LinReTraCe – Tutorial

Matthias Pickem 2022

System requirements:
Modern GNU/Linux Distribution (Linux Kernel >= 4.x + Python3, e.g., Ubuntu 22.04 LTS)
Fortran Compiler with quadruple precision support
System prerequisites: pip, git, cmake, Fortran95 compiler (e.g., gfortran)
Packages obtainable, e.g, under Ubuntu via `sudo apt-get install pip` etc.
You need admin rights to do so, or you have to ask your computer admin.
Pip can be also obtained via the get-pip.py script, circumventing some of the root requirements. (https://pip.pypa.io/en/stable/installation/#get-pip-py)

LinReTraCe installation from a clean Ubuntu 22.04 LTS installation:

1) `sudo apt-get install git pip gfortran cmake`
2) `pip install numpy scipy h5py matplotlib ase spglib`
3) `pip install boltztrap2`
4) **HDF5 installation** (USER=your username)
   - `cd` # or choose a custom directory where to install the library
   - `mkdir -p opt`
   - `wget` https://support.hdfgroup.org/ftp/HDF5/releases/hdf5-1.13/hdf5-1.13.1/src/hdf5-1.13.1.tar.gz
   - `tar xf hdf5-1.13.1.tar.gz`
   - `cd hdf5-1.13.1`
   - `CC=gcc`
   - `FC=gfortran`
   - `./configure --enable-fortran --prefix=/home/USER/opt/hdf5-1.13.1_gcc`
   - `make`
   - `make install`
5) **LinReTraCe installation**
   - `cd` # or choose a custom directory where to install the code
   - `git clone` https://github.com/linretrace/linretrace
   - `cd linretrace`
   - with root rights: `sudo python3 setup.py install`
   - without root rights: `python3 setup.py install --user`
   - `touch make_include`
   - save the following into `make_include` (see folder `make_include_examples/` for examples, e.g., for a compilation with parallel computing (MPI) capabilities)

```
FC = gfortran
FCDG = gfortran
FFLAGS = -O3
HDF5 = -I/home/USER/opt/hdf5-1.13.1_gcc/include
HDF5 += -L/home/USER/opt/hdf5-1.13.1_gcc/lib -lhdf5_fortran -lhdf5hl_fortran
```

   - `make validate`

- make linretrace
- make install
- echo 'export PATH=/home/USER/bin:$PATH' >> ~/.bashrc
- echo ‘export LD_LIBRARY_PATH=/home/USER/opt/hdf5-1.13.1_gcc/lib:$LD_LIBRARY_PATH’ >> ~/.bashrc
- source ~/.bashrc

Installation complete.

The linretrace binary will be located in $HOME/bin.
The Python3 packages will be located either in
/usr/local/lib/python*X.Y*/site-packages
or
$HOME/.local/lib/python*X.Y*/site-packages
depending on how setup.py was called.
(see https://docs.python.org/3/install/ for a detailed discussion)

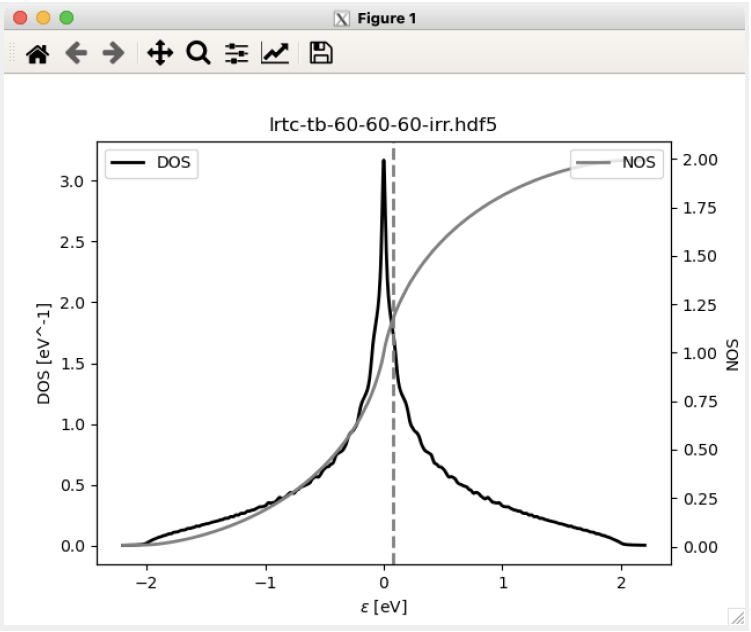
First LinReTraCe calculation: body centered-cubic tight-binding calculation

Setting up the energy file:

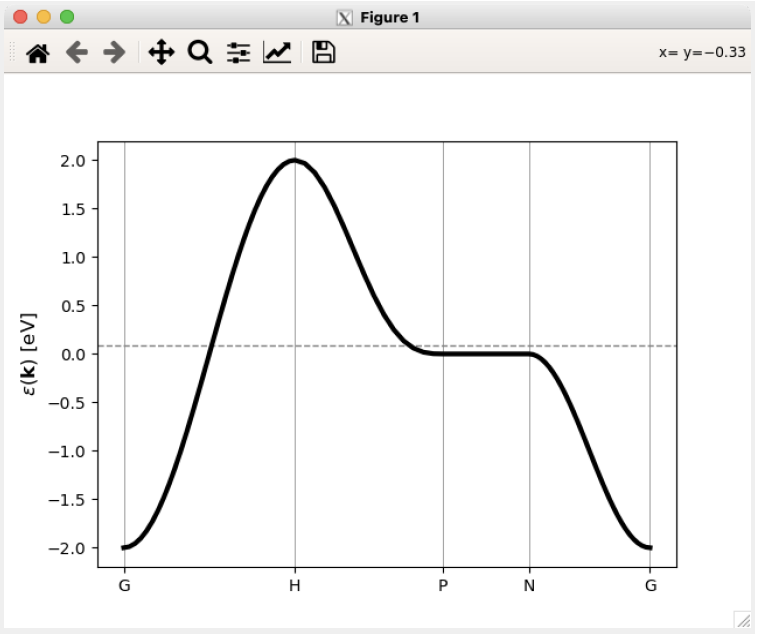
- cd
- mkdir test
- cd test
- ltb ~/linretrace/templates/bcc.tbdata 60 60 60 1.2

Inspecting energy file:

- lprint lrtc-tb-60-60-60-irr.hdf5 dos -p to plot the density of states:



- lprint lrtc-tb-60-60-60-irr.hdf5 path GHPNG -p to plot the band structure:



Setting up config file:

- lconfig

Starts up the following interactive prompt: Enter the highlighted inputs:

INTERACTIVE GENERATION OF LRTC CONFIG FILES

energy file: lrtc-tb-60-60-60-irr.hdf5
output file: output.hdf5
calculate intra-band quantities [y,n]: y
calculate inter-band quantities [y,n]: n
calculate boltzmann quantities [y,n]: y
calculate magnetic field quantities [y,n]: y
calculate quadruple precision [y,n]: y

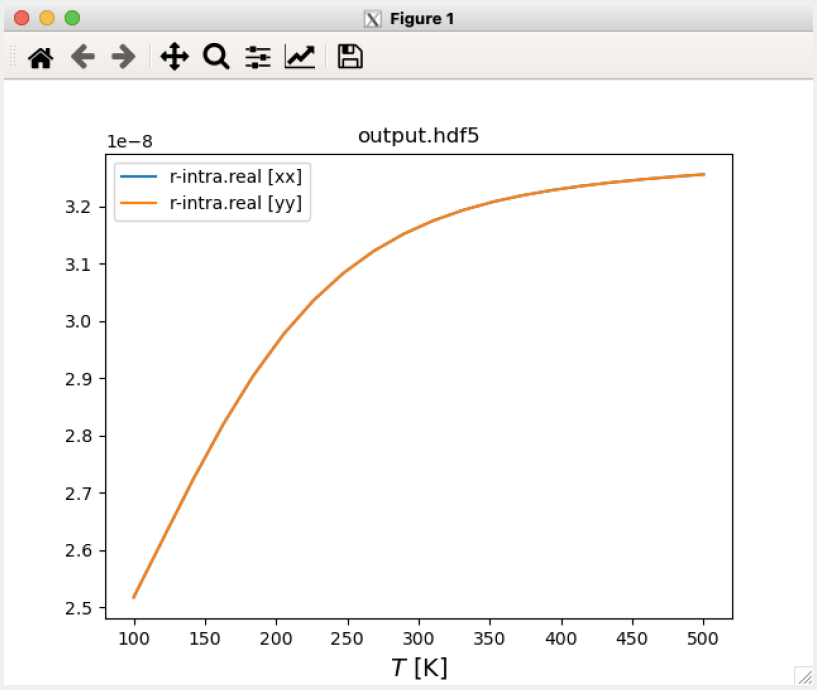
run mode (temp [1], mu [2]): 1
use Scattering file [y,n]: n

TEMP-MODE configuration:
chemical potential (fermi [1], digamma [2]): 1
temperature starting point [K]: 100
temperature ending point [K]: 500
temperature points: 20
logarithmic temperature steps [y,n]: n
scattering coefficients (separated by space): 1e-2
quasiparticle coefficients (separated by space): 1

config.lrtc successfully created.

Running LinReTraCe and inspecting output data:

- `linretrace config.lrtc` to execute the program
- `lprint -p latest r-intra xx yy` to plot the resistivity



- `lprint -p latest n-intra xyz` to plot the Nernst coefficient