Sfit4 Outputs

Two foci of sfit4 Development

1. Flexibility – Exploratory analysis tool
   i. S_a (S_a^{-1}) definition / direct input
   ii. Background parameters (slope, curvature, zero)
   iii. Shifts, by species, by fit
   iv. Channeling
   v. SNR by region
   vi. Multiple regions / SZA
   vii. Fit gas by region
   viii. Phase, ME
   ix. Isotope separation
   x. Solar background /shift
   xi. Levenberg-Marquardt non-linear iteration scheme
   xii. Emission spectra
   xiii. Log(vmr) retrieval
   xiv. Line mixing (co2, ch4 soon…)
   xv. SDV speed dependent Voigt lineshape
   xvi. Spectra output by layer / gas
   xvii. O2 CIA line data included

2. Process & I/O Speed – NDACC operational processing
   i. Standard layering
   ii. Binary HITRAN input
   iii. Binary output for HDF ?

outputs

- Output can be set to 3 levels of detail
  - Plus any given output file can be switched off or on
- Any output file (other than sfit4.dtl – detail file) can be renamed
- Many output files have been reformatted for easy read / write by batch scripts
- All output files have version tag and timestamp
- *Direct binary or hdf output still planned*

output files

See: docs/output_descrip_v4.docx

- output level set to 1
  - Statevevctor file
  - Apriori profiles
  - Retrieved profiles
  - Final Calculated, observed and difference spectra
  - Fit summary
  - Averaging kernels
  - Complete Sa matrix
- output level set to 2
  - K matrix
  - K_b matrix
  - AB matrix
  - Measurement error
  - Sa Inverse matrix
  - Se inverse matrix
  - Shat matrix
  - Retrieval-Calculated Smoothing error
  - Parameter array by iteration
  - Spectra by gas
- output level set to 3
  - Channel spectra diagnostic
  - Raytracing diagnostics
  - Solar spectra calculation
  - L-M diagnostics
  - Cross-section diagnostics
- gas spectra type
  - =1 final spectra by gas, and fit
  - =2 and by atmospheric level
- raytrace type
  - =3 verbose output
  - =2 obsolete fastcode output

Common Header

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

Common Parameters for indexing file contents

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 Switches

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 1/2

out.statevec
statevec - initial and retrieved values of the retrieved parameters - mostly unchanged from sfit2 except first line contains several variables and flags:
Key Line: 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.
Key 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
Key line is: nmol, nlev, nret, retrieved_gas_name(1:nret)

Output Level 1 2/2

out.pbpfile
pbpfile - observed, calculated and difference spectra,
Key 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!)
Key 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.
Key line is nvar, nvar.

Output Level 2

out.ak_matrix
averaging kernels matrix - for target gas only, **Key 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. **Key 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. **Keyline is nlev, nlev.**

out.sainv_matrix
inverse of sa matrix as used in the retrieval. **Key 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. **Key line is nfits, 1**

Output Level 2 2/2

out.shat_matrix
final sa matrix - a posterior covariance on the retrieved parameters.
Key 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. **Key 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. **Key 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

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

Output Level 3

1

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