FHI-aims File Format Description: geometry.in

Version 2020/06/01 – Volker Blum

1 Overview

The FHI-aims input file `geometry.in` specifies the system geometry (placement and type of atoms, unit cell vectors, etc.) of a molecule or solid and any information that is linked directly to the system geometry, to the system's physical environment, or to specific atoms. No other technical information should be part of `geometry.in`. Instead, any other technical information is provided to FHI-aims as part of the codes' other input file `control.in`.

In its simplest form, `geometry.in` is a generic format specification for files conveying the atomic structure of molecules or solids. This basic form is thus equivalent to other, code-agnostic file specifications containing atomic structure information, such as .xyz, .cif, or .pdb. Like these other file formats, `geometry.in` can also contain technical information beyond the actual atomic structure.

The present document focuses on aspects related to the basic atomic structure information (including information on specified initial spin moments, which may result in physically different outcomes for the structure in question). The information provided below should be sufficient to understand how to convert FHI-aims' `geometry.in` format to and from other utilities and codes. A full listing of all keywords related to `geometry.in` may be found in the FHI-aims code manual.

2 Examples

Any molecular geometry in FHI-aims requires only cartesian atomic coordinates of the position of a nucleus (in Å) and of the atomic species (usually, the chemical element) found at that position. No other information is required. Any `geometry.in` file that does not include a unit cell specification is automatically considered to correspond to the definition of an isolated molecule.

The `geometry.in` file for an isolated N_2 molecule might look like this:

```
atom 0. 0. 0.      N
atom 0. 0. 1.0976  N
```

Periodic systems are defined by specifying three lattice repeat vectors in cartesian units (Å). The `geometry.in` file for the primitive two-atom cell of a GaAs periodic crystal might look like this:

```
lattice_vector  2.826650         2.826650         0.000000
lattice_vector  0.000000         2.826650         2.826650
lattice_vector  2.826650         0.000000         2.826650

atom  0.000000         0.000000         0.000000  Ga
atom  1.413325         1.413325         1.413325  As
```

The previous version specifies the cartesian atomic coordinates in Å (`atom` keyword). Alternatively, a specification in fractional coordinates (units of the lattice vectors) is possible as well:

```
lattice_vector  2.826650         2.826650         0.000000
lattice_vector  0.000000         2.826650         2.826650
lattice_vector  2.826650         0.000000         2.826650
```

```
atom_frac  0.              0.              0.        Ga
atom_frac  0.25            0.25            0.25      As
```

The relation between lattice vectors $\{\boldsymbol{a}_k\}$, cartesian atomic coordinates $\{\boldsymbol{R}_I\}$ of atom I and fractional atomic coordinates $\{\boldsymbol{f}_I\}$ is

$$R_{I,j} = \sum_k f_{I,k} a_{k,j} \tag{1}$$

The index j denotes the cartesian coordinates of the kth lattice vector in the order provided in `geometry.in`.

3 Format and Keywords

In `geometry.in`, whitespace separates keywords and their values. Empty lines are ignored and comment lines can be inserted starting with the '#' character. The order of lines is generally arbitrary, with the exception of keywords that pertain to a specific atom. Keywords that pertain to a specific atom (such as an `initial_moment` spin moment specification or a constraint on the atomic position) must be specified after the `atom` or `atom_frac` line of that atom, and before the `atom` or `atom_frac` line indicating the next atom.

Keywords descriptions:
(restricted to the keywords that do not refer to code-specific technical features)

`atom`

Usage: `atom x y z species_name`

Purpose: Specifies the initial location and type of an atom.

`x`, `y`, `z` are real-valued numbers (in Å) which specify the atomic position.

`species_name` is a string descriptor which names the element on this atomic position; when used in FHI-aims, it must match one of the species descriptions defined in `control.in`.

`atom_frac`

Usage: `atom_frac` f_1 f_2 f_3 `species_name`

Purpose: Specifies the initial location and type of an atom in fractional coordinates.

f_k is a real-valued multiplier to `lattice_vector` k. `species_name` is a string descriptor which specifies the chemical element (or, more broadly, atomic species type) at this atomic position; when used in FHI-aims, it must match one of the `species` descriptions defined in `control.in`. Fractional coordinates are only meaningful in periodic calculations.

As noted above (but here in vector notation and for a given atom), conversion of fractional atomic positions into cartesian coordinates, $\boldsymbol{R}$, is achieved by

$$\boldsymbol{R} = \sum_{k=1}^{3} f_k \cdot \boldsymbol{a}_k, \tag{2}$$

where $\boldsymbol{a}_k$ is a unit cell vector specified by the `lattice_vector` keyword.

`lattice_vector`

Usage: `lattice_vector x y z`

Purpose: Specifies one lattice vector for periodic boundary conditions.

`x`, `y`, `z` are real numbers (in Å) which specify the direction and length of a unit cell vector.

If up to three lattice vectors are specified, FHI-aims automatically assumes periodic boundary conditions in those directions. *Note* that the order of lattice vectors matters, as the order of k space divisions (given in `control.in`) depends on it!

`initial_moment`

Usage: `initial_moment moment`

Purpose: Allows to place an initial spin moment on an `atom` in file `geometry.in`.

`moment` is a real number, referring to the electron difference $N^{\uparrow} - N^{\downarrow}$ in the up ($\uparrow$) and down ($\downarrow$) spin channels of the atom on that site. Default: Zero, unless `default_initial_moment` is set explicitly in `control.in`.

The `initial_moment` keyword always applies to the immediately preceding `atom` specified in input file `geometry.in`. The moment is introduced by using a spin-polarized instead of an unpolarized spherical free-atom density on that site in the initial superposition-of-free-atoms density. In FHI-aims, initial charge densities are generated by the functional specified with `xc` for DFT-LDA/GGA, but refer to `pw-lda` densities (i.e., free-atom densities computed using the 1991 parameterization of the local-density approximation to the exchange-correlation functional by Perdew and Wang) for all other density functionals (hybrid functionals, Hartree-Fock, ...).

`velocity`

Usage: `velocity vx vy vz`

Purpose: Specifies a velocity for the immediately preceding `atom` in file `geometry.in`.

`vx`, `vy`, `vz` : x, y, and z components of the velocities, in Å/ps.

In `geometry.in`, the line containing the velocity must follow the line containing the `atom` that the velocity refers to. This can be used, e.g., to initialize a molecular dynamics run, or for analysis purposes later. Note that, for molecular dynamics, the FHI-aims standard output prints this information in the proper format, as part of a particular geometry associated with a molecular dynamics trajectory.