Brief description of output files
20200709 / v1.0

The file.out. section allows renaming of the output file names. The out. section determines which files are output by a grouping and individually as well. Each file has a header that can identify the retrieval. For instance from a parm.out file:

SFIT4:v1.0.8 :Off-Release -- June 2020 RUNTIME:20200709-11:11:24 STATE VECTOR FACTORS BY ITERATION N VECTOR

word 1 is the version:
SFIT4:v1.0.8

word 2 is the runtime this file was made
RUNTIME: 20200709-11:11:24

the rest of the line is a description of the file:
STATE VECTOR FACTORS BY ITERATION N VECTOR

All files so far are ascii. Here are some variables used in the file headers to help dimensioning and reading.

NLEV - number of layers in retrieval grid
NVAR - number of retrieval parameters
NFIT - number of spectral points fit
NKB - number of model parameters other jacobians were calculated for
NMOL - number of all possible molecules from reference.prf
NRET - number of retrieved gases profile + column
NBAND - number of micro-windows
NFITS - number of spectra * number of bands
ISMIX - next index in retrieval parameter array is the start of vmr's

Output Files Section

out.level	= 1
out.gas_spectra	= T
out.gas_spectra.type	= 1
out.sa_matrix	= T
out.statevec	= T
out.k_matrix	= T
out.shat_matrix	= F
out.retprofiles	= T
out.aprprofiles	= T
out.ab_matrix	= F
out.ak_matrix	= T
out.summary	= T

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out.pbpfile                = T
out.channel                = F
out.parm_vectors           = T
out.seinv_vector           = F
out.sainv_matrix           = F
out.smeas_matrix           = F
out.ssmooth_matrix         = F
out.raytrace               = F
out.raytrace.type          = 0
out.solarspectrum          = F
out.levmardet              = F
out.xscdetail              = F
```

output. Level = 1:
out.statevec
statevec - initial and retrieved values of the retrieved parameters - mostly unchanged from sfit2 except first line contains several variables and flags: nlev, iter, itrmax, iftemp, converge, divwarn

out.aprprofiles
apriori profiles - a table of the alt, temperature, pressure, airmass and vmrs after raytracing and isotope separation at the start of the retrieval on the retrieval grid. First line is: nmol, nlev, nret, retrieved_gas_name(1:nret)

out.retprofiles
retrieved profiles - a table of the alt, temperature, pressure, airmass and vmrs after the retrieval - same format as the apriori files
First line is: nmol, nlev, nret, retrieved_gas_name(1:nret)

out.pbpfile
pbpfile - observed, calculated and difference spectra, first line is nfits, nband

out.summary
summary - summary of retrieval details in table form (still needs work)

out.k_matrix
retrieved parameters final jacobian matrix (array transposed from sfit2 k.out!) first line is nfit, nvar, ismix, nlev

out.sa_matrix
apriori covariance matrix - full covariance as computed before and used in retrieval - except in cases where the inverse cannot be calculated, that section is read in later. First line is nvar, nvar.

Output.level = 2:

out.ak_matrix
averaging kernels matrix - for target gas only, first line has nlev, nlev

out.ab_matrix
G*Kb matrix - write out Ab (G*Kb) in fractions of A priori, corresponds to formula 3.16 page 48 in Rodgers and can directly be used for the error calculation. The first line has: nlev, nkb, -1 -1

out.smeas_matrix
measurement error matrix - measurement error with retrieval se nlev x nlev matrix for target gas only. First line is nlev, nlev.

out.sainv_matrix
inverse of sa matrix as used in the retrieval. First line is nvar, nvar.

out.seinv_matrix
inverse of spectra error covariance (diagonal) matrix as used for instance after any de-weighting has been imposed. First line is nfits, 1

out.shat_matrix
final sa matrix - a posterior covariance on the retrieved parameters. First line is nvar, nvar.

out.ssmooth_matrix
smooth error matrix on the target gas nlev x nlev using retrieval parameters - may not be too useful. First line is nlev, nlev.

out.parm_vectors
parameters by iteration - these may be parameter values or scale factors depending on how the variable is used internally. First line is nvar.

out.gas_spectra
gas spectra - ascii files of spectra for each gas, solar spectra and all non-retrieved gases with the calculated background, shifts etc. see type.

out.gas_spectra.type
gas spectra type
1 - files are output by gas, band and scan for the final iteration
2 - files are output by gas, band and scan for every iteration

The calculation is performed assuming only GAS is present in the atmosphere, everything else is set to zero. NOTE: the spectra for the single files do not add up to give the final spectrum, because the spectral contributions ar enot additive.

Those file are named spc.GAS.01.01.01

meaning the spectrum for the gas GAS first microwindow, first scan, first iteration

GAS can be
ALL – the complete forward spectrum
REST – The spectrum of all gases except the retrieved gases
SOL – the calculated solar spectrum
the gasname of a retrieved gas (from the lists gas.profile or gas.column in sfit4.ctl)

The format of the file is the same as the format for file.in.spectrum, except the first two lines are empty and the third line describes what is in the file itself, e.g.

in the file spc.sol.01.01.03
GAS SOLAR BAND 1 SCAN 1 ITER 3

Output level = 3:
These are mostly very low-level code debugging outputs.

out.channel
channel spectra - mainly useful for debugging channel calculation

out.raytrace
raytrace detail - see raytrace type (not fully implemented yet)

out.raytrace.type
raytrace type:
1 - prints raytrace.sa a series of possible vmr sa's based on the retrieval grid
2 - prints old .mix, .pt, .ms files
3 - prints detailed raytracing output

out.solarspectrum
solar spectra - from solar calculation module - slightly different format from out.gas files

out.levmardet
levenberg-marquardt details - limited extra info on lm calculations

out.xscdetail
cross-section details - limited extra information on cross-section calculations