SFIT4 – Quickstart HOWTO

Mathias Palm

Bremen, 2020

Contents

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 dierectory is given, the current directory is used.
3. sent them to one or all people listet 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 descritions 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.llllll-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 refered 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 calclating 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 SFTI4 is interpolated to the altitudes given in file.in.stalayers, i.e. its range has to be equal or larger

LLLLL.llllll-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 is fw.solarspectrum = T. Is a linelist of solar lines and part of the spectroscopy which comes with SFIT4

file.in.modulation_fcn needed is 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 separetly 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 recomment 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
- 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)