

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	

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	

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		has to be specified	Lineshape model 0 - depreciated and removed 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	

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	
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	

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	
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	

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	

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	out.gas_spectra = T		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.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.ak_matrix.type	out.ak_matrix = T	1	Type of AK matrix file 1 - (default) AVK matrix only for the target species 2 -AK matrix for the full retrieval	
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