How to use the GreenALM code

Introduction to hands-on workshop

Oleg E. Peil
Materials Center Leoben GmbH

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General interface design

The interface is provided via **Python 3.x**

Parameters are read from an input file

Two modes of operation:

- Use input file as a template, vary parameters **in a script**

  Example:

```
from gfalm import main
from gfalm.utils import read_input_file
input_data = read_input_file('fcc-Al.in')
input_data['struct_params']['ws_radius'] = (2.9, 'au')
status = main.run(**input_data)
```

- Run the code **from command line** with an input file

```
> python -m gfalm.main fcc-Al.in
> gfalm fcc-Al.in
```

Input file parameters

Parameters are grouped into sections:

- **[Control]:** job control, DFT iterations, etc.
- **[Structure]:** crystal structure
- **[Alloy]:** alloy sublattices (pseudo-species) for a CPA calculation
- **[Kpoints]:** Brillouin zone sampling
- **[Contour]:** parameters of the complex contour
- **[Atomic]:** parameters of the radial mesh
- **[DOS]:** parameters of the density of states calculations
- **[BSF]:** parameters of the Bloch spectral function calculations

Section [Control]

Important parameters:

- **Mandatory:**
  - `job_type`: type of the job (‘sc’, ‘dos’)
  - `job_name`: will be used for directory names
- `spin_polarized`: `yes` or `no`
- `max_iter`: maximum number of DFT iterations
- `etot_tol, chd_tol, spd_tol, ef_tol`: tolerances for errors
- Mixing parameters:
  - `chd_mixing`: `chd_type` (`anderson`, `linear`), `chd_params`
  - `pot_mix`: potential mixing
- `restart`: restart mode (`force`, `soft`, forbid`)

Section [Structure]

Important parameters:

- **Mandatory:**
  - `lattice`**:** lattice vectors
  - `sites_frac` **or** `sites_cart`**:** atom positions
  - `lattice_scale` **or** `ws_radius`**:** linear scale (`3.6 A` or `2.6 au`)
- `name`: name of the structure (used for the structure constants file)
- `path`: directory to which the structure constants file is stored
- `poscar`: use POSCAR file to input a structure
- `lmax`: orbital number cut-off

Each site is specified by:

- **Mandatory:**
  - `x y z`**:** coordinates (fractional or Cartesian)
  - `El` **or** `${name}`**:** element or alloy sublattice (given in [Alloy])
- `mom`**:** initial spin splitting
- `lsm_mode` **:** “local spin moment mode” (`dlm` and / or `lsf` / `fxm`)

Section [Alloy]

Each species is defined similar to a site in [Structure]:

```
name =
       Cu    0.3   <optional parameters>
       Ni    0.7   <optional parameters>
```

- **Mandatory:**
  - `El`: element symbol
  - `conc`: atomic fraction of the element
- `mom`: initial spin splitting
- `lsm_mode` : “local spin moment mode” (`dlm` and / or `lsf`)
- `al_scr, bet_scr`: CPA screening parameters

Section [Kpoints]

Only a couple of parameters are available:

- **Mandatory:**
  - `mesh_size`: number of k-points in each direction
- `bz_type`: irreducible or full BZ (`ibz` or `fbz`)
- `time_reversal`: time reversal is present (`yes`, `no`)

Section [Contour]

There is a rare need to touch anything in this section except two parameters

For the default contour type (circular) the only parameters worth changing are

- **`nz_sections`:** number of points on contour sections (circular has one)
- **`depth`:** depth of the contour (e.g.,`1.2 Ry` or `15 eV`)

Section [DOS]

DOS calculation is defined by a linear energy mesh along the real axis shifted by a small imaginary value

The parameters of the DOS mesh are

- `e_range`: boundary of the mesh (e.g., -0.8 0.2)
- `n_points`: number of points of the mesh
- `im_delta` : small imaginary shift (typically of order 0.003-0.03)

Section [BSF]

Bloch spectral function is defined at each (k, e)-point and there are two basic uses

- Fermi surface section: $\mathbf{A}(k_1, k_2)$, energy is fixed, k-points belong to a 2D manifold (**section**)
- Band structure: $\mathbf{A}(E, k)$, energy mesh, k-points belong to a 1D manifold (**line**)

General parameters (`kset_params`)

- `type`: **segments** ("spaghetti") or **sections** ("Fermi surface")
- `segment_len` or `section_size`: parameters of k-point meshes

Specific parameters

- Fermi surface section: energy is fixed, k-points belong to a 2D manifold (**section**)
  - `e_range` : set to one point (relative to the Fermi level, e.g., [0.0, 0.0])
  - `n_points`: number of points in the energy mesh (typically 1)
  - `sections`: define 2D cross sections in reciprocal space

- Band structure: k-points belong to a 2D manifold (**section**)
  - `e_range` : defines the energy mesh bounds (as for DOS)
  - `n_points`: number of points in the energy mesh
  - `kpoints`: end points of line segments

Common parameters

- `im_delta` : small imaginary shift (typically of order 0.003-0.03)