Basic Fleur workflows

Apr 12, 2021 | **Gregor Michalicek** | Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

MAX DRIVING THE EXASCALE TRANSITION

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Outline

- Invoking Fleur
- Reaching self-consistency
- Calculating a band structure
- Calculating a density of states

g.michalicek@fz-juelich.de

Invoking Fleur

- Fleur uses different parallelization schemes: MPI and OpenMP
- OpenMP parallelization can be controlled by setting the OMP_NUM_THREADS environment variable, e.g.,
  - export OMP_NUM_THREADS=3
- Invoking Fleur without MPI parallelization
  - call **fleur** or **fleur_MPI**
- Invoking Fleur with MPI parallelization
  - call **mpirun -np 2 fleur_MPI**
  - MPI command depends on the machine: Also **srun** or **mpiexec**.
- On supercomputers the parallelization is partially controlled by the jobscript.
- More details on the parallelization schemes in Fleur in separate talk by Uliana Alekseeva.

g.michalicek@fz-juelich.de

Reaching self-consistency

Sometimes running Fleur does not yield well-behaved progress in the convergence process

```
Iteration:           1  Distance:   11.625649453388078
Iteration:           2  Distance:   9.3735022175314953
Iteration:           3  Distance:   9.4073604146575747
Iteration:           4  Distance:   5.1871680279159609
Iteration:           5  Distance:   5.3222708799839786
Iteration:           6  Distance:   5.5609892143282025
Iteration:           7  Distance:   5.9511958373075702
Iteration:           8  Distance:   5.9622832176342566
Iteration:           9  Distance:   5.7344112384776889
Iteration:          10  Distance:   9.3641887701414674

****************************************
Run finished successfully
Stop message:
  all done
****************************************
```


g.michalicek@fz-juelich.de

Reaching self-consistency

Sometimes running Fleur does not yield well-behaved progress in the convergence process

Options in such a case:

- Continue calculation by invoking Fleur again
- Delete mixing_history files, then continue the calculation.
- Delete mixing_history files, change scfLoop parameters to a more defensive setup, then continue the calculation.
- Check output files on hints what went wrong.
  - There may be a problem in the setup.
  - There may be a ghost states.
  - Are the electrons where they are supposed to be?
  - If problem is found fix input and start over again.
- For large unit cells the usage of the preconditioner may help.
  - See Fleur documentation and article by Miriam Winkelmann et al. (Phys. Rev. B **102**, 195138 (2020))

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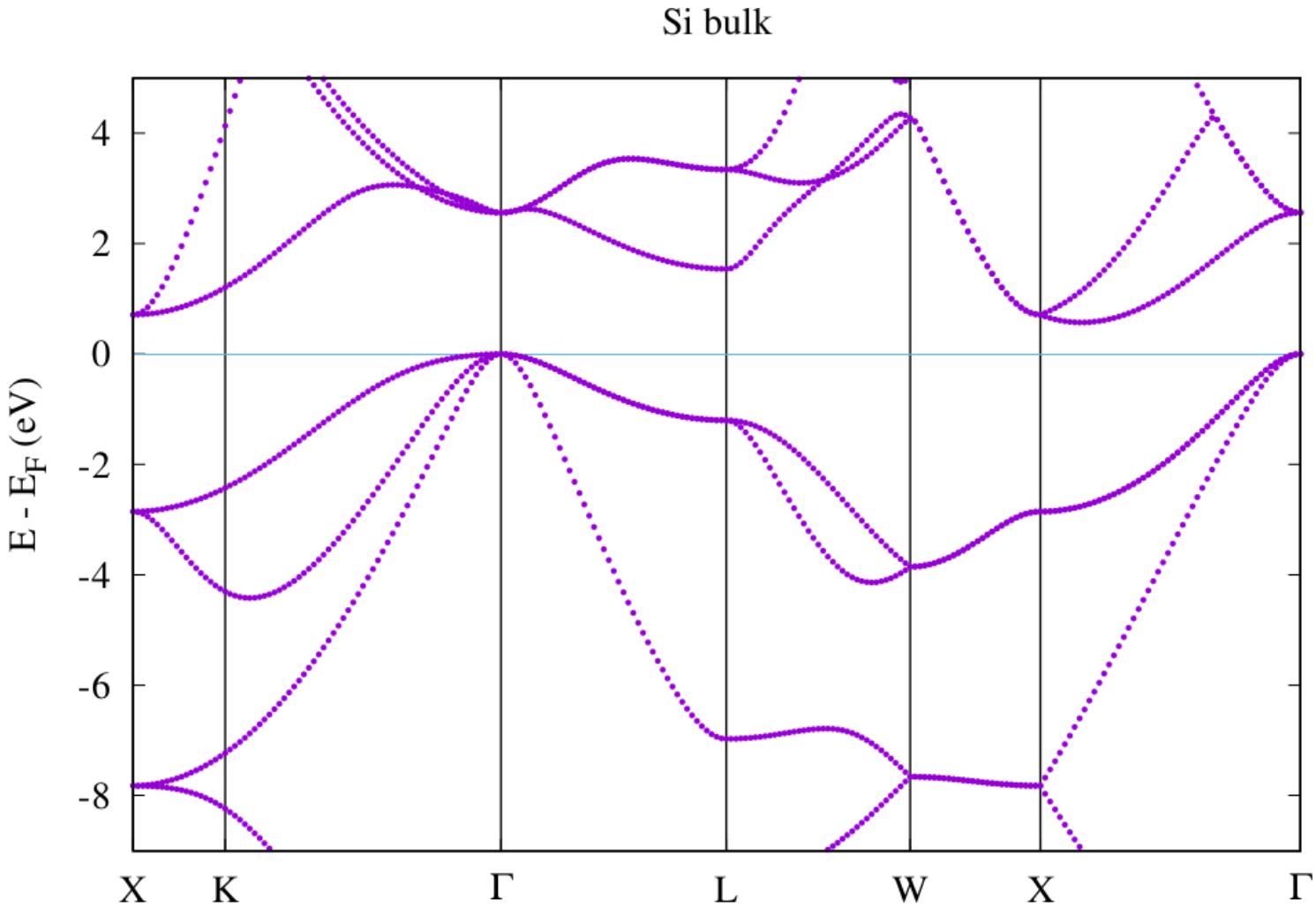
Band structure calculations

1. Reach self-consistency.
2. Select an adequate k-point path in the inp.xml file.
   - For most unit cells there is a default k-point path for band structure calculations generated.
   - You may also generate an additional k-point path, e.g., with:
     - **inpgen -inp.xml -kpt band=60**
     - **inpgen -inp.xml -kpt band=100 -kptsPath "gamma=0,0,0;x=0.5,0.5,0.5"**
3. Set band switch in inp.xml to "T".
4. Run Fleur.
   - Fleur will generate **bands.1** (and **bands.2**) files and a gnuplot script **band.gnu**.
   - with HDF5: Also a **banddos.hdf** file.
5. Run gnuplot script:
   - gnuplot < band.gnu > bands.ps

g.michalicek@fz-juelich.de

Band structure calculations: gnuplot script visualization



g.michalicek@fz-juelich.de

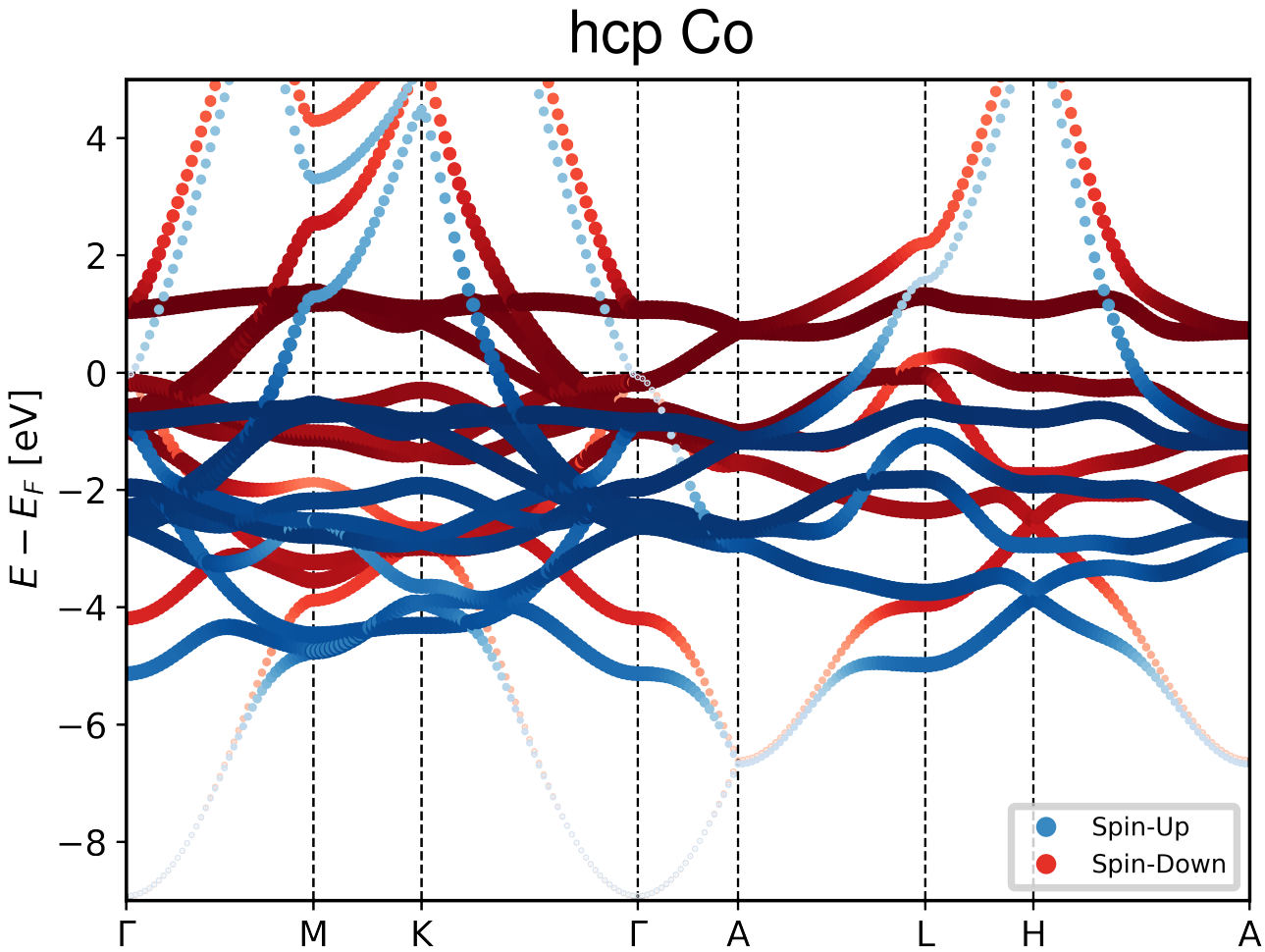
Band structure calculations: Alternative plotting with masci-tools

- The **masci-tools** provide an easy-to-use way of extracting and plotting the data in the **banddos.hdf** file.
- https://pypi.org/project/masci-tools/

```
from masci_tools.io.parsers.hdf5 import HDF5Reader
from masci_tools.io.parsers.hdf5.recipes import FleurBands
from masci_tools.vis.fleur import plot_fleur_bands

filepath='banddos.hdf'

with HDF5Reader(filepath) as h5reader:
    data, attributes = h5reader.read(recipe=FleurBands)

# We are interested in each state's d-projection in
# the MT sphere of the 1st atom type.
weightName = "MT:1d"

# Plot the bandstructure and save to a file bandstructure.png
plot_fleur_bands(data, attributes,
                 weight=weightName,
                 limits={'y': (-10, 5)},
                 show=False, save_plots=True)
```


g.michalicek@fz-juelich.de

Band structure calculations: masci-tools visualization with d character highlighting



g.michalicek@fz-juelich.de

Density of states calculations

1. Reach self-consistency
2. Adjust several parameters in inp.xml to your needs for the DOS:
   - /cell/bzIntegration/@mode (”hist” or ”tria”)
   - /output/bandDOS/@minEnergy (lower energy for the DOS generation)
   - /output/bandDOS/@maxEnergy (upper energy for the DOS generation)
   - /output/bandDos/@sigma (smoothen the DOS)
3. (Generate and) select an adequate k-point set for the DOS calculation.
4. Activate the dos switch in inp.xml
5. Run Fleur
6. Data is stored in **Local.1** (and **Local.2**) and **banddos.hdf**
   - See Fleur documentation on the extraction of the data

g.michalicek@fz-juelich.de

Density of states calculations: The art of producing a nice DOS (1)

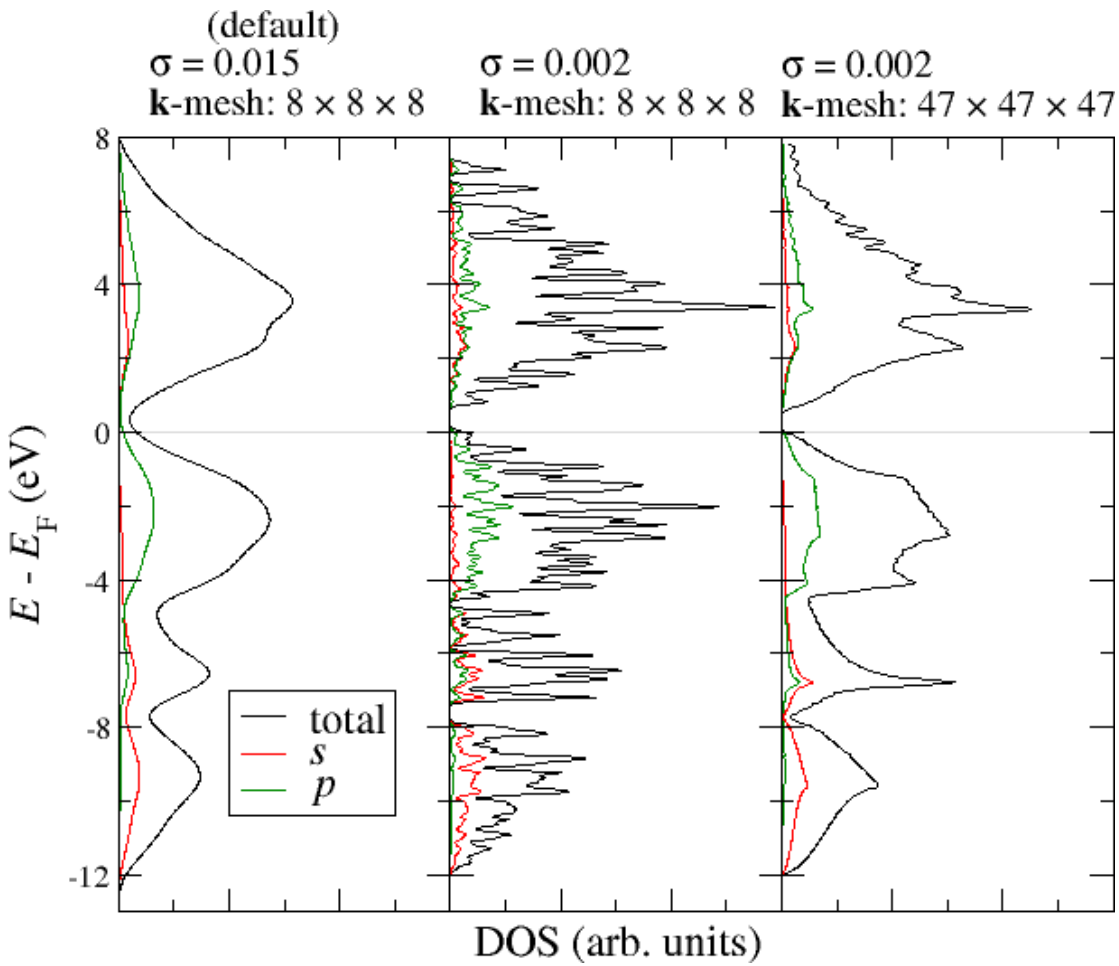
The quality of the DOS depends on the interplay of many different parameters and material properties:

- k-point set
- BZ integration mode
- Band dispersion
- Choice of DOS energy window
- Choice of number of energy mesh points
- Smearing of the DOS

g.michalicek@fz-juelich.de

Density of states calculations: The art of producing a nice DOS (2)

- DOS for Si
- Left: Smearing too large to see features or even the band gap
- Center: k-point set too coarse for band dispersion and smearing
- Right: Smearing, dispersion, and k-point set match



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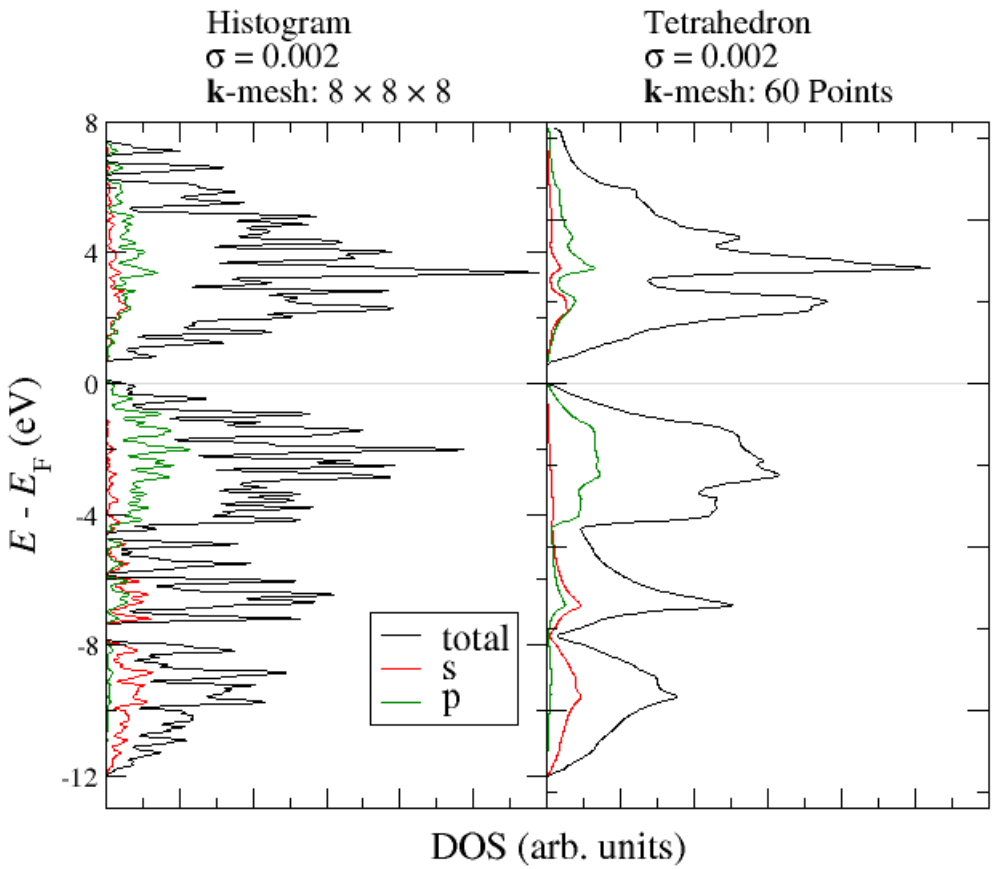
Density of states calculations: The art of producing a nice DOS (3)

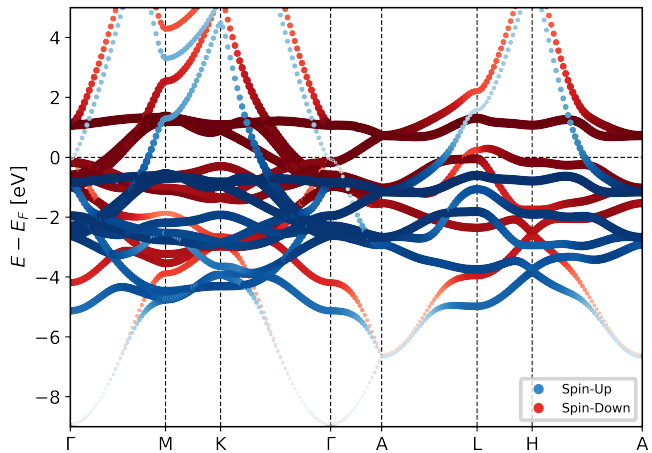
- DOS for Si
- Left: Default ”hist” mode
  - like center plot above
- Right: Tetrahedron method (use ”tria” mode)
  - special k-point set required.
- equal number of k points for both plots



g.michalicek@fz-juelich.de

Conclusion

- Invoking Fleur
- Reaching self-consistency
- Band structures
- Density of states

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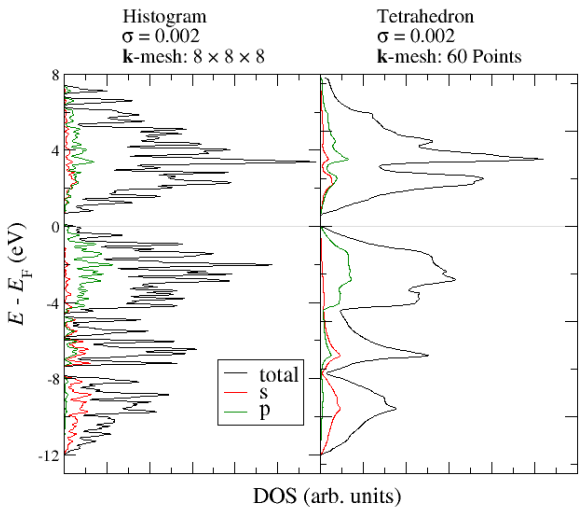

g.michalicek@fz-juelich.de