Brief description of output files
20130502 / v0.9.2

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:V0.9.2:20130502 RUNTIME:05/02/2013-14:27:17 STATE VECTOR FACTORS BY ITERATION N VECTOR

word 1 is the version:
SFIT4:V0.9.2:20130502

word 2 is the runtime this file was made
RUNTIME:05/02/2013-14:27:17

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

```
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.

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

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