

Initialisation of sfit4

The general format is
Keyword1.keyword2.keyword3 = value

Keyword 1

Defines general section under which keyword2,3,4,... are defining more detailed parameters

file defines in and output files. All output files are also set to default values by the code.

gas defines parameters for the retrieval gases

fw all parameters for the forward model are defined in this section

kb is set to true if Kb matrizes are calculated at the end of the talk.

rt in this section the retrieval parameters are defined, except for the S_A matrices for the gases which are defined in the gas section. If rt is set to F, no retrieval is performed but only a forward calculation.

band the parameters for all MW bands are defined.

sp contains additional noise information for the spectra, i.e. for deweighting

out more details of output are defined

Do not rely on default values for in and output to make the program forward compatible

| Key | Dependency | Default | Description | versions |
|------------------------|---|--------------------|--|----------|
| file.in.spectrum | | t15asc.4 | File containing the spectrum in ASCII | |
| file.in.stalayers | | station.layers | File containing the layering | |
| File.in.refprofile | | reference.prf | File containing the atmosphere | |
| file.in.modulation_fcn | fw.apod_fcn = T | modulation_gcn.dat | empirical apodization function fw.apod_fcn.type=: table containing the apodisation versus the OPD fw.apod_fcn.type = 2,3: coefficients of the polynomial or Fourier series. fw.apod_fcn.type = 4: Output of lft (modulat.dat) | |
| file.in.phase_fcn | fw.phase_fcn = T | Phase.dat | empirical phase function fw.phase_fcn.type=1: table of values version OPD fw.phase_fcn.type = 2: coefficients of the polynomial, Must be one more than ft.phase_fcn.order. The first coefficient is the 0 th order (constant over the whole interferogram) fw.phase_fcn.type = 4: Output of lft (modulat.dat) | >= 1.0 |
| file.in.sa_matrix | gas.x.correlation = T gas.x.correlation.type = 4 | sainv.input | file containing a full sa matrix | |
| | gas.x.correlation = T gas.x.correlation.type = 5 | sainv.input | file containing fill inverse matrix S_a^{-1} | |
| file.in.isotope | fw.isotope_separation = T | isotope.input | containg the isotope description | |
| file.in.solarlines | fw.solspectrum = T | solar_data.input | containg solar lines | |
| file.in.linelist | | none | file containing spectral data, created with hbin | |

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|----------------------------------|---|----------------|---|-------|
| file.in.transmission | fw.filter_transmission = T | none | A file containing a measured transmission. The format is the same as file.in.spectrum | |
| | | | | |
| file.out.solarspectrum | fw.solar_spectrum=T | solspec.dat | Calculated solar spectrum | |
| file.out.summary | | summary | | |
| file.out.pbpfile | | pbpfile | | |
| file.out.statevec | | statevec | | |
| file.out.k_matrix | | k.out | | |
| file.out.g_matrix | | d.complete | | |
| file.out.shat_matrix | | shat.complete | | |
| file.out.sa_matrix | | sa.complete | | |
| file.out.retprofiles | | rprfs.table | | |
| file.out.aprprofiles | | aprfs.table | | |
| file.out.ak_matrix | | ak.out | | |
| file.out.ab_matrix | | ab.out | | |
| file.out.parm_vectors | | parm.vectors | Internal statevector per iteration | |
| file.out.seinv_vector | | seinv.out | | |
| file.out.sainv_matrix | | sainv.out | | |
| file.out.smeas_matrix | | smeas.target | | |
| file.out.ssmooth_matrix | | ssmooth.target | | |
| file.out.kb_matrix | | kb.out | | |
| | | | | |
| gas.layers | | | Nr of layers the gas is retrieved on. Must match the number of layers in file.statlayers | |
| gas.profile.list | | empty | names of the gases for which profiles are retrieved | |
| gas.column.list | | empty | names of the gases for which columns are retrieved | |
| gas.profile.x.correlation | | F | T for calculation of off diagonal correlation | |
| gas.profile.x.correlation.type | gas.profile.x.correlation = T | | definition of off diagonal correlation in the S _a -matrix 1 - Gaussian shape 2 - Exponential shape 4 - the S _a matrix is read in from file.sa_matrix 5 - the inverse, S _a ⁻¹ , matrix is read from file.sa_matrix 6 - an L1 redularization matrix is created | >=1.0 |
| gas.profile.x.correlation.width | gas.profile.x.correlation = T gas.profile.x.correlation.type = 1,2 | | width of the correlation in km | |
| gas.profile.x.correlation.minalt | gas.profile.x.correlation = T gas.profile.x.correlation.type = 1,2 | | correlation calculation starts at given altitude | |
| gas.profile.x.correlation.maxalt | gas.profile.x.correlation = T gas.profile.x.correlation.type = 1,2 | | correlation calculation ends at given altitude | |

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|----------------------------------|--|------|--|--|
| Gas.profile.x.correlation.lambda | gas.profile.x.correlation = T gas.profile.x.correlation = 6 | type | Regularisation parameter for L1 regularisation | |
| gas.profile.x.logstate | | F | If T the statevector is ln(VMR) | |
| gas.profile.x.scale | | | a priori scaling of the VMR | |
| gas.profile.x.sigma | gas.x.ifoff=0,1,2 | | diagonals of Sa matrix in fractions of the a priori Nr of entries must correspond to the number of layers defined in the statlayers | |
| | gas.x.ifoff=5 | | the corresponding rows of the read matrix are multiplied by the inverse value of the sigma | |
| | | | | |
| fw.tips | | T | Turn TIPS On or Off. TIPS (as of HITRAN 2016) is slow but more accurate calculation of partition sums. | |
| fw.isotope_separation | | F | Isotopes are separated, see file <file.in.isotope> for a definition of the isotope separation | |
| fw.delnu | | | Half width of integration interval for cross section calculation | |
| fw.lshapemodel | | 0 | Lineshape model 0 - depends on the spectroscopic values given 1 - always Voigt 2 - Galatry if BETA_T is given, if not Voigt 3 - LM calculation using the Voigt profile by Boone (2012) 4 - Use the pCqSDHC lineshape model Tran(2013) | |
| fw.lshapemodel.sdv | fw.lshapemodel = 4 | F | Use the SDV approximation in the pCqSDHC model. | |
| fw.linemixing | fw.lshapemodel = 3,4 | F | if T and parameters found, linemixing is included currently only 1 st order approximation (Rosenkranz, 1975) | |
| fw.linemixing.gas | | | gas for which linemixing is calculated | |
| fw.solar_spectrum | | F | if T inclusion of solar lines (files.solarlines) | |
| fw.pressure_shift | | F | Pressure induced line shift T - read from linelist F - no shift | |
| fw.apod_fcn | | F | Calculate apodization function | |
| fw.apod_fcn.type | fw.apod_fcn = T | | Empirical apodization 0 - no empirical apodization 1 - tabular function is read in 2 - polynomial 3 - fourier series 4 - linefit output is read in An extra file in file.in.apod_fcn has to be supplied if type <> 0. Format of this file depends on the type. | |
| fw.apod_fcn.order | fw.apod_fcn.type = 2 o. 3 | | Order of polynomial/fourier series | |
| fw.phase_fcn | | F | T if empirical phase is calculated | |
| fw.phase_fcn.type | fw.phase_fcn = T | | Empirical phase error 0 - no empirical phase 1 - tabular function is read in 2 - polynomial 4 - linefit output An extra file in file.in.phase_fcn has to be supplied if type <> 0. Format of this file depends on the type. (compare documentation sfit4_EAPOD_EPHASE | |

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| fw.phase_fcn.order | fw.phase_fcn = T fw.phase_fcn.type = 2 | | Order of polynomial | |
| fw.emission | | F | if T emitted radiation from the atmosphere is calculated | |
| fw.emission.T_infinity | | n | Temperature (in K) of the radiating object outside the atmosphere Moon = 370.0 Sun = 6000.0 None = 2.7 | |
| fw.emission.object | fw.emission = T | | Reflexion of solar light off object .e. only emission is calculated, no reflection .m. reflection of solar light of the moon (pre-alpha) | |
| fw.emission.normalized | fw.emission = T | | spectra are normalized to one (T) or not normalized (F) | |
| fw.rayonly | | F | if T only calculate raytracing | |
| fw.filter_transmission | | F | If T applies the measured transmission contained in file.in.transmission to the calculated spectrum | |
| | | | | |
| Cell | | x | Number (placeholders) for cell | |
| Cell.x.temperature | | | Temperature of CELL in K | |
| Cell.x.pressure | | | Pressure in CELL in hPa. This is the total pressure, not the partial pressure of the gas. | |
| Cell.x.gas | | | GAS in CELL. For more than one GAS, a seperate CELL has to be defined. | |
| Cell.x.vmr | | | VMR of the gas in CELL | |
| Cell.x.path | | | Path of the cell in cm | |
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| kb | | F | T if Kb matrix entries are calculated, if the respective statevector entries are not retrieved, i.e. given kb.slope = T the Kb row for the slopes are only calculated if slope is not retrieved. | |
| kb.profile | | F | Calculates AB matrix for a wrong assumed profile if the retrieved gas is a column | |
| kb.profile.gas | kb.profile | | For which gas an error for the retrieved profile is calculated? | |
| kb.sza | | F | T if Kb calculation of the SZA | |
| kb.line | | F | T if Kb calculation for line intensities | |
| kb.line.gas | | | for which gases line parameters are calculated, default: all gases which are retrieved predefined values: target - calculation only for the target gas retrieval - kb are calculated for each gas which is retrieved. individual gasnames are also possible | |
| kb.line.type | | | 1 if all line parameters of a gas are perturbed together with the same perturbation (this is the only parameter supported so far) Kb are calculated for: <ul style="list-style-type: none">• Intensity• Pressure broadening• Temperature dependency of pressure broadening | |

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| kb.temperature | | | | |
| kb.slope | | | | |
| kb.curvature | | | | |
| kb.zshift | | | | |
| kb.omega | | | | |
| kb.max_opd | | | | |
| kb.solstrnth | | | | |
| kb.solshift | | | | |
| kb.phase | | | | |
| kb.apod_fnc | | | if fw.apod_fcn = F a three order three order polynomial is assumed as the empirical apodisation function. If the apodisation function is read in as a table, no kb matrix is calculated (yet) | |
| kb.phase_fcn | | | if fw.phase_fcn = F a three order three order polynomial is assumed as the empirical apodisation function. If the phase function is read in as a table, no kb matrix is calculated (yet). | |
| kb.wshift | | | not recommended (usually retrieved) | |
| kb.dwshift | | | not recommended | |
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| rt | | | Switch on (T) or off (F) Retrieval, if F only a forward model calculation is performed | |
| rt.lm | | F | Switch on (T) or off (F) LM iteration scheme | |
| rf.lm.gamma_start | rt.lm = T | | Start value for gamma | |
| rf.lm.gamma_inc | rt.lm = T | | Increase gamma by value if step was succesful | |
| rf.lm.gamma_dec | rt.lm = T | | Decrease gamma if step failed | |
| rt.convergence | | | convergence is reached if change in cost function is smaller than value | |
| rt.tolerance | rt.lm = F OR rt.convergance not given | | convergence cirterion used by sfit2. Convergence is reached if the proposed change in the spectrum is smaller than the noise * rt.tolerance | |
| rt.max_iteration | | | maximal number of iterations | |
| rt.wshift | | F | T if a wavenumver shift is retrieved. | |
| rt.wshift.type | rt.wshift = T | | 0 - no shift for any bandpass 1 - single shift for each bandpass 2 - independent shift for each bandpass 3 - idependent shift for each bandpass and scan | |
| rt.wshift.apriori | rt.wshift = T | | apriori of the additional scaling for all microwindows -1. Internally it is added to band.x.wavfac, the scaling which is applied to microwindow x as apriori is band.x.wavfac + rt.wshift.apriori after retrieval the value is found in statevec as IWNUMSHFT_X hence the scaling applied in a MW is band.x.wavfac + IWNNumShft_x | |

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| rt.wshift.sigma | rt.wshift = T | | its sa | |
| rt.slope | | F | slope is retrieved if T | |
| rt.slope.apriori | rt.slope = T | | a priori of slope | |
| rt.slope.sigma | rt.slope = T | | sa of slope | |
| rt.curvature | | F | curvature on spectrum is retrieved if T | |
| rt.curvature.apriori | rt.curvature = T | | a priori of curvature | |
| rt.curvature.sigma | rt.curvature = T | | sa of curvature | |
| rt.phase | | F | simple phase correction retrieved if T | |
| rt.phase.apriori | rt.phase = T | | | |
| rt.phase.sigma | rt.phase = T | | | |
| rt.phase_fcn | fw.phase_fcn = T fw.phase_fcn.type=2 | F | Empirical phase function retrieved if T | |
| rt.phase_fcn.apriori | rt.phase_fcn = T | | | |
| rt.phase_fcn.phase | rt.phase_fcn = T | | | |
| rt.apod_fcn | fw.apod_fcn = T fw.apod_fcn.type=2,3 | F | Empirical phase function retrieved if T | |
| rt.apod_fcn.apriori | rt.apod_fcn = T | | | |
| rt.apod_fcn.phase | rt.apod_fcn = T | | | |
| rt.solshift | fw.solar_spectrum = T | F | retrieve shift in solar lines if T | |
| rt.solshift.apriori | rt.solshift = T | | | |
| rt.solshift.sigma | rt.solshift = T | | | |
| rt.solstrnth | fw.solar_spectrum = T | F | retrieve strength of solar lines if T | |
| rt.solstrnth.apriori | rt.solshift = T | | | |
| rt.solstrnth.sigma | rt.solshift = T | | | |
| rt.dwshift | | F | if T retrieval of line shifts for each retrieved gas | |
| | | | | |
| rt.temperature | | F | if T, temperature is retrieved | |
| rt.temperature.sigma | rt.temperature = T | | diagonals of sa matrix for temperature for each layer in state vector | |
| rt.temperature.lambda | rt.temperature = T rt.temperature.sigma not given | | strength of L1 regularisation | |
| | | | | |
| band | | | = 1..2 MWs that are included in the calculation | |
| band.x.nu_start | | | smallest frequency of MW | |
| band.x.nu_stop | | | argest frequency of MW | |
| band.x.calc_point_space | | | spacing for spectrum calculation | |
| band.x.wave_factor | | 1.0 | scaling of wave factor in this band | |
| band.x.opd_max | | | maximal OPD for this band | |
| band.x.omega | | | FOV for this band | |
| band.x.apodization_code | | 0 | Imposed Apodization Code 0 - Boxcar 1 -3 Norton Beer (weak, med., strng) 4 - Denver data 5 - Triangle 6 - Happ - Genzel 7 - KPNO Atmospheric Spectra A 8 - KPNO Atmospheric Spectra B 9 - Hamming function | |

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| band.x.zshift | | F | T if an offset is retrieved in this band | |
| band.x.zshift.type | band.1.zshift = T | | 0 - use the a priori as given 1 - allow to retrieve for each bad 2 - use zero level from first band in list | |
| band.x.zshift.apriori | band.1.zshift = T | | apriori of shift of the zero line | |
| band.x.zshift.sigma | band.1.zshift = T band.1.zshift.type = {1,2} | | sa of the zero line shift | |
| band.x.beam | | empty | Number of beams beams included two lines for each beam | |
| band.x.beam.y.apriori | band.1.beam /= 0 | | Four values: amp, freq, phase, slope | |
| band.x.beam.y.sigma | band.1.beam /= 0 | | Its standart deviation, if set to 0.0 not retrieved but fixed | |
| band.x.beam.model | | | Channel model PS - phase model IP - interferogram pertubation model | |
| band.x.gasb | | | gases which are retrieved from this band, must be contained in gas (see above) | |
| band.x.tempretb | rt.temperature = T | F | T if temperature is retrieved in this band | |
| band.x.snr | | | initial default snr for all scans in this band. Over ridden by snr from t15asc file and sp window | |
| | | | | |
| sp.snr = x | | | which additional snr windows are taken into account e.g. = 1, the lines containing an 1 are read in, all other lines are ignored. example = 1 2 3 this over rides all previous snr values in this window | |
| sp.snr.x.nu_start | spectrum.snr not empty | | low wavenumber for snr window x | |
| sp.snr.x.nu_stop | | | high wavenumber for snr window x | |
| sp.snr.x.snr | | | snr value for window x | |
| | | | | |
| out.level | | 0 | Output level, a predefined set of putput files | |
| out.gas_spectra | | F | T for write gasfiles | |
| out.gas_spectra.type | | | Type of GASFILE 1 - only the final spectrum, the spectrum of each gas and the solar spectrum will be printed out. The files are named like gas1.1.1, allgases.1.1 and solar 1.1 2 - spectra will be printed out for each iteration. The names are like above,but an extra number is appended denoting the iteration number the numbers appended to the files are "nr of window", "nr of scan" and "nr of iteration" The information of for band nr, gas and iteration number are also contained in the file header | |

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| Additionally to the predefined output acc to the level given in <output> the following quantities can be written out. If such a key is given the resp quantity is written out to the file defined by the parameter string (e.g. output.k-matrix = kk.out - the Kmatrix is written out to kk.out) | | | | |
| out.k_matrix | | F | <filename> matrices written in file (now only: K.out) | |
| Out.g_matrix | | F | Write out complete Gain matrix | |
| out.sa_matrix | | F | <filename> write out SA-matrix (now only: SA.out) | |
| out.smeas_matrix | | F | <filename> write out SM-matrix (error on profile due to the measurement noise (now only: SM.out) | |
| out.shat_matrix | | F | | |
| out.refprofiles | | F | | |
| out.aprprofiles | | F | | |
| out.ak_matrix | | F | | |
| out.ab_matrix | | F | | |
| out.summary | | F | | |
| out.pbpfile | | F | | |
| out.channel | | F | | |
| out.parm_vectors | | F | | |
| out.ssmooth_matrix | | F | | |
| out.sainv_matrix | | F | | |
| out.seinv_vector | | F | | |
| out.raytrace | | F | Write out raytrace | |
| out.raytrace.type | | | Type of raytracing output 1: SA's only 2: Detailed output of the raytrace calculation 3: Old style output files: MIX, MS, PT | |

Output description

Files which may appear but are not described here are a legacy and are subject to modification or removal in the future, so dont relay on them, but notify the maintainers of sfit4 if you need the information contained in them.

| OUTPUT | Contained in Output level | Description |
|----------|---------------------------|---|
| PRFS.out | 0 | contains all profiles of the retrieval gases together with the alitude grid, pressure , temperature and airmass (vertical). For each gas there are five columns: VMR Apriori VMR Retrieved SIGMA VMR RETRIEVED PARTIAL COLUMN A priori PARTIAL COLUMN Retrieved |
| pbpfile | 0 | contains the retrieved, measured spectra and the difference thereof |
| AK.out | 0 | Averaging kernel in units of the internal statevector, i.e. x/x_a |
| Ab.out | 0 | Contains the $G_y K_b$ matrix (see formula 3.16 page 48 in Rodgers (2000) |
| Kb.out | 1 | contains the K_b matrix for all parameters which are not retrieved (and contained in the K-matrix) |
| SM.out | 1 | contains the full matrix of the retrieval noise |
| spc.* | 1 | contains the spectra calculated for each retrieval gas, each iteration (if output.gas_spectra.type = 2) and each microwindow |

References

Boone, C. D.; Walker, K. A. & Bernath, P. F. An efficient analytical approach for calculating line mixing in atmospheric remote sensing applications J. Quant. Spectrosc. Radiat. Transfer, 2011, 112, 980 – 989
Rosenkranz PW. Shape of the 5 mm oxygen band in the atmosphere. IEEE Trans Antennas Propag 1975;AP-23:498–506.
Tran, H.; Ngo, N. & Hartmann, J.-M. Efficient computation of some speed-dependent isolated line profiles Journal of Quantitative Spectroscopy and Radiative Transfer, 2013