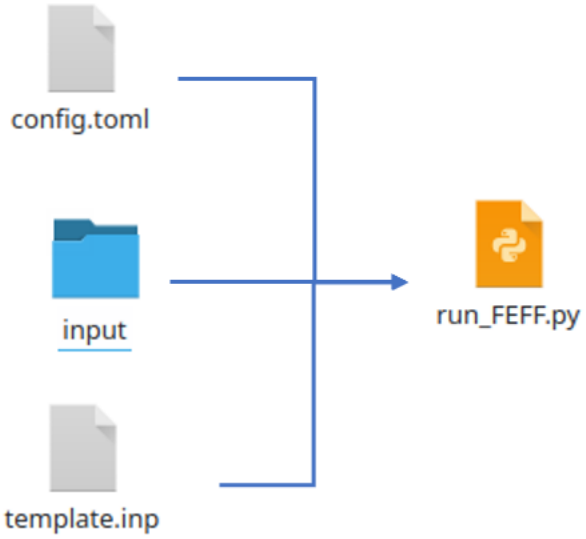
DOCUMENT of Multi-task FEFF calculation

1. The required files



Config.toml contains the configurations of this calculation.

```
template_dir = "template.inp"
#scratch = "/gpfs/scratch/kaifzheng/FEFF"
scratch = "/data/scratch/kz/FEFF"
CA = "Ni"
radius = 14
mode = "mpi_seq"
cores = 2
tasks = 10
site = [0]
pos_filename = ""
average = true
file_type="*.xyz"
symmetry=true
site_rule="""site=int(readfiles.split('.')[0].split('site_')[1])"""
```

Template_dir: the location of feff.inp template
Scratch: the location of scratch folder
CA: absorbing atom
Radius: the size of particle for calculating spectrum. For non-periodic samples(nanoparticles), the value requires to be large enough to cover all atoms of the particle or the distance where is enough to calculate stable spectrum.
Mode: the calculation mode, there are 4 different modes: mpi_seq,mpi_multi,seq_seq, and seq_multi. **The _seq** means the program will calculate spectrum for different site or sample one by one. _multi means the program will calculate the spectrum in a batch, the size of batch is defined by tasks.

Cores: the number of cpus for mpirun
Tasks: number of tasks run simultaneously.
Site: the site we are trying to calculate(still under developed)
File_type: the input file type, can be *.xyz,*.POSCAR, *.cif
Symmetry: True means the calculation will find inequivalent sites by point group(only work for molecule—xyz file)
Site_rule: This is a paragraph of python program to define how to get the site index, which will execute in the python program by exec(). For example, if you want to use site in config.toml, you can write: site_rule=""""site=site[0]""""(I delete it for now, it may come later.)

2. How to run

2.1 use module

cd /home/ames/module

module use FEFF10

module load 10

Then, you can run feff: **feffmpi** 8 #8 cores

Or: **feff** #seq run

2.2 write input files

Go to `/home/ames/kzheng/FEFF_works/test`

```
python run_FEFF.py -h
```

```
calculation configuration

optional arguments:
  -h, --help        show this help message and exit
  -w, --write_file  write FEFF input file
  -r, --run_file    run FEFF calculation
```

The python script has two arguments: -w and -r

If run `python run_FEFF.py -w,` the program will write feff input files(if symmetry=True, it will write input files for inequivalent sites) automatically to a new folder called FEFF_inp.

2.3 run FEFF

To run FEFF correctly, first needs to check template.inp, and then check config.toml.
Then run it `python  run_FEFF.py -r`
The results will be stored in json file separately in output folder.

output

Note: Sometimes cluster cannot finish all calculations, you may need to restart it, then you need to change config.toml file:
restart=true
In other case, keep restart=false

3. **A small test on 55-atom Ni particle**
`(/home/ames/kzheng/FEFF_works/test)`
For multi-task computing, I used 2 cores for mpi, and the maximum number of tasks can be submitted is 10, but we only have 5 tasks in this case, so it will submit all tasks simutanously.

```
mode = "mpi_multi"
cores = 2
tasks = 10
```

In this case, it takes

```
End in 3.089505743980408 min
```

For single-task computing(one by one)
The value of tasks is not matter.

```
mode = "mpi_seq"
cores = 2
```

It takes 9 minutes for all 5 tasks finished.

```
End in 9.40652873913447 min
```