**Siesta+DMFT User Manual**

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As of now we are only able to run self consistent calculations within DMFT. We would hope to have self consistency with both DFT+DMFT for siesta eventually.

First, setup the DMFT framework as you would for vasp+DMFT.   
I created a documentation for that which is available here:

<https://github.com/uthpalah/DMFTwDFT/blob/master/Documentation/DFTDMFT_code.ipynb>

Steps for DMFT calculations with siesta  
  
I am assuming you have siesta already. If not get it from here.

https://launchpad.net/siesta

Let’s take the example case of SrVO3 for this procedure.

We would be working in /siestaDMFT/runs/SrVO3 directory.

1. Initially, run siesta to find the Fermi energy and the Total energy. We need this for the DMFT calculation.

For this initial run, you may comment out the wannier blocks in your .fdf file.

**siesta<SrVO3.fdf>SrVO3.out**

Read SrVO3.out and find something similar to the following towards the end of the file:

**Total = -2318.571072**

**Fermi = -6.491889**

Save Fermi energy in **DFT\_mu.out** and Total energy in **siesta\_ETOT.**

Once we have self consistency in siesta+DMFT, these files would be automatically updated with each DFT+DMFT iteration.

2. Modify the .win file required for the wannier projections.

The DMFT code calculates the required wannier projections for the material you use as your input in INPUT.py and writes it in SrVO3.win. However, siesta+wannier90 does not write the unit\_cell\_cart, atoms\_cart, mp\_grid or kpoints blocks in this file. It would be quite easy to automate writing this since we could get all this information from the siesta input file and even generate a kmesh grid from the kmesh.pl utility provided with wannier90. But for now we will use the provided SrVO3.win.

3. Run **RUNDMFT\_siesta.py**

Don’t forget to include the path to your DMFT bin directory at the top of this file. For example:

**sys.path.insert(0,"/home/uthpala/projects/DMFT/bin/")**

You might also have to add the environmental variable WIEN\_DMFT\_ROOT in your .bashrc which points to your DMFT bin directory if you haven’t already. For example:

**export WIEN\_DMFT\_ROOT="/home/uthpala/projects/DMFT/bin/"**

Make the modifications in **INPUT.py** as you would for a vasp+DMFT run.

To enable parallelization, modify the line **para\_com="mpirun -np 4"** in RUNDMFT\_siesta.py. Otherwise leave it blank.

Finally run the program:  
  
**python RUNDMFT\_siesta.py**

Note that this works for python2 and not python3.