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