(new_struc)
voro_calc_aux.use_parameters(kkrcalc_converged.inputs.parameters)
voro_calc_aux.store_all()
voro_calc_aux.submit()
### !!! use queue name if necessary !!! ###
# voro_calc_aux.set_queue_name('<quene_name>')

# wait for calculation to finish
wait_for_it(voro_calc_aux)

# then create impurity startpot using auxiliary voronoi calc and converged host␣
↪potential

from aiida_kkr.tools.common_workfunctions import neworder_potential_wf

potname_converged = kkrcalc_converged._POTENTIAL
potname_imp = 'potential_imp'
neworder_pot1 = [int(i) for i in loadtxt(GF_host_calc.outputs.retrieved.get_abs_path(
↪'scoef'), skiprows=1)[:,3]-1]
potname_impvorostart = voro_calc_aux._OUT_POTENTIAL_voronoi
replacelist_pot2 = [[0,0]]

settings_dict = {'pot1': potname_converged,  'out_pot': potname_imp, 'neworder':␣
↪neworder_pot1,
                 'pot2': potname_impvorostart, 'replace_newpos': replacelist_pot2,
↪'label': 'startpot_KKRimp',
                 'description': 'starting potential for Au impurity in bulk Cu'}
settings = Dict(dict=settings_dict)

startpot_Au_imp_sfd = neworder_potential_wf(settings_node=settings,
                                            parent_calc_folder=kkrcalc_converged.out.
↪remote_folder,
                                            parent_calc_folder2=voro_calc_aux.out.
↪remote_folder)

# now create KKRimp calculation and run first (some simple mixing steps) calculation

# needed to link to host GF writeout calculation
GF_host_output_folder = GF_host_calc.out.remote_folder

# create new KKRimp calculation
from aiida_kkr.calculations.kkrimp import KkrimpCalculation
kkrimp_calc = KkrimpCalculation()
```

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```
### !!! use your code name !!! ###
kkrimp_code = Code.get_from_string('KKRimp@my_mac')

kkrimp_calc.use_code(kkrimp_code)
kkrimp_calc.use_host_Greenfunction_folder(GF_host_output_folder)
kkrimp_calc.use_impurity_potential(startpot_Au_imp_sfd)
kkrimp_calc.set_resources(resources)
kkrimp_calc.set_computer(kkrimp_code.get_computer())

# first set 20 simple mixing steps
kkrimp_params = kkrparams(params_type='kkrimp')
kkrimp_params.set_multiple_values(SCFSTEPS=20, IMIX=0, MIXFAC=0.05)
ParamsKKRimp = Dict(dict=kkrimp_params.get_dict())
kkrimp_calc.use_parameters(ParamsKKRimp)

# store and submit
kkrimp_calc.store_all()
kkrimp_calc.submit()

# wait for calculation to finish
wait_for_it(kkrimp_calc)


#####################################################
# continued KKRimp calculation until convergence
#####################################################

kkrimp_calc_converge = kkrimp_code.new_calc()
kkrimp_calc_converge.use_parent_calc_folder(kkrimp_calc.out.remote_folder)
kkrimp_calc_converge.set_resources(resources)
kkrimp_calc_converge.use_host_Greenfunction_folder(kkrimp_calc.inputs.GFhost_folder)

kkrimp_params = kkrparams(params_type='kkrimp', **kkrimp_calc.inputs.parameters.get_
↪dict())
kkrimp_params.set_multiple_values(SCFSTEPS=99, IMIX=5, MIXFAC=0.05)
ParamsKKRimp = Dict(dict=kkrimp_params.get_dict())
kkrimp_calc_converge.use_parameters(ParamsKKRimp)

### !!! use queue name if necessary !!! ###
# kkrimp_calc_converge.set_queue_name('<quene_name>')

# store and submit
kkrimp_calc_converge.store_all()
kkrimp_calc_converge.submit()

wait_for_it(kkrimp_calc_converge)
```

KKRimp DOS (starting from converged parent KKRimp calculation)

Script running host GF step for DOS contour first before running KKRimp step and plotting.

Download: `this example script`

```
#!/usr/bin/env python

# connect to aiida db
from aiida import load_profile
load_profile()
# load essential aiida classes
from aiida.orm import DataFactory, load_node
Dict = DataFactory('parameter')


# some settings:
#DOS contour (in Ry units), emax=EF+dE_emax:
emin, dE_emax, npt = -0.2, 0.1, 101
# kkrimp parent (converged imp pot, needs to tbe a KKRimp calculation node)
kkrimp_calc_converge = load_node(25025)

# derived quantities:
GF_host_calc = kkrimp_calc_converge.inputs.GFhost_folder.inputs.remote_folder
kkr_converged_parent_folder = GF_host_calc.inputs.parent_calc_folder

# helper function
def wait_for_it(calc, maxwait=300):
    from time import sleep
    N = 0
    print 'start waiting for calculation to finish'
    while not calc.has_finished() and N<(maxwait/2.):
        N += 1
        if N%5==0:
            print('.')
        sleep(2.)
    print('waiting done after {} seconds: {} {}'.format(N*2, calc.has_finished(),␣
↪calc.has_finished_ok()))

################################################################################
↪##########

# first host GF with DOS contour
from aiida_kkr.tools.kkr_params import kkrparams
params = kkrparams(**GF_host_calc.inputs.parameters.get_dict())
params.set_multiple_values(EMIN=emin, EMAX=GF_host_calc.res.fermi_energy+dE_emax,␣
↪NPOL=0, NPT1=0, NPT2=npt, NPT3=0)
ParaNode = Dict(dict=params.get_dict())

code = GF_host_calc.get_code() # take the same code as in the calculation before
GF_host_doscalc= code.new_calc()
resources = GF_host_calc.get_resources()
GF_host_doscalc.set_resources(resources)
GF_host_doscalc.use_parameters(ParaNode)
GF_host_doscalc.use_parent_folder(kkr_converged_parent_folder)
GF_host_doscalc.use_impurity_info(GF_host_calc.inputs.impurity_info)

# store and submit
GF_host_doscalc.store_all()
GF_host_doscalc.submit()

# wait for calculation to finish
print 'host GF calc for DOS contour'
```

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```
wait_for_it(GF_host_doscalc)

# then KKRimp step using the converged potential

kkrimp_doscalc = kkrimp_calc_converge.get_code().new_calc()
kkrimp_doscalc.use_host_Greenfunction_folder(GF_host_doscalc.out.remote_folder)
kkrimp_doscalc.use_parent_calc_folder(kkrimp_calc_converge.out.remote_folder)
kkrimp_doscalc.set_resources(kkrimp_calc_converge.get_resources())

# set to DOS settings
params = kkrparams(params_type='kkrimp', **kkrimp_calc_converge.inputs.parameters.get_
↪dict())
params.set_multiple_values(RUNFLAG=['lmdos'], SCFSTEPS=1)
ParaNode = Dict(dict=params.get_dict())

kkrimp_doscalc.use_parameters(ParaNode)

# store and submit calculation
kkrimp_doscalc.store_all()
kkrimp_doscalc.submit()

# wait for calculation to finish

print 'KKRimp calc DOS'
wait_for_it(kkrimp_doscalc)

# Finally plot the DOS:

# get interpolated DOS from GF_host_doscalc calculation:
from masci_tools.io.common_functions import interpolate_dos
dospath_host = GF_host_doscalc.out.retrieved.get_abs_path('')
ef, dos, dos_interpol = interpolate_dos(dospath_host, return_original=True)
dos, dos_interpol = dos[0], dos_interpol[0]

# read in impurity DOS
from numpy import loadtxt
impdos0 = loadtxt(kkrimp_doscalc.out.retrieved.get_abs_path('out_lmdos.interpol.
↪atom=01_spin1.dat'))
impdos1 = loadtxt(kkrimp_doscalc.out.retrieved.get_abs_path('out_lmdos.interpol.
↪atom=13_spin1.dat'))
# sum over spins:
impdos0[:,1:] = impdos0[:,1:]*2
impdos1[:,1:] = impdos1[:,1:]*2

# plot bulk and impurity DOS
from matplotlib.pyplot import figure, fill_between, plot, legend, title, axhline,␣
↪axvline, xlim, ylim, ylabel, xlabel, title, show
figure()
fill_between((dos_interpol[:,0]-ef)*13.6, dos_interpol[:,1]/13.6, color='lightgrey',␣
↪lw=0, label='bulk Cu')
plot((impdos0[:,0]-ef)*13.6, impdos0[:,1]/13.6, label='Au imp')
plot((impdos0[:,0]-ef)*13.6, impdos1[:,1]/13.6, label='1st Cu neighbor')
plot((impdos0[:,0]-ef)*13.6, (impdos1[:,1]-dos_interpol[:,1])/dos_interpol[:,1], '--',
↪ label='relative difference in 1st Cu neighbor')
legend()
title('DOS of Au impurity embedded into bulk Cu')
axhline(0, lw=1, color='grey')
```

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```
axvline(0, lw=1, color='grey')
xlim(-8, 1)
ylim(-0.5,8.5)
xlabel('E-E_F (eV)')
ylabel('DOS (states/eV)')
show()
```

KKR bandstructure

Script running a bandstructure calculation for which first from the structure node the kpoints of the high-symmetry lines are extracted and afterwards the bandstructure (i.e. `qdos`) calculation is started. Finally the results are plotted together with the DOS data (taken from KKRimp DOS preparation step).

Download: `this example script`

```
#!/usr/bin/env python

# connect to aiida db
from aiida import load_profile
load_profile()
# load essential aiida classes
from aiida.orm import Code, DataFactory, load_node
StructureData = DataFactory('structure')
Dict = DataFactory('parameter')

# helper function:
def wait_for_it(calc, maxwait=300):
    from time import sleep
    N = 0
    print 'start waiting for calculation to finish'
    while not calc.has_finished() and N<(maxwait/2.):
        N += 1
        if N%5==0:
            print('.')
        sleep(2.)
    print('waiting done after {} seconds: {} {}'.format(N*2, calc.has_finished(),␣
↪calc.has_finished_ok()))


# some settings (parent calculations):

# converged KKR calculation (taken form bulk Cu KKR example)
kkr_calc_converged = load_node(24951)
# previous DOS calculation started from converged KKR calc (taken from KKRimp DOS␣
↪example, i.e. GF host calculation with DOS contour)
host_dos_calc = load_node(25030)


# generate kpoints for bandstructure calculation

from aiida_kkr.calculations.voro import VoronoiCalculation
struc, voro_parent = VoronoiCalculation.find_parent_structure(kkr_calc_converged.out.
↪remote_folder)

from aiida.tools.data.array.kpoints import get_explicit_kpoints_path
```

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```
kpts = get_explicit_kpoints_path(struc).get('explicit_kpoints')


# run bandstructure calculation

# create bandstructure calculation reusing old settings (including same computer and␣
↪resources in this example)
kkrcode = kkr_calc_converged.get_code()
kkrcalc = kkrcode.new_calc()
kkrcalc.use_kpoints(kpts) # pass kpoints as input
kkrcalc.use_parent_folder(kkr_calc_converged.out.remote_folder)
kkrcalc.set_resources(kkr_calc_converged.get_resources())
# change parameters to qdos settings (E range and number of points)
from aiida_kkr.tools.kkr_params import kkrparams
qdos_params = kkrparams(**kkr_calc_converged.inputs.parameters.get_dict()) # reuse␣
↪old settings
# reuse the same emin/emax settings as in DOS run (extracted from input parameter␣
↪node)
qdos_params.set_multiple_values(EMIN=host_dos_calc.inputs.parameters.get_dict().get(
↪'EMIN'),
                                EMAX=host_dos_calc.inputs.parameters.get_dict().get(
↪'EMAX'),
                                NPT2=100)
kkrcalc.use_parameters(Dict(dict=qdos_params.get_dict()))

# store and submit calculation
kkrcalc.store_all()
kkrcalc.submit()

wait_for_it(kkrcalc, maxwait=600)


# plot results

# extract kpoint labels
klbl = kpts.labels
# fix overlapping labels (nicer plotting)
tmp = klbl[2]
tmp = (tmp[0], '\n'+tmp[1]+' ')
klbl[2] = tmp
tmp = klbl[3]
tmp = (tmp[0], '  '+tmp[1])
klbl[3] = tmp

#plotting of bandstructure and previously calculated DOS data

# load DOS data
from masci_tools.io.common_functions import interpolate_dos
dospath_host = host_dos_calc.out.retrieved.get_abs_path('')
ef, dos, dos_interpol = interpolate_dos(dospath_host, return_original=True)
dos, dos_interpol = dos[0], dos_interpol[0]

# load qdos file and reshape
from numpy import loadtxt, sum, log
qdos_file = kkrcalc.out.retrieved.get_abs_path('qdos.01.1.dat')
q = loadtxt(qdos_file)
nepts = len(set(q[:,0]))
```

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```
data = q[:,5:].reshape(nepts, len(q)/nepts, -1)
e = (q[::len(q)/nepts, 0]-ef)*13.6

# plot bandstructure
from matplotlib.pyplot import figure, pcolormesh, show, xticks, ylabel, axhline,␣
↪axvline, gca, title, plot, ylim, xlabel, suptitle
figure(figsize=((8, 4.8)))
pcolormesh(range(len(q)/nepts), e, log(sum(abs(data), axis=2)), lw=0)
xticks([i[0] for i in klbl], [i[1] for i in klbl])
ylabel('E-E_F (eV)')
axhline(0, color='lightgrey', lw=1)
title('band structure')

# plot DOS on right hand side of bandstructure plot
axBand = gca()
from mpl_toolkits.axes_grid1 import make_axes_locatable
divider = make_axes_locatable(axBand)
axDOS = divider.append_axes("right", 1.2, pad=0.1, sharey=axBand)

plot(dos_interpol[:,1]/13.6, (dos_interpol[:,0]-ef)*13.6)

ylim(e.min(), e.max())

axhline(0, color='grey', lw=1)
axvline(0, color='grey', lw=1)

axDOS.yaxis.set_tick_params(labelleft=False, labelright=True, right=True, left=False)
xlabel('states/eV')

title('DOS')
suptitle(struc.get_formula(), fontsize=16)

show()
```

Workflows

This page can contain a short introduction to the workflows provided by `aiida-kkr`.

Density of states

The density of states (DOS) workflow `kkr_dos_wc` automatically sets the right parameters in the input of a KKR calculation to perform a DOS calculation. The specifics of the DOS energy contour are set via the `wf_parameters` input node which contains default values if no user input is given.

Note: The default values of the `wf_parameters` input node can be extraced using `kkr_dos_wc.get_wf_defaults()`.

Inputs:

- `kkr` (*aiida.orm.Code*): KKRcode using the `kkr.kkr` plugin
- `remote_data` (*RemoteData*): The remote folder of the (converged) calculation whose output potential is used as input for the DOS run

- `wf_parameters` (*ParameterData*, optional): Some settings of the workflow behavior (e.g. number of energy points in DOS contour etc.)
- `options` (*ParameterData*, optional): Some settings for the computer you want to use (e.g. *queue_name*, *use_mpi*, *resources*, ...)
- `label` (*str*, optional): Label of the workflow
- `description` (*str*, optional): Longer description of the workflow

Returns nodes:

- `dos_data` (*XyData*): The DOS data on the DOS energy contour (i.e. at some finite temperature)
- `dos_data_interpol` (*XyData*): The interpolated DOS from the line parallel to the real axis down onto the real axis
- `results_wf` (*ParameterData*): The output node of the workflow containing some information on the DOS run

---

Note: The *x* and *y* arrays of the `dos_data` output nodes can easily be accessed using:

```
x = dos_data_node.get_x()
y = dos_data_node.get_y()
```

where the returned list is of the form `[label, numpy-array-of-data, unit]` and the *y*-array contains entries for total DOS, s-, p-, d-, ..., and non-spherical contributions to the DOS, e.g.:

```
[(u'interpolated dos tot', array([[...]]), u'states/eV'),
 (u'interpolated dos s', array([[...]]), u'states/eV'),
 (u'interpolated dos p', array([[...]]), u'states/eV'),
 (u'interpolated dos d', array([[...]]), u'states/eV'),
 (u'interpolated dos ns', array([[...]]), u'states/eV')]
```

Note that the output data are 2D arrays containing the atom resolved DOS, i.e. the DOS values for all atoms in the unit cell.

Example Usage

We start by getting an installation of the KKRcode:

```
from aiida.orm import Code
kkrcode = Code.get_from_string('KKRcode@my_mac')
```

Next load the remote folder node of the previous calculation (here the *converged calculation of the Cu bulk test case*) from which we want to start the following DOS calculation:

```
# import old KKR remote folder
from aiida.orm import load_node
kkr_remote_folder = load_node(22852).out.remote_folder
```

Then we set some settings of the workflow parameters (this step is optional):

```
# create workflow settings
from aiida.orm import DataFactory
ParameterData = DataFactory('parameter')
```

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```
workflow_settings = ParameterData(dict={'dos_params':{'emax': 1, 'tempr': 200, 'emin
↪': -1,
                                                       'kmesh': [20, 20, 20], 'nepts':␣
↪81}})
```

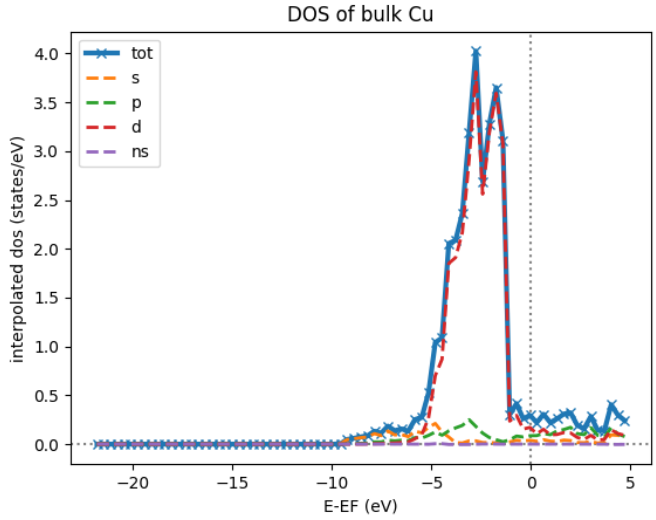
Finally we run the workflow:

```
from aiida_kkr.workflows.dos import kkr_dos_wc
from aiida.work import run
run(kkr_dos_wc, _label='test_doscal', _description='My test dos calculation.',
    kkr=kkrcode, remote_data=kkr_remote_folder, wf_parameters=workflow_settings)
```

The following script can be used to plot the total interpolated DOS (in the `dos_data_interpol` output node that can for example be access using `dos_data_interpol = <kkr_dos_wc-node>.out.dos_data_interpol` where `<kkr_dos_wc-node>` is the workflow node) of the calculation above:

```
def plot_dos(dos_data_node):
    x = dos_data_node.get_x()
    y_all = dos_data_node.get_y()

    from matplotlib.pylab import figure, xlabel, ylabel, axhline, axvline, plot,␣
↪legend, title

    figure()

    # loop over contributions (tot, s, p, d, ns)
    for y in y_all:
        if y==y_all[0]: # special line formatting for total DOS
            style = 'x-'
            lw = 3
        else:
            style = '--'
            lw = 2
        plot(x[1][0], y[1][0], style, lw=lw, ms=6, label=y[0].split('dos ')[1])

    # add axis labels etc
    xlabel(x[0]+' ({})'.format(x[-1]))
    ylabel(y[0].replace(' ns','')+' ({})'.format(y[-1]))
    axhline(0, color='grey', linestyle='dotted', zorder=-100)
    axvline(0, color='grey', linestyle='dotted', zorder=-100)
    legend(loc=2)
    title('DOS of bulk Cu')

plot_dos(dos_data_interpol)
```

which will produce the following plot:



Generate KKR start potential

Workflow: `kkr_startpot_wc`

Inputs:

- `structure` (*StructureData*):
- `voronoi` (*Code*):
- `kkr` (*Code*):
- `wf_parameters` (*ParameterData*, optional):
- `options` (*ParameterData*, optional): Some settings for the computer you want to use (e.g. *queue_name*, *use_mpi*, *resources*, ...)
- `calc_parameters` (*ParameterData*, optional):
- `label` (*str*, optional):
- `description` (*str*, optional):

Note: The default values of the `wf_parameters` input node can be extraced using `kkr_dos_wc.get_wf_defaults()` and it should contain the following entries:

General settings:

- `r_cls` (*float*):
- `natom_in_cls_min` (*int*):
- `fac_cls_increase` (*float*):
- `num_rerun` (*int*):

Computer settings:

- `walltime_sec` (*int*):
- `custom_scheduler_commands` (*str*):
- `use_mpi` (*bool*):

- `queue_name` (*str*):
- `resources` (*dict*): `{'num_machines': 1}`

Settings for DOS check of starting potential:

- `check_dos` (*bool*):
- `threshold_dos_zero` (*float*):
- `delta_e_min` (*float*):
- `delta_e_min_core_states` (*float*):
- **`dos_params` (*dict*): with the keys**
  - `emax` (*float*):
  - `tempr` (*float*):
  - `emin` (*float*):
  - `kmesh` ([*int*, *int*, *int*]):
  - `npts` (*int*):

Output nodes:

- `last_doscal_dosdata` (*XyData*):
- `last_doscal_dosdata_interpol` (*XyData*):
- `last_doscal_results` (*ParameterData*):
- `last_params_voronoi` (*ParameterData*):
- `last_voronoi_remote` (*RemoteData*):
- `last_voronoi_results` (*ParameterData*):
- `results_vorostart_wc` (*ParameterData*):

Example Usage

First load KKRcode and Voronoi codes:

```
from aiida.orm import Code
kkrcode = Code.get_from_string('KKRcode@my_mac')
vorocode = Code.get_from_string('voronoi@my_mac')
```

Then choose some settings for the KKR specific parameters (LMAX cutoff etc.):

```
from aiida_kkr.tools.kkr_params import kkrparams
kkr_settings = kkrparams(NSPIN=1, LMAX=2)
```

Now we create a structure node for the system we want to calculate:

```
# create Copper bulk aiida Structure
from aiida.orm import DataFactory
StructureData = DataFactory('structure')
alat = 3.61 # lattice constant in Angstroem
bravais = alat*array([[0.5, 0.5, 0], [0.5, 0, 0.5], [0, 0.5, 0.5]]) # Bravais matrix␣
↪in Ang. units
```

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```
Cu = StructureData(cell=bravais)
Cu.append_atom(position=[0,0,0], symbols='Cu')
```

Finally we run the `kkr_startpot_wc` workflow (here using the defaults for the workflow settings):

```
from aiida_kkr.workflows.voro_start import kkr_startpot_wc
from aiida.work import run
ParameterData = DataFactory('parameter')
run(kkr_startpot_wc, structure=Cu, voronoi=vorocode, kkr=kkrcode, calc_
↪parameters=ParameterData(dict=kkr_settings.get_dict()))
```

KKR scf cycle

Workflow: `kkr_scf_wc`

Inputs:

```
{'strmix': 0.03, 'brymix': 0.05, 'init_pos': None, 'convergence_criterion': 1e-08,
 'custom_scheduler_commands': '', 'convergence_setting_coarse': {'npol': 7, 'tempr':␣
↪1000.0,
                                                                 'n1': 3, 'n2': 11,
↪'n3': 3,
                                                                 'kmesh': [10, 10,␣
↪10]},
 'mixreduce': 0.5, 'mag_init': False, 'retreive_dos_data_scf_run': False,
 'dos_params': {'emax': 0.6, 'tempr': 200, 'nepts': 81, 'kmesh': [40, 40, 40], 'emin
↪': -1},
 'hfield': 0.02, 'queue_name': '', 'threshold_aggressive_mixing': 0.008,
 'convergence_setting_fine': {'npol': 5, 'tempr': 600.0, 'n1': 7, 'n2': 29, 'n3': 7,
                              'kmesh': [30, 30, 30]},
 'use_mpi': False, 'nsteps': 50, 'resources': {'num_machines': 1}, 'delta_e_min': 1.0,
 'walltime_sec': 3600, 'check_dos': True, 'threshold_switch_high_accuracy': 0.001,
 'kkr_runmax': 5, 'threshold_dos_zero': 0.001}

_WorkChainSpecInputs({'_label': None, '_description': None, '_store_provenance': True,
                      'dynamic': None, 'calc_parameters': None, 'kkr': None, 'voronoi
↪': None,
                      'remote_data': None, 'wf_parameters': <ParameterData: uuid:␣
↪b132dfc4-3b7c-42e7-af27-4083802aff40 (unstored)>,
                      'structure': None})
```

Outputs:

```
{'final_dosdata_interpol': <XyData: uuid: 0c14146d-90aa-4eb8-834d-74a706e500bb (pk:␣
↪22872)>,
 'last_InputParameters': <ParameterData: uuid: 28a277ad-8998-4728-8296-75fd3b0c4eb4␣
↪(pk: 22875)>,
 'last_RemoteData': <RemoteData: uuid: d24cdfc1-938a-4308-b273-e0aa8697c975 (pk:␣
↪22876)>,
 'last_calc_out': <ParameterData: uuid: 1c8fab2d-e596-4874-9516-c1387bf7db7c (pk:␣
↪22874)>,
 'output_kkr_scf_wc_ParameterResults': <ParameterData: uuid: 0f21ac18-e556-49f8-aa26-
↪55260d013fac (pk: 22878)>,
 'results_vorostart': <ParameterData: uuid: 93831550-8775-493a-907b-27a470b52dc8 (pk:␣
↪22877)>,
```

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```
 'starting_dosdata_interpol': <XyData: uuid: 54fa57ad-f559-4837-ba1e-7db4ed67d5b0␣
↪(pk: 22873)>}
```

Example Usage

Case 1: Start from previous calculation

```
from aiida.orm import Code
kkrcode = Code.get_from_string('KKRcode@my_mac')
vorocode = Code.get_from_string('voronoi@my_mac')
```

```
from aiida_kkr.tools.kkr_params import kkrparams
kkr_settings = kkrparams(NSPIN=1, LMAX=2)
```

```
from aiida.orm import load_node
kkr_startpot = load_node(22586)
last_vorono_remote = kkr_startpot.get_outputs_dict().get('last_voronoi_remote')
```

```
from aiida_kkr.workflows.kkr_scf import kkr_scf_wc
from aiida.work import run
ParameterData = DataFactory('parameter')
run(kkr_scf_wc, kkr=kkrcode, calc_parameters=ParameterData(dict=kkr_settings.get_
↪dict()), remote_data=last_vorono_remote)
```

Case 2: Start from structure and run voronoi calculation first

```
# create Copper bulk aiida Structure
fro numpy import array
from aiida.orm import DataFactory
StructureData = DataFactory('structure')
alat = 3.61 # lattice constant in Angstroem
bravais = alat*array([[0.5, 0.5, 0], [0.5, 0, 0.5], [0, 0.5, 0.5]]) # Bravais matrix␣
↪in Ang. units
Cu = StructureData(cell=bravais)
Cu.append_atom(position=[0,0,0], symbols='Cu')
```

```
run(kkr_scf_wc, structure=Cu, kkr=kkrcode, voronoi=vorocode, calc_
↪parameters=ParameterData(dict=kkr_settings.get_dict()))
```

KKR flex (GF calculation)

The Green's function writeout workflow performs a KKR calculation with runoption `KKRFLEX` to write out the `kkr_flexfiles`. Those are needed for a `kkrimp` calculation.

Inputs:

- `kkr` (*aiida.orm.Code*): KKRcode using the `kkr.kkr` plugin
- `remote_data` (*RemoteData*): The remote folder of the (converged) kkr calculation

- `imp_info` (*ParameterData*): ParameterData node containing the information of the desired impurities (needed to write out the `kkr_flexfiles` and the `scoef` file)
- `options` (*ParameterData*, optional): Some settings for the computer (e.g. computer settings)
- `wf_parameters` (*ParameterData*, optional): Some settings for the workflow behaviour
- `label` (*str*, optional): Label of the workflow
- `description` (*str*, optional): Longer description of the workflow

Returns nodes:

- `workflow_info` (*ParameterData*): Node containing general information about the workflow (e.g. errors, computer information, ...)
- `GF_host_remote` (*RemoteData*): RemoteFolder with all of the `kkrflexfiles` and further output of the workflow

Example Usage

We start by getting an installation of the KKRcode:

```
from aiida.orm import Code
kkrcode = Code.get_from_string('KKRcode@my_mac')
```

Next load the remote folder node of the previous calculation (here the *converged calculation of the Cu bulk test case*) from which we want to start the following KKRFLEX calculation:

```
# import old KKR remote folder
from aiida.orm import load_node
kkr_remote_folder = load_node(<pid of converged calc>).out.remote_folder
```

Afterwards, the information regarding the impurity has to be given (in this example, we use a Au impurity with a cutoff radius of 2 alat which is placed in the first labelled lattice point of the unit cell). Further keywords for the `impurity_info` node can be found in the respective part of the documentation:

```
# set up impurity info node
imps = ParameterData(dict={'ilayer_center':0, 'Rcut':2, 'Zimp':[79.]})
```

Then we set some settings of the options parameters (this step is optional):

```
# create workflow settings
from aiida.orm import DataFactory
ParameterData = DataFactory('parameter')
options = ParameterData(dict={'use_mpi':'false', 'queue_name':'viti_node', 'walltime_
↪sec' : 60*60*2,
                              'resources':{'num_machines':1, 'num_mpiprocs_
↪per_machine':1}})
```

Finally we run the workflow:

```
from aiida_kkr.workflows.gf_writeout import kkr_flex_wc
from aiida.work import run
run(kkr_flex_wc, label='test_gf_writeout', description='My test KKRflex calculation.',
    kkr=kkrcode, remote_data=kkr_remote_folder, options=options, wf_parameters=wf_
↪params)
```

KKR impurity self consistency

This workflow performs a KKRimp self consistency calculation starting from a given host-impurity startpotential and converges it.

Note: This workflow does only work for a non-magnetic calculation without spin-orbit-coupling. Those two features will be added at a later stage. This is also just a sub workflow, meaning that it only converges an already given host-impurity potential. The whole kkrimp workflow starting from scratch will also be added at a later stage.

Inputs:

- `kkrimp` (*aiida.orm.Code*): KKRimpcode using the `kkr.kkrimp` plugin
- `host_imp_startpot` (*SinglefileData*, optional): File containing the host impurity potential (potential file with the whole cluster with all host and impurity potentials)
- `remote_data` (*RemoteData*, optional): Output from a KKRflex calculation (can be extracted from the output of the GF writeout workflow)
- `kkrimp_remote` (*RemoteData*, optional): RemoteData output from previous kkrimp calculation (if given, `host_imp_startpot` is not needed as input)
- `impurity_info` (*ParameterData*, optional): Node containing information about the impurity cluster (has to be chosen consistently with `imp_info` from GF writeout step)
- `options` (*ParameterData*, optional): Some general settings for the workflow (e.g. computer settings, queue, ...)
- `wf_parameters` (*ParameterData*, optional) : Settings for the behavior of the workflow (e.g. convergence settings, physical properties, ...)
- `label` (*str*, optional): Label of the workflow
- `description` (*str*, optional): Longer description of the workflow

Returns nodes:

- `workflow_info` (*ParameterData*): Node containing general information about the workflow (e.g. errors, computer information, ...)
- `host_imp_pot` (*SinglefileData*): Converged host impurity potential that can be used for further calculations (DOS calc, new input for different KKRimp calculation)

Example Usage

We start by getting an installation of the KKRimpcode:

```
from aiida.orm import Code
kkrimpcode = Code.get_from_string('KKRimpcode@my_mac')
```

Next, either load the remote folder node of the previous calculation (here the KKRflex calculation that writes out the GF and KKRflexfiles) or the output node of the gf_writeout workflow from which we want to start the following KKRimp calculation:

```
# import old KKRFLEX remote folder
from aiida.orm import load_node
```

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```
GF_host_output_folder = load_node(<pid of KKRFLEX calc>).out.remote_folder # 1st␣
↪possibility
# GF_host_output_folder = load_node(<pid of gf_writeout wf output node>) # 2nd␣
↪possibility: take ``GF_host_remote`` output node from gf_writeout workflow
```

Now, load a converged calculation of the host system (here Cu bulk) as well as an auxiliary voronoi calculation (here Au) for the desired impurity:

```
# load converged KKRcalc
kkrcalc_converged = load_node(<pid of converged KKRcalc (Cu bulk)>)
# load auxiliary voronoi calculation
voro_calc_aux = load_node(<pid of voronoi calculation for the impurity (Au)>)
```

Using those, one can obtain the needed host-impurity potential that is needed as input for the workflow. Therefore, we use the `neworder_potential_wf` workfunction which is able to generate the startpot:

```
## load the neccessary function
from aiida_kkr.tools.common_workfunctions import neworder_potential_wf
import numpy as np

# extract the name of the converged host potential
potname_converged = kkrcalc_converged._POTENTIAL
# set the name for the potential of the desired impurity (here Au)
potname_imp = 'potential_imp'

neworder_pot1 = [int(i) for i in np.loadtxt(GF_host_calc.out.retrieved.get_abs_path(
↪'scoef'), skiprows=1)[:,3]-1]
potname_impvorostart = voro_calc_aux._OUT_POTENTIAL_voronoi
replacelist_pot2 = [[0,0]]

# set up settings node to use as argument for the neworder_potential function
settings_dict = {'pot1': potname_converged,  'out_pot': potname_imp, 'neworder':␣
↪neworder_pot1,
                 'pot2': potname_impvorostart, 'replace_newpos': replacelist_pot2,
↪'label': 'startpot_KKRimp',
                 'description': 'starting potential for Au impurity in bulk Cu'}
settings = ParameterData(dict=settings_dict)

# finally create the host-impurity potential (here ``startpot_Au_imp_sfd``) using the␣
↪settings node as well as
the previously loaded converged KKR calculation and auxiliary voronoi calculation:
startpot_Au_imp_sfd = neworder_potential_wf(settings_node=settings,
                                            parent_calc_folder=kkrcalc_converged.out.
↪remote_folder,
                                            parent_calc_folder2=voro_calc_aux.out.
↪remote_folder)
```

Note: Further information how the neworder potential function works can be found in the respective part of this documentation.

Afterwards, the information regarding the impurity has to be given (in this example, we use a Au impurity with a cutoff radius of 2 alat which is placed in the first labelled lattice point of the unit cell). Further keywords for the `impurity_info` node can be found in the respective part of the documentation:

```
# set up impurity info node
imps = ParameterData(dict={'ilayer_center':0, 'Rcut':2, 'Zimp':[79.]})
```

Then, we set some settings of the options parameters on the one hand and specific wf_parameters regarding the convergence etc.:

```
options = ParameterData(dict={'use_mpi':'false', 'queue_name':'viti_node', 'walltime_
↪sec' : 60*60*2,
                              'resources':{'num_machines':1, 'num_mpiprocs_per_machine
↪':20}})
kkrimp_params = ParameterData(dict={'nsteps': 50, 'convergence_criterion': 1*10**-8,
↪'strmix': 0.1,
                                    'threshold_aggressive_mixing': 3*10**-2,
↪'aggressive_mix': 3,
                                     'aggrmix': 0.1, 'kkr_runmax': 5})
```

Finally we run the workflow:

```
from aiida_kkr.workflows.kkr_imp_sub import kkr_imp_sub_wc
from aiida.work import run
run(kkr_imp_sub_wc, label='kkr_imp_sub test (CuAu)', description='test of the kkr_imp_
↪sub workflow for Cu, Au system',
    kkrimp=kkrimpcode, options=options, host_imp_startpot=startpot_Au_imp_sfd,
    remote_data=GF_host_output_folder, wf_parameters=kkrimp_params)
```

KKR impurity workflow

This workflow performs a KKR impurity calculation starting from an `impurity_info` node as well as either from a coverged calculation remote for the host system (1) or from a GF writeout remote (2). In the two cases the following is done:

- (1): First, the host system will be converged using the `kkr_scf` workflow. Then, the GF will be calculated using the `gf_writeout` workflow before calculating the auxiliary startpotential of the impurity. Now, the total impurity-host startpotential will be generated and then converged using the `kkr_imp_sub` workflow.
- (2): In this case the two first steps from above will be skipped and the workflow starts by calculating the auxiliary startpotential.

Note: This workflow is different from the `kkr_imp_sub` workflow that only converges a given impurity host potential. Here, the whole process of a KKR impurity calculation is done automatically.

Inputs:

- `kkrimp` (*aiida.orm.Code*): KKRimpcode using the `kkr.kkrimp` plugin
- `voronoi` (*aiida.orm.Code*): Voronoi code using the `kkr.voro` plugin
- `kkr` (*aiida.orm.Code*): KKRhost code using the `kkr.kkr` plugin
- `impurity_info` (*ParameterData*): Node containing information about the impurity cluster
- `remote_data_host` (*RemoteData*, optional): RemoteData of a converged host calculation if you want to start the workflow from scratch
- `remote_data_gf` (*RemoteData*, optional): RemoteData of a GF writeout step (if you want to skip the convergence of the host and the GF writeout step)

- `options` (*ParameterData*, optional): Some general settings for the workflow (e.g. computer settings, queue, ...)
- `wf_parameters` (*ParameterData*, optional) : Settings for the behavior of the workflow (e.g. convergence settings, physical properties, ...)
- `voro_aux_parameters` (*ParameterData*, optional): Settings for the usage of the `kkr_startpot` sub workflow needed for the auxiliary voronoi potentials
- `label` (*str*, optional): Label of the workflow
- `description` (*str*, optional): Longer description of the workflow

Returns nodes:

- `workflow_info` (*ParameterData*): Node containing general information about the workflow
- `last_calc_info` (*ParameterData*): Node containing information about the last used calculation of the workflow
- `last_calc_output_parameters` (*ParameterData*): Node with all of the output parameters from the last calculation of the workflow

Example Usage

We start by getting an installation of the codes:

```
from aiida.orm import Code
kkrimpcode = Code.get_from_string('KKRimpcode@my_mac')
kkrcode = Code.get_from_string('KKRcode@my_mac')
vorocode = Code.get_from_string('vorocode@my_mac')
```

Then, set up an appropriate `impurity_info` node for your calculation:

```
# set up impurity info node
imps = ParameterData(dict={'ilayer_center':0, 'Rcut':2, 'Zimp':[79.]})
```

Next, load either a `gf_writeout_remote` or a `converged_host_remote`:

```
from aiida.orm import load_node
gf_writeout_remote = load_node(<pid or uuid>)
converged_host_remote = load_node(<pid or uuid>)
```

Set up some more input parameter nodes for your workflow:

```
# node for general workflow options
options = ParameterData(dict={'use_mpi': False, 'walltime_sec' : 60*60*2,
                              'resources':{'num_machines':1, 'num_mpiprocs_per_machine
↪':1}})
# node for convergence behaviour of the workflow
kkrimp_params = ParameterData(dict={'nsteps': 99, 'convergence_criterion': 1*10**-8,
↪'strmix': 0.02,
                                    'threshold_aggressive_mixing': 8*10**-2,
↪'aggressive_mix': 3,
                                    'aggrmix': 0.04, 'kkr_runmax': 5, 'calc_orbmom':␣
↪False, 'spinorbit': False,
                                    'newsol': False, 'mag_init': False, 'hfield': [0.
↪05, 10],
                                    'non_spherical': 1, 'nspin': 2})
```

(continues on next page)

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```
# node for parameters needed for the auxiliary voronoi workflow
voro_aux_params = ParameterData(dict={'num_rerun' : 4, 'fac_cls_increase' : 1.5,
↪'check_dos': False,
                                      'lmax': 3, 'gmax': 65., 'rmax': 7., 'rclustz':␣
↪2.})
```

Finally, we run the workflow (for the two cases depicted above):

```
from aiida_kkr.workflows.kkr_scf import kkr_scf_wc
from aiida_kkr.workflows.voro_start import kkr_startpot_wc
from aiida_kkr.workflows.kkr_imp_sub import kkr_imp_sub_wc
from aiida_kkr.workflows.gf_writeout import kkr_flex_wc
from aiida_kkr.workflows.kkr_imp import kkr_imp_wc
from aiida.work.launch import run, submit

# don't forget to set a label and description for your workflow

# case (1)
wf_run = submit(kkr_imp_wc, label=label, description=description, voronoi=vorocode,␣
↪kkrimp=kkrimpcode,
                kkr=kkrcode, options=options, impurity_info=imps, wf_
↪parameters=kkrimp_params,
                voro_aux_parameters=voro_aux_params, remote_data_gf=gf_writeout_
↪remote)

# case (2)
wf_run = submit(kkr_imp_wc, label=label, description=description, voronoi=vorocode,␣
↪kkrimp=kkrimpcode,
                kkr=kkrcode, options=options, impurity_info=imps, wf_
↪parameters=kkrimp_params,
                voro_aux_parameters=voro_aux_params, remote_data_host=converged_host_
↪remote)
```

KKR impurity density of states

This workflow calculates the density of states for a given host impurity input potential.

Inputs:

- `kkrimp` (*aiida.orm.Code*): KKRimpcode using the `kkr.kkrimp` plugin
- `kkr` (*aiida.orm.Code*): KKRhost code using the `kkr.kkr` plugin
- `host_imp_pot` (*SinglefileData*): converged host impurity potential from impurity workflow
- `options` (*ParameterData*, optional): Some general settings for the workflow (e.g. computer settings, queue, . . .)
- `wf_parameters` (*ParameterData*, optional) : Settings for the behavior of the workflow (e.g. convergence settings, physical properties, . . .)
- `label` (*str*, optional): Label of the workflow
- `description` (*str*, optional): Longer description of the workflow

Returns nodes:

- `workflow_info` (*ParameterData*): Node containing general information about the workflow

- `last_calc_info` (*ParameterData*): Node containing information about the last used calculation of the workflow
- `last_calc_output_parameters` (*ParameterData*): Node with all of the output parameters from the last calculation of the workflow

Example Usage

We start by getting an installation of the codes:

```
from aiida.orm import Code
kkrimpcode = Code.get_from_string('KKRimpcode@my_mac')
vorocode = Code.get_from_string('vorocode@my_mac')
```

Next, load the converged host impurity potential:

```
from aiida.orm import load_node
startpot = load_node(<pid or uuid of SinglefileData>)
```

Set up some more input parameter nodes for your workflow:

```
# node for general workflow options
options = ParameterData(dict={'use_mpi': False, 'walltime_sec' : 60*60*2,
                              'resources':{'num_machines':1, 'num_mpiprocs_per_machine
↪':1}})
# node for convergence behaviour of the workflow
wf_params = ParameterData(dict={'ef_shift': 0. ,
                                'dos_params': {'nepts': 61,
                                               'tempr': 200,
                                               'emin': -1,
                                               'emax': 1,
                                               'kmesh': [30, 30, 30]},
                                'non_spherical': 1,
                                'born_iter': 2,
                                'init_pos' : None,
                                'newsol' : False})
```

Finally, we run the workflow (for the two cases depicted above):

```
from aiida_kkr.workflows.kkr_imp_dos import kkr_imp_dos_wc
from aiida.work.launch import run, submit

# don't forget to set a label and description for your workflow
wf_run = submit(kkr_imp_dos_wc, label=label, description=description,␣
↪kkrimp=kkrimpcode,
                kkrcode=kkrcode, options=options, wf_parameters=wf_params)
```

Equation of states

Workflow: `aiida_kkr.workflows.eos`

Warning: Not implemented yet!

Check KKR parameter convergence

Workflow: `aiida_kkr.workflows.check_para_convergence`

Warning: Not implemented yet!

Idea is to run checks after convergence for the following parameters:

- RMAX
- GMAX
- cluster radius
- energy contour
- kmesh

Find magnetic ground state

Workflow: `aiida_kkr.workflows.check_magnetic_state`

Warning: Not implemented yet!

The idea is to run a Jij calculation to estimate if the ferromagnetic state is the ground state or not. Then the unit cell could be doubled to compute the antiferromagnetic state. In case of noncollinear magnetism the full Jij tensor should be analyzed.

Workfunctions

Here the workfunctions provided by the aiida-kkr plugin are presented. The workfunctions are small tools useful for small tasks performed on aiida nodes that keep the provenance in the database.

update_params_wf

The workfunktion `aiida_kkr.tools.common_workfunctions.update_params_wf` takes as an input a *ParameterData* node (`parameternode`) containing a KKR parameter set (i.e. created using the `kkrparams` class) and updates the parameter node with new values given in the dictionary of the second *ParameterData* input node (`updatenode`).

Input nodes:

- `parameternode` (ParameterData): aiida node of a KKR parameter set
- `updatenode` (ParameterData): aiida node containing parameter names with new values

Output node:

- `updated_parameter_node` (ParameterData): new parameter node with updated values

---

Note: If the `updatenode` contains the keys `nodename` and/or `nodedesc` then the label and/or description of the output node will be set accordingly.

Example Usage:

```
# initial KKR parameter node
input_node = ParameterData(dict=kkrparams(LMAX=3, EMIN=0))
input_node.store()
# update some values (e.g. change EMIN)
updated_params = ParameterData(dict={'nodename': 'my_changed_name', 'nodedesc': 'My␣
↪description text', 'EMIN': -1, 'RMAX': 10.})
new_params_node = update_params_wf(input_node, updated_params)
```

neworder_potential_wf

The workfunction `aiida_kkr.tools.common_workfunctions.neworder_potential_wf` creates a *SingleFileData* node that contains the new potential based in a potential file in the *RemoteFolder* input node (`settings_node`) which is braught to a new order according to the workfunction settings in the *ParameterData* input node (`parent_calc_folder`).

Input nodes:

- `settings_node` (ParameterData): Settings like filenames and neworder-list
- `parent_calc_folder` (RemoteData): folder where initial potential file is found
- `parent_calc_folder2` (RemoteData, optional): folder where second potential is found

Output node:

- `potential_file` (SingleFileData): output potential in new order

Note:

The settings_dict should contain the following keys:

- `pot1`, mandatory: <*filename_input_potential*>
- `out_pot`, mandatory: <*filename_output_potential*>
- `neworder`, mandatory: *[list of intended order in output potential]*
- `pot2`, mandatory if `parent_calc_folder2` is given as input node: <*filename_second_input_file*>
- `replace_newpos`, mandatory if `parent_calc_folder2` is given as input node: *[[position in neworder list which is replace with potential from pot2, position in pot2 that is chosen for replacement]]*
- `label`, optional: *label_for_output_node*
- `description`, optional: *longer_description_for_output_node*

---

prepare_VCA_structure_wf

Warning: Not implemented yet!

prepare_2Dcalc_wf

Warning: Not implemented yet!

Tools

Here the tools provided by `aiida-kkr` are described.

Plotting tools

Visualize typical nodes using `plot_kkr` from `aiida_kkr.tools.plot_kkr`. The `plot_kkr` function takes a node reference (can be a pk, uuid or the node itself or a list of these) and creates common plots for a quick visualization of the results obtained with the `aiida-kkr` plugin.

Usage example:

```
from aiida_kkr.tools.plot_kkr import plot_kkr
# use pk:
plot_kkr(999999)
# use uuid:
plot_kkr('xxxxx-xxxxx')
# used actual aiida node:
from aiida.orm import load_node
plot_kkr(load_node(999999))
# give list of nodes which goups plots together
plot_kkr([999999, 999998, 'xxxx-xxxxx', load_node(999999)])
```

The behavior of `plot_kkr` can be controled using keyword arguments:

```
plot_kkr(99999, strucplot=False) # do not call ase`s view function to visualize␣
↪structure
plot_kkr(99999, silent=True) # plots only (no printout of inputs/outputs to node)
```

List of `plot_kkr` specific keyword arguments:

- `silent` (*bool*, default: `False`): print information about input node including inputs and outputs
- `strucplot` (*bool*, default: `True`): plot structure using ase's `view` function
- `interpol` (*bool*, default: `True`): use interpolated data for DOS plots
- `all_atoms` (*bool*, default: `False`): plot all atoms in DOS plots (default: plot total DOS only)
- `l_channels` (*bool*, default: `True`): plot l-channels in addition to total DOS
- `logscale` (*bool*, default: `True`): plot rms and charge neutrality curves on a log-scale

Other keyword arguments are passed onto plotting functions, e.g. to modify line properties etc. (see matplotlib documentation for a reference of possible keywords to modify line properties):

```
plot_kkr(99999, marker='o', color='r') # red lines with 'o' markers
```

Examples

Plot structure node

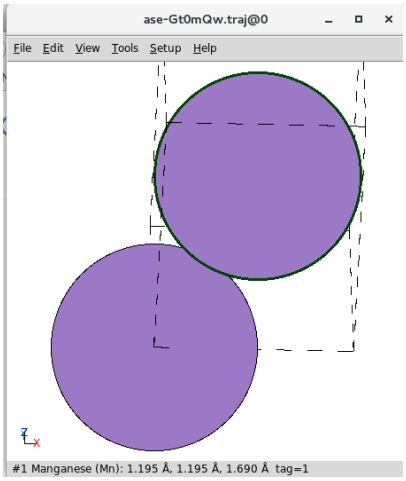

Fig. 1: Visualize a structure node (also happens as sub-parts of workflows that have a structure as input if `strucplot` is not set to `False`). Shown is a screenshot of the ouput produced by ase's `view`.

Plot output of a KKR calculation

Plot output of `kkr_dos_wc` workflow

Plot output of `kkr_startpot_wc` workflow

Plot output of `kkr_scf_wc` workflow

Plot output of `kkr_eos_wc` workflow

Plot multiple KKR calculations at once in the same plot

```
plot_kkr([34157,31962, 31974], silet=True, strucplot=False, logscale=False)
```

1.1.2 Modules provided with aiida-kkr (API reference)

1.1.2.1 Modules provided with aiida-kkr (API reference)

Calculations

Voronoi

KKRcode

KKRcode - calculation importer

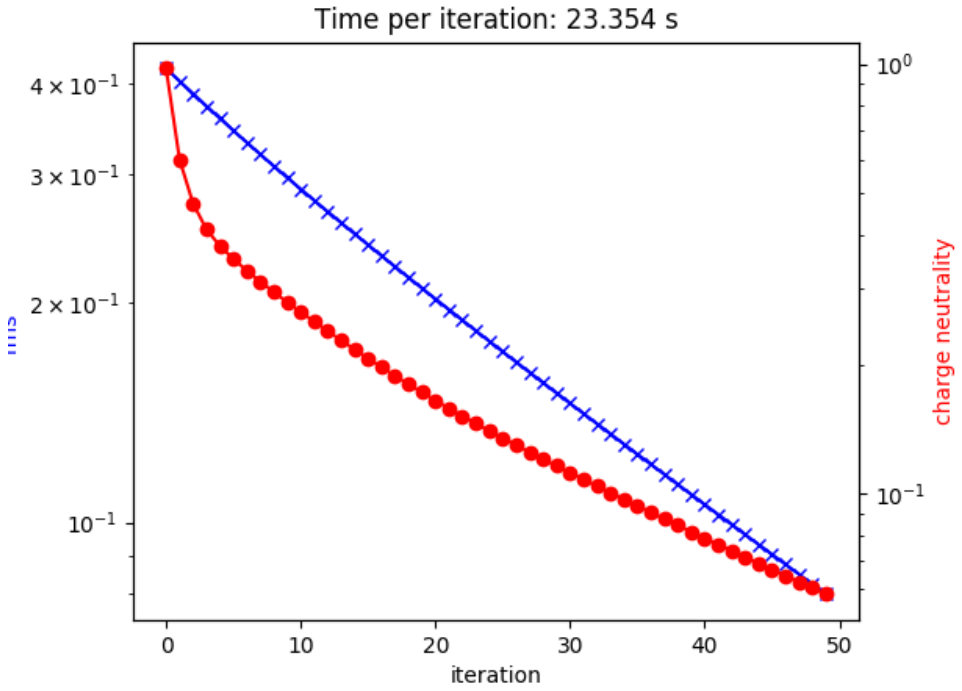

Fig. 2: Visualize the output of a `KkrCalculation`.

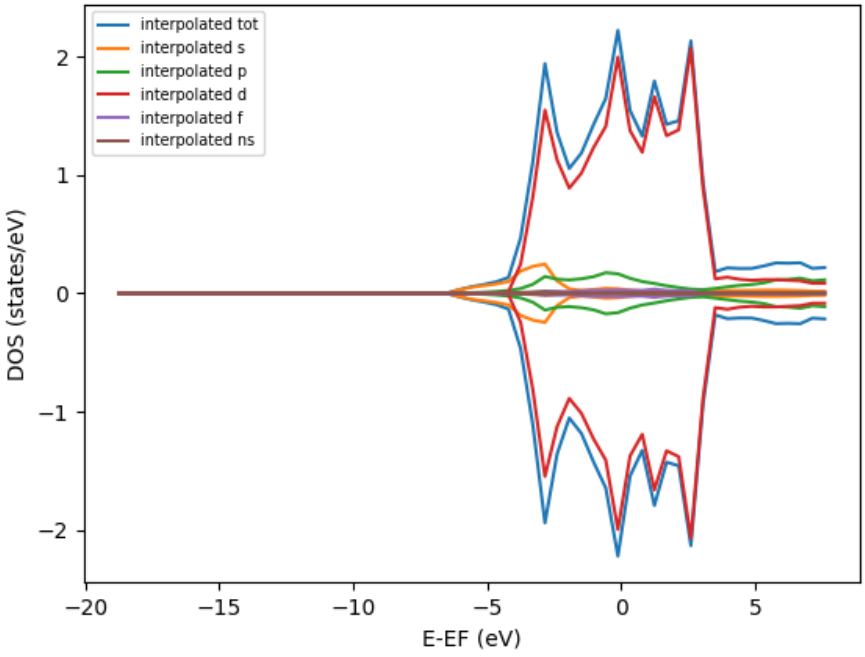

Fig. 3: Visualize the output of a `kkr_dos_wc` workflow.

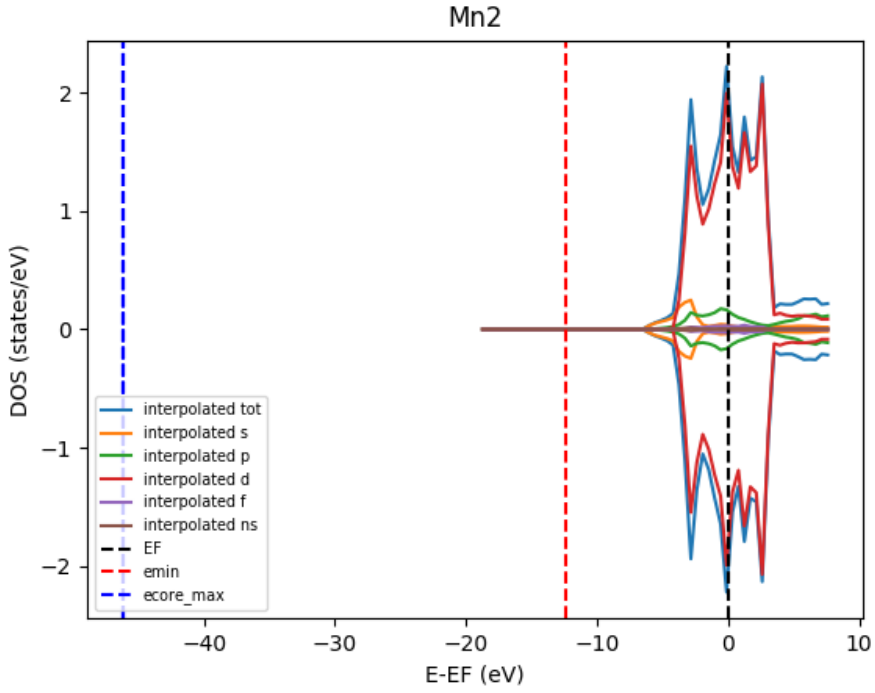

Fig. 4: Visualize the output of a `kkr_startpot_wc` workflow. The starting DOS is shown and the vertical lines indicate the position of the highest core states, the start of the ernergy contour and the Fermi level.

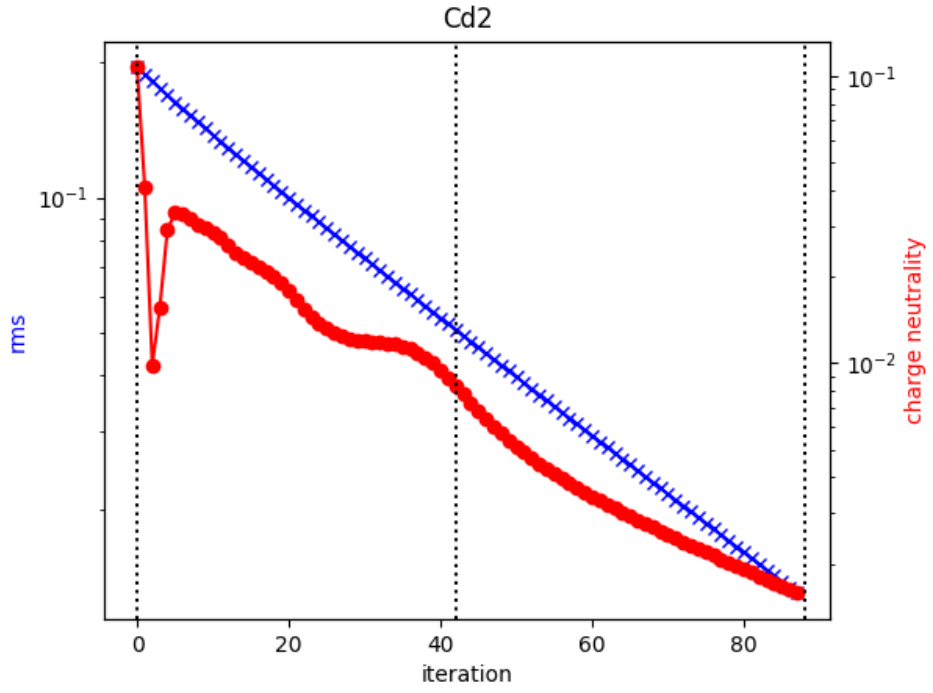

Fig. 5: Visualize the output of an unfinished `kkr_scf_wc` workflow. The vertical lines indicate where individual calculations have started and ended.

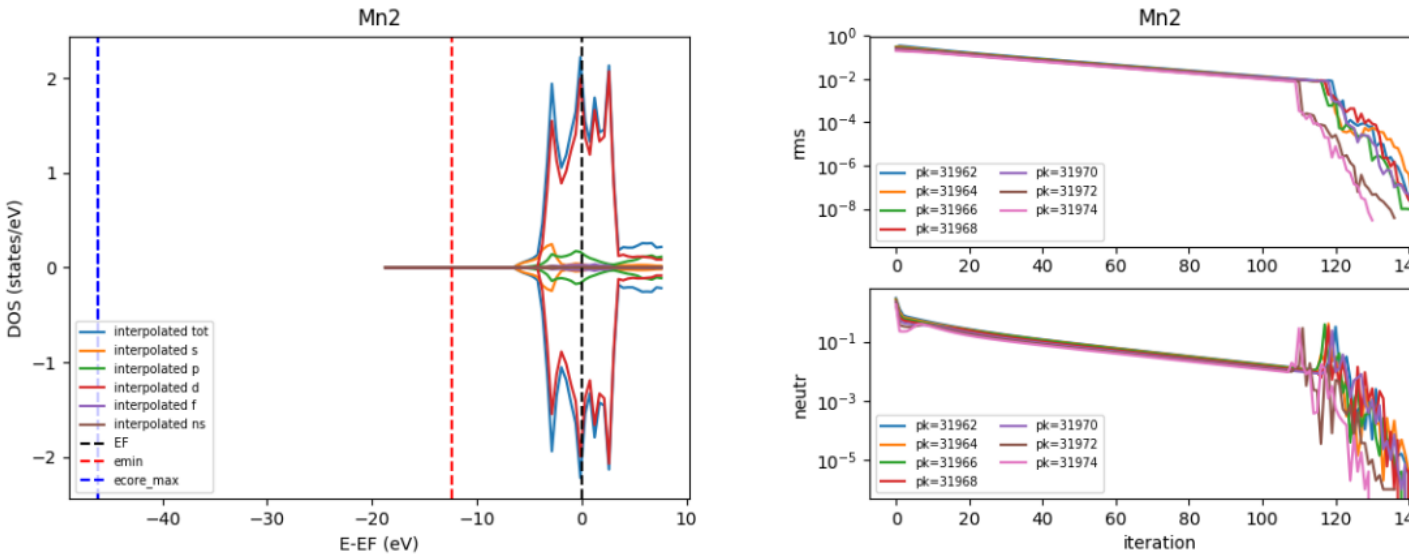

Fig. 6: Visualize the output of a `kkr_eos_wc` workflow.

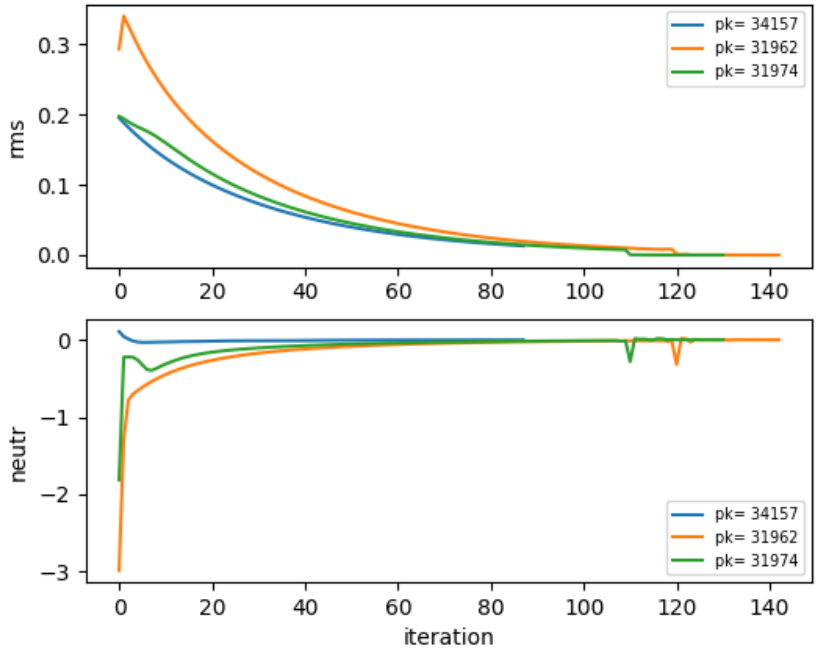

Fig. 7: Visualize the output of multiple `kkr_scf_wc` workflows without plotting structure.

KKRimp

Workflows

This section describes the aiida-kkr workflows.

Generate KKR start potential

KKR scf cycle

Density of states

Equation of states

Check KKR parameter convergence

Find magnetic ground state

Find Green Function writeout for KKRimp

KKRimp self-consistency

KKRimp complete calculation

Calculation parsers

This section describes the different parsers classes for calculations.

Voronoi Parser

KKRcode Parser

KKRcode - calculation importer Parser

KKRimp Parser

Voronoi Parser

Tools

Here the tools provided by `aiida_kkr` are described.

Common (work)functions that need aiida

KKRimp tools

Plotting tools

CHAPTER 2

Indices and tables

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- modindex
- search