

LinReTraCe – Tutorial

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System requirements:

Modern GNU/Linux Distribution (Linux Kernel $\geq 4.x$ + 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_config`
 - save the following into `make_config` (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/pythonX.Y/site-packages`

or

`$HOME/.local/lib/pythonX.Y/site-packages`

depending on how setup.py was called.

(see <https://docs.python.org/3/install/> for a detailed discussion)

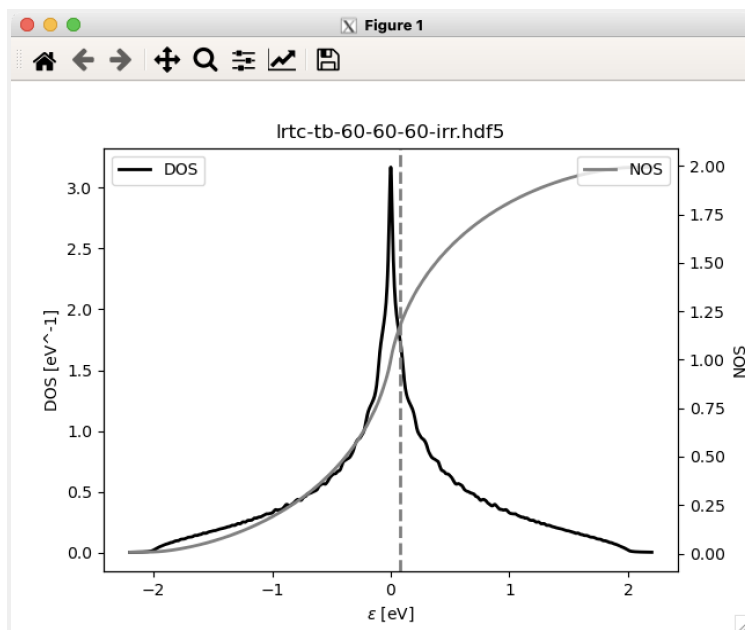
First LinReTraCe calculation: body centered-cubic tight-binding calculation

Setting up the energy file:

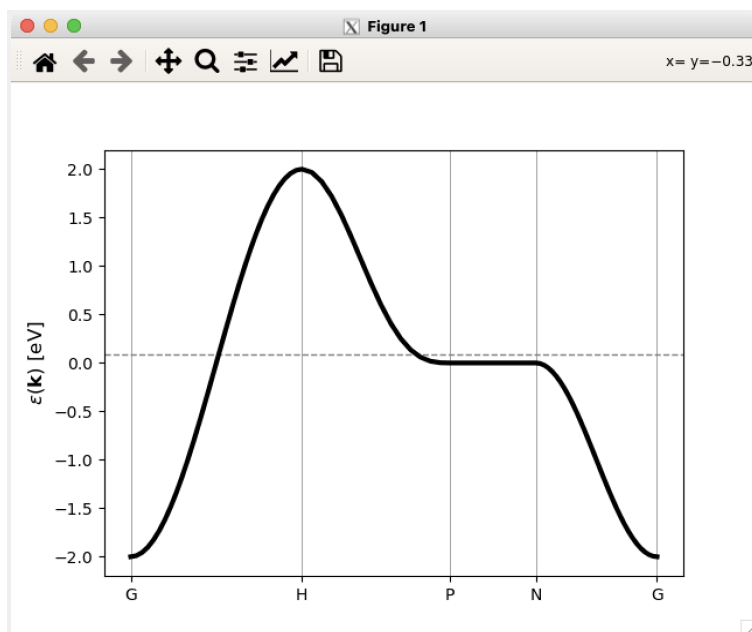
- `cd`
- `mkdir test`
- `cd test`
- `lrb ~/linretrace/templates/bcc.tbdata 60 60 60 1.2`

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

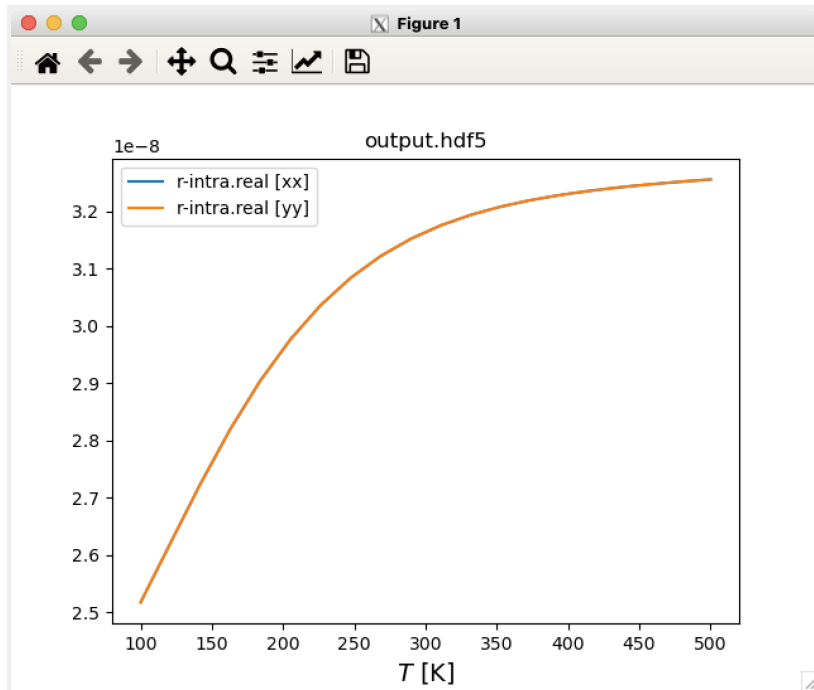
scattering coefficients (separated by space): 1e-2

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

