

SFIT4 – Quickstart HOWTO

Mathias Palm

Bremen, 2020

Contents

- ▶ Contact and getting help
- ▶ Other documentation files and what they contain
- ▶ Files needed and where to get them
- ▶ Build sfit4, hbin and pspec
- ▶ Create the spectral file LLLLLL.IIIIII-HHHHHH.hhhhhh.hbin
- ▶ Create a setup for your own station

Contact and getting help

1. make sure you have the latest SFIT4 version (check on <https://wiki.ucar.edu/display/sfit4/>)
2. Pack a full testcase, i.e.
 - 2.1 sfit4.ctl
 - 2.2 hbin.ctl
 - 2.3 all files the section file.in. point to
 - 2.4 sfit4.dtl if it exists.
 - 2.5 a screenshot of the output.

you may use the script in tools/Create_testcase. It is called by

```
python3 Create_testcase_repository <DIR>
```

where <DIR> is the testcase directory. If no directory is given, the current directory is used.
3. sent them to one or all people listed in the CONTACT section of <https://wiki.ucar.edu/display/sfit4/>.
4. We rely on bug reports to improve the program further. Many bugs tend to be subtle and turn up only in very special circumstances.

Other descriptions and what they contain

[sfit4_init/sfit4_init.pdf](#) The tentative description of the keys in the sfit4.ctl file and their interdependencies

[hbin/sfit4-hbin_ctl.docx](#) describes the structure of the hbin.ctl file (input file of hbin) to create the file
LLLLL.IIIII-HHHHH.hhhhhh.hbin

[Linelist/sfit4-isotope_descrip.docx](#) contains the structure of the file.in.isotope file

[Linelist/sfit4-isotope_descrip.docx](#) contains the structure of the file.in.isotope file

[ForwardModel/sfit4-lineshapes.pdf](#) summarizes the lineshape options available in SFIT4.

[ForwardModel/Workshop2019-Palm-sfit4-fwdmodel-params.pdf](#) contains many descriptions of forward model parameters. Is referred to as
FWDMODEL-PARAMS.

Files needed and where to get them

Files always necessary

The section `file.in` contains the names of the input files. The structure of the files is described on extra slides later on.

`file.in.spectrum` The measured spectrum. This file is created using `pspec` or any other tool. Is also needed for calculating a synthetic spectrum, because it defines the spectral grid, SFIT4 is working on.

`file.in.stalayers` The file containing the altitude bins for the forward model and the retrieval. This file defines the altitude grid which is used in SFIT4.

`file.in.refprofile` Contains the atmosphere and is created by the processing environment or elsewhere. The atmosphere used in SFIT4 is interpolated to the altitudes given in `file.in.stalayers`, i.e. its range has to be equal or larger

`LLLLL.IIIII-HHHHH.hhhhhh.hbin` Contains the spectral data and is created by `hbin` (part of the `sfit4` package, check `sfit4-hbin_ctl.docx`)

Files needed and where to get them

Files needed for certain optional calculations

`file.in.solarlines` needed if `fw.solarspectrum = T`. Is a linelist of solar lines and part of the spectroscopy which comes with SFIT4

`file.in.modulation_fcn` needed if `fw.apod_fcn = T`. Parameters of the empirical apodisation function. See file `FWDMODEL_PARAMS` slide 3ff.

`file.in.phase_fcn` needed if `fw.phase_fcn = T`, Parameters of empirical phase function. See file `FWDMODEL_PARAMS` slide 3ff.

`file.in.isotope` needed if `fw.isotope_separation = T`. Contains definitions necessary for treating isotopes separately from the main isotope of the retrieved gas. Check the file `sfit4-isotope_descrip.docx` for its structure and contents. Files for the most common isotopes are part of the spectroscopy which comes with SFIT4.

Download and build SFIT4, HBIN and PSPEC

From <<https://wiki.ucar.edu/display/sfit4/>->SFIT 4 Version 1.0.+ (Pre) Release> download the following files:

[sfit4_v1.0.zip](#) contains the sfit4, hbin and pspec programs

[linelist-core-20200715.tar.gz](#) contains the linelist which are used with SFIT4

1. unpack both archives
2. in the directory sfit-core-code/src: type
make clean
make

SFIT4 has been tested with gfortran version 9.3.0. Most of the gfortran builds work, but we would recommend to use at least gfortran version 8.0.

3. go into directory sfit-core-code/sfit4_testbed, modify test.cfg and run
python2.7 script/run_testcases.py

If test.cfg is still filled in with the place-holders it will ask for the directories. Details are found in the README file.

Download and build SFIT4, HBIN and PSPEC (cont'd)

4. After it finishes it compares the results to the results stored in `sfit4_testbed/results_v1.0` and prints out the differences if they are any. The differences should be small (fractions of a percent) if not, use another compiler.
5. in the `hbin.ctl` set the key `file.in.linelist` to your linelist directory.
6. run some or all of the testcases in `test_cases_NDACC`. It is better you start modifying testcases rather than building up a new one from scratch.

Create a setup for the station you are interested in

- ▶ Start from a testcase from test_cases_NDACC
- ▶ Make sure, the hbin is a recent one, preferably the one taken from the linelist
<LINELIST-DIR>/templates/hbin.ctl_hit2016)
- ▶ Create the reference profile for your station. You find WACCM runs at
<https://wiki.ucar.edu/display/sfit4/Whole+Atmosphere+Community>
- ▶ Download the profiles for your station.
- ▶ If your station is not there, you may:
 - ▶ choose a station with the same latitude and altitude
 - ▶ write an email to the contact and ask for the run for your station
- ▶ Use the tool
tools/Create_Refprofile/Create_REF_from_WACCM.py to create an example refprofile and copy the station.layers file in the sfit4 directory.
- ▶ use pspec to create a spectrum
(docs/Processing/sfit4-pspec_descrip.pdf)