SIESTA POSTPROCESSING

An overview.

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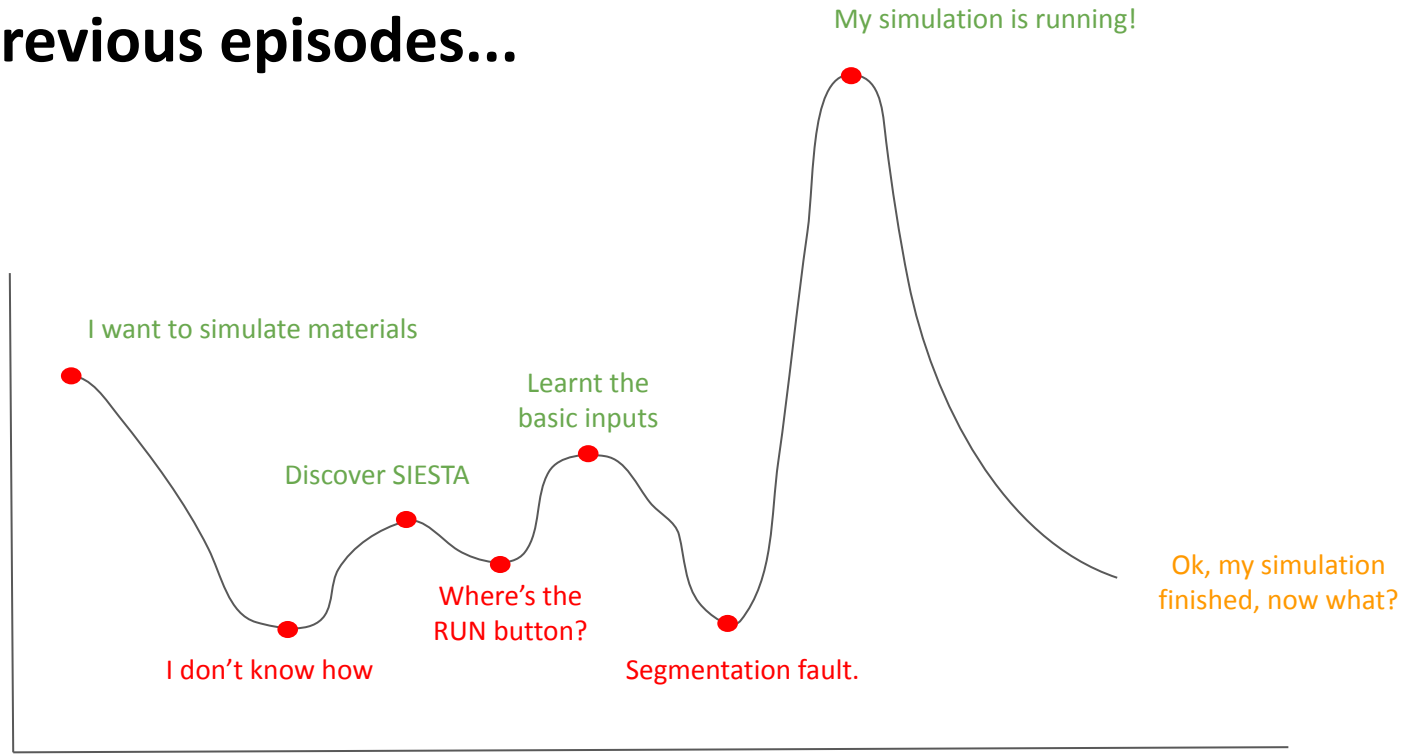
In previous episodes...



What can I analyze?

- Bands
- Fatbands
- Density of States
- Projected density of states
- Local density of states/STM
- Wavefunctions
- Electronic density
- Potential profiles
- Partial charges
- COOP/COHP
- ...

The list is endless...

Where are the tools?

Fortran utils

```
(base) pfebrer@pfebrer-P65-Creator-8SE:~/siesta$ cd Util/
(base) pfebrer@pfebrer-P65-Creator-8SE:~/siesta/Util$ ls
Bands          COPYING        Grimme       MPI_test    Projections       Sockets
build_all.sh   Denchar        Helpers      ON          PyAtom            SpPivot
clean_all.sh   DensityMatrix  HSX          Optical     README            STM
CMLComp        dep_all.sh     JobList      Optimizer   SCF               TS
Contour        Eig2DOS        Macroave     pdosxml     Scripting         VCA
Contrib        Gen-basis      MD           PEXSI       sies2arc          Vibra
COOP           Grid           MM_Examples  Plrho       SiestaSubroutine  WFS
```

execute to install (after SIESTA compilation)

Sisl (python package)

```
:~$ pip install sisl
```

or if you are using conda

```
:~$ conda install sisl
```

In general, there's more than one way to get the same analysis

How do I use them?

Fortran utils

There's either a *README* or a *.tex* file in each util's directory.

```
(base) pfebrer@pfebrer-P65-Creator-8SE:~/siesta/Util/Denchar/Docs$ ls
CHANGES  denchar.tex  README
```

From the *.tex* file you can get a *pdf* of the documentation:

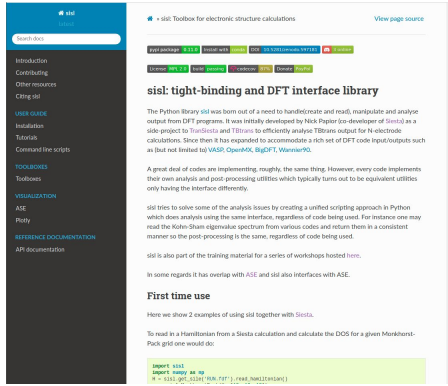
```
:~/siesta/Util/Denchar/Docs$ pdflatex denchar.tex
```

```
(base) pfebrer@pfebrer-P65-Creator-8SE:~/siesta/Util/Denchar/Docs$ ls
CHANGES      denchar.log  denchar.tex  README
denchar.aux  denchar.pdf  denchar.toc
```

Very well explained tutorials:
https://personales.unican.es/junqueraj/JavierJunquera_files/Metodos/Full-STO/Full-STO.html

Sisl

https://zerothi.github.io/sisl/docs/latest/index.html



Some tutorials:
https://github.com/zerothi/ts-tbt-sisl-tutorial

Number 1 advice: **PLAN in advance**

Output files can get VERY big

SIESTA ouputs information on demand

Always better to know what you need.

READ SIESTA'S USER GUIDE AND EACH TOOL'S DOCUMENTATION!

Hamiltonian:

```
TS.HS.Save t
```

Potentials/density:

```
SaveTotalPotential t
SaveRho t
```

Bands:

```
%block BandLines
  1 1.000 1.000 1.000 L
  20 0.000 0.000 0.000 \Gamma
%endblock BandLines
```

PDOS:

```
%block ProjectedDensityOfStates
  -20.00 10.00 0.200 500 eV
%endblock ProjectedDensityOfStates
```

Charges:

```
WriteHirshfeldPop t
```

SIESTA outputs

Unformatted files

You need scripts to read them.

- Hamiltonian and overlap (.HSX or .TSHS)
- Density matrix (.DM or .TSDE)
- Real space grids (.RHO, .VT, .LDOS...)
- Wavefunction files (.WFSX)
- ...

Formatted files

They are human-readable.
(often better to use scripts anyway)

- Main output
- Structures (.xyz, .XV, .STRUCT_OUT...)
- Forces (.FA)
- Density of states (.DOS, .PDOS...)
- Bands (.bands)
- ...

Real space grids: Understanding them

They are **evenly spaced 3d meshes** of a certain quantity inside the unit cell.

Input flag	Without netcdf support	With netcdf support
SaveRho	SystemLabel.RHO	Rho.grid.nc
SaveTotalPotential	SystemLabel.VT	TotalPotential.grid.nc
...	...	...

Softwares such as VESTA or XCrysDen can help you visualize these grids,
but first they need to be **converted to a format they understand**.

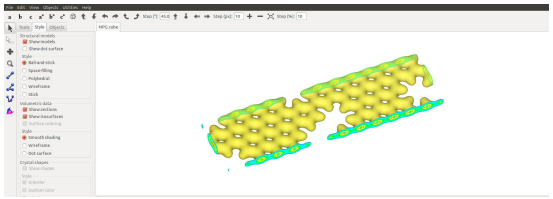
Real space grids: Visualizing them.

Util/Grid: *grid2cube* (docs in grid2cube.f)

Sisl:

```
:~$ sgrid SystemLabel.RHO SystemLabel.cube
```

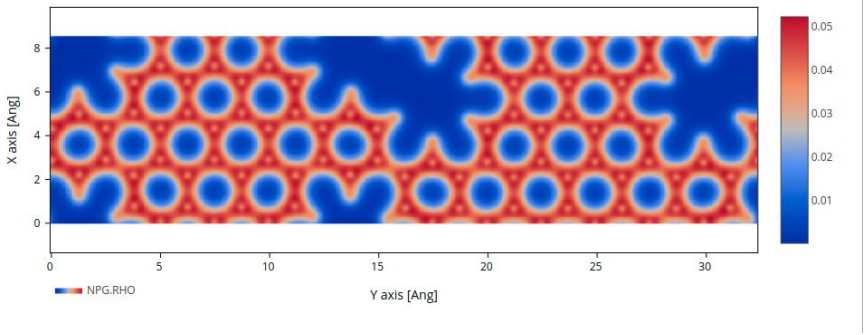
VESTA or XCrysDen



Visualize directly with sisl:

(you can also process the grid)

```
In [5]: sisl.get_sile("SystemLabel.RHO").plot(axes=[1,0])
```



An example: **Charge density**