Initialisation of sfit4

The general format is

Keyword1.keyword2.keyword3 = value

First keyword:

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 SA 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.

In the section **band** the parameters for all MW bands are defined.

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

In **out** more details of output are defined

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

Key	Dependency	Default	Description
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.modulation_fcn = 4	ils.dat	empirical apodization (measured)
file.in.phase_fcn	fw.phase_fcn = 4	ils.dat	empirical phase error (measured),
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		full inverse matrix
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
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.gain_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, in file.refprofile and file.isotope
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 sa-matrix 1 – Gaussian shape 2 – Exponential shape 4 - the sa matrix is read in from file.sa_matrix 5 – the inverse Sa matrix is read from file.sa_matrix
gas.profile.x.correlation.width	gas.profile.x.correlation = T gas.profile.x.correlation.type =1,2		width of the correlation
gas.profile.x.correlation.minalt	gas.profile.x.correlation = T		correlation calculation starts at altitude

gas.profile.x.correlation.maxalt	gas.profile.x.correlation = T		correlation calculation ends at altitude
gass.profile.x.logstate		F	T if the statevector is ln(VMR)
gas.profile.x.scale			apriori 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=4,5		factor the entries in file.sa_matrix are multiplied
fw.isotope_separation		F	Isotopes are separated
fw.delnu			Half width of integration interval for crosssection calculation
fw.lshapemodel		0	Lineshape model 0 – depends on the spectroscopic values given 2 - Galatry if BETA_T is given, if not Voigt 3 - SDV, if parameters are given
fw.linemixing		F	if T and parameters found, linemixing is included
fw.linemixing.gas			currently only CO2 possible, 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 0 - read from linelist 1 - no shift
fw.apod_fcn		F	Calculate apodization function
fw.apod_fcn.type	fw.apod_fcn = T		Empirical apodiziation

			0 - no empirical apodiziation 1 - tabular function is read in 2 - polynomial 3 - fourier series 4 - linfit output is read in
fw.apod_fcn.order	fw.apod_fcn.type = 2 o. 3		Order of polynomial/fourier series
fw.phase_fcn		F	T if emirical 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
fw.phase_fcn.order	fw.phase_fcn = T fw.phase_fcn.type = 2		Order of polynomial if fw.iephs = 2
fw.emission		F	if T emitted radiation from the atmosphere is calculated
fw.emission.T_infinity	fw.emission = T		Temperatur (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 ligh of the moon (pre-alpha)
fw.emission.normalized	fw.emission = T		spectra are normalized to one (T) or not normalized (F)
fw.raytonly		F	if T only calculate raytracing
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 it 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 retreived 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 lineparameters are calculated, default: all gases which are retrieved predefined values: target – calculation only for the target gas retreival – kb are calculated for each gas which is retrieved.
kb.line.type			1 if all lineparameters of a gas are perturnbed together with the same perturbation (this is the only parameter supported so far) Kb are calculated for: • Intensity • Pressure broadening • Temperature depency of pressure braodening
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 fit
rt.wshift.apriori	rt.wshift = T		apriori of all types of wavenumber shift in [cm^-1]
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_fcn		F	simple phase correction retrieved if T

rt.phase.apriori	rt.phase = T		
rt.phase.sigma	rt.phase = T		
rt.phase_fcn		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		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		F	retrieve shift in solar lines if T
rt.solshift.apriori	rt.solshift = T		
rt.solshift.sigma	rt.solshift = T		
rt.solstrnth		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
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 4 – Triangle 5 - Happ – Genzel 6 – KPNO Atmospheric Spectra 7 – Hamming function
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 o.o 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
sp.snr			which additional snr windows are taken into account e.g. = 1, the lines containing an 1 are read in, all other lines are ignored
sp.snr.x.win.nu_start	spectrum.snr not empty		
sp.snr.x.win.nu_stop			
sp.snr.x.win.snr			
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
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.level		F	0,1,2 for the level of the output (see below)
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.gas_spectra		F	T calculated spectra for each retrieved gas and each band are printed out
out.gas_spectra.type	output.gas_spectra = T	F	1. gas spectra are only for the final iteration written out 2. gas spectra are written out for each iteration
out.raytrace		F	Write out raytrace
Out.raytrace.type			Type of raytracing output

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	Description

	Output level	
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_yK_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 S_ϵ 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