

SFit4 Updates for 2013

J Hannigan, M. Palm, N. Jones



Jan/28/2013



IRWG/NORS Error Analysis Workshop,
NCAR, January 2013

Two foci of sfit4 Development

1. Flexibility – Exploratory analysis tool

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

2. Process & I/O Speed – NDACC operational processing

- i. Standard layering
- ii. Binary HITRAN input
- iii. Binary output for HDF ?

Sfit4 current version d0.9.2.1

- log scaling of vmr by gas
- include emission of atmosphere & source (moon)
- analytic derivatives for vmrs
- Levenberg-Marquardt iterative scheme
- internal raytracing module
- line mixing for CO₂ (ch₄...)
- speed dependent Voigt (from C Boone)
- tagged - variable input format
- arbitrary SZA / μ window / resolution
 - Spectral process code to support it
- binary HITRAN input – end of cfl files
- Pre-raytrace isotope separation scheme
- spectra-centric parameters in ascii spectra data file

required inputs

sfit4.ctl

Retrieval specific params:

- *Region*
- *Species*
- *State vector*

t15asc4

- *Spectrum specific params:*
- *Date/Time*
- *Solar zenith angle*
- *N spectra*

stations.layers

- *Layering for each site*
- *From WACCM*

reference.prf

- *Z-p-T for reference profiles*
- *Reference (apriori) chemical profiles*

Binary (HITRAN) Line list file

required output

sit4.dtl (detail file)

- *Step-by-step of retrieval process*

sfit4
raytracing
retrieval

auxiliary inputs

- *isotope separation data (new format)*
- instrument phase function
- instrument modulation function
- retrieval mixing ratio predefined covariance
- retrieval mixing ratio predefined inverse covariance
- solar line list

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
 - Statevector 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

new HITRAN data input scheme

See: docs/hbin_descrip_v4.docx

Predefined directory structure:

```
001_H2O:
  01_hit08.par
  01_hit08.zip
  01_hit09.par
  01.H2O
002_CO2:
  02_hit08_f53.par
  02_hit08_f53+LM.par
  02_hit08.zip
  02.CO2
  co2_lm.dat
  read_out_example.txt
.
.
.
```

Stand alone code *hbin.f90* compiled with *sfit4* is run before *sfit4* call.

*hbin** reads files:

- *sfit4.ctl*
- *hbin.input*
- *isotope.input*
- Hitran files directly

hbin is run
once for a
specified
retrieval

Writes file: *lllll.dddddd-hhhhh.dddddd.hbin*
Sorts all lines in wavenumber order, edits id numbers, separates isotopes, can choose gases and adds flags for:

- CIA
- line mixing parameters
- Galatry parameters
- SVD parameters

(slightly) new isotope separation input scheme

See: docs/isotope_descrip_v4.docx

Main differences:

- I. Profile for new gas is now on pre-raytrace or 'refmod' grid
- II. There are no default pre-separated species
- III. You can add subsequent isotopes to the new species that will use the new profile eg.
 - a. H_2O 1/4 \rightarrow HDO 80/1 (HD^{16}O)
 - b. H_2O 1/5 \rightarrow HDO 80/2 (HD^{18}O)
 - c. H_2O 1/6 \rightarrow HDO 80/3 (HD^{17}O)

(slightly) new ascii spectral data file

header for each block:

```
37.26100 6385.44500 40.03800 254.76000 402.3
    2011    6    23    16    24    11
06/23/2011 16:24:11UT Z:37.261 A:284.29 D:0101.7 R:0.0035 P:BX F:01.9139mr
4881.8975000000000 4888.1025000000000 2.5000000000000005E-003 2483
0.315438E+00
0.293434E+00
0.285126E+00
0.271612E+00
0.240477E+00
.
```

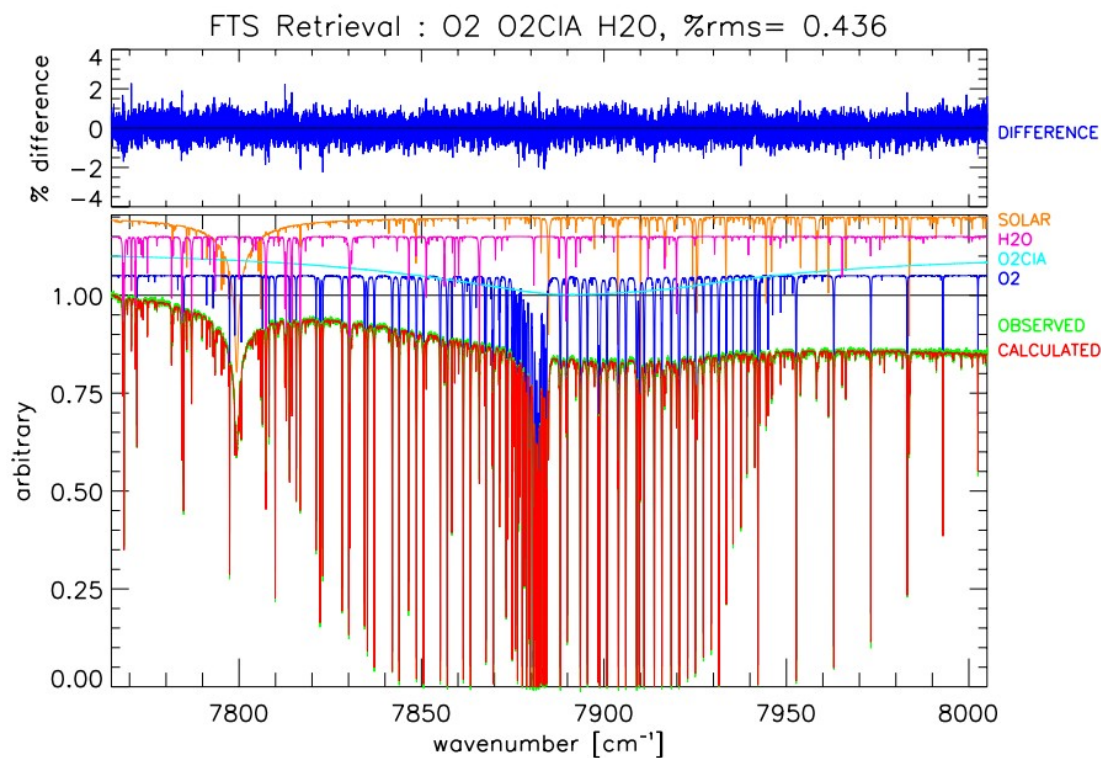
KEY:

SZA° radius_of_earth [km] latitude [°N] longitude [°E] SNR
YYYY MM DD HH MM SS
arbitrary ascii comment, 80 characters
start_wn end_wn point_spacing Npoints
spectra values...

- ✓ Any number of blocks are ok
- ✓ All blocks with spectra within sfit4.ctl band limits will be fit
- ✓ Spectra will be truncated to sfit4.ctl band limits

Calculated Kb

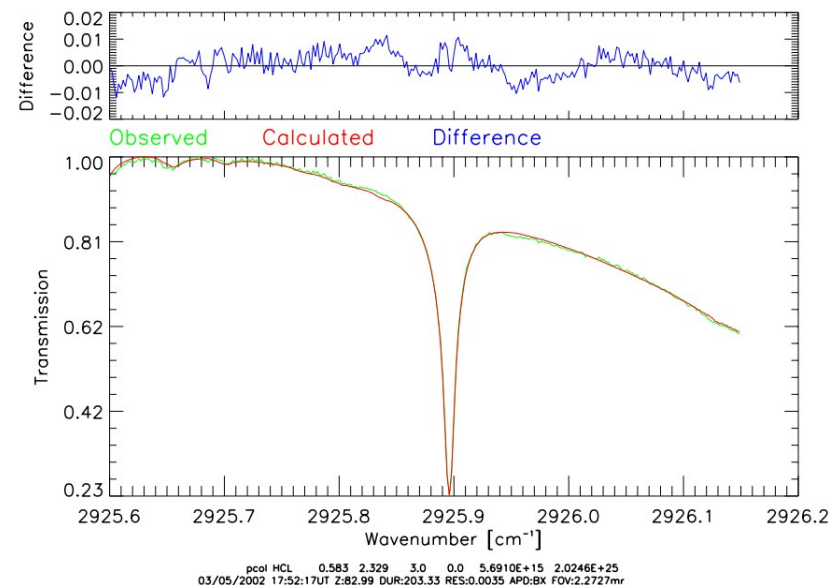
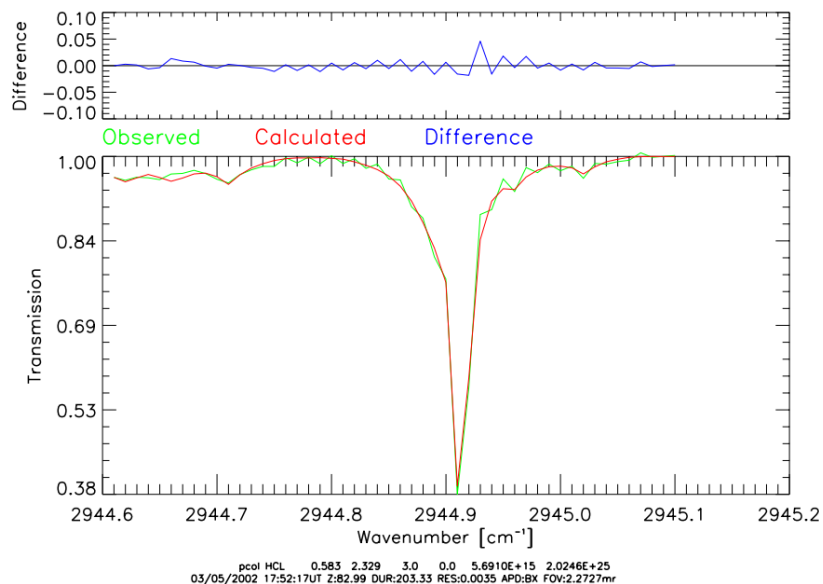
- temperature
- background
 - Slope
 - curvature
- solar shift
- solar line strength
- phase
- differential wavenumber shift
- wavenumber shift
- apodization function
- phase function
- zero level shift
- solar zenith angle
- field of view
- optical path difference
- hitran line parameters for retrieval or target gas
 - Strength
 - Pressure broadening
 - Broadening temperature dependence



Sample Retrieval O₂, O₂CIA & H₂O

Self & Foreign CIA lines use same O₂ profile

– Wollongong data



Example: HCl

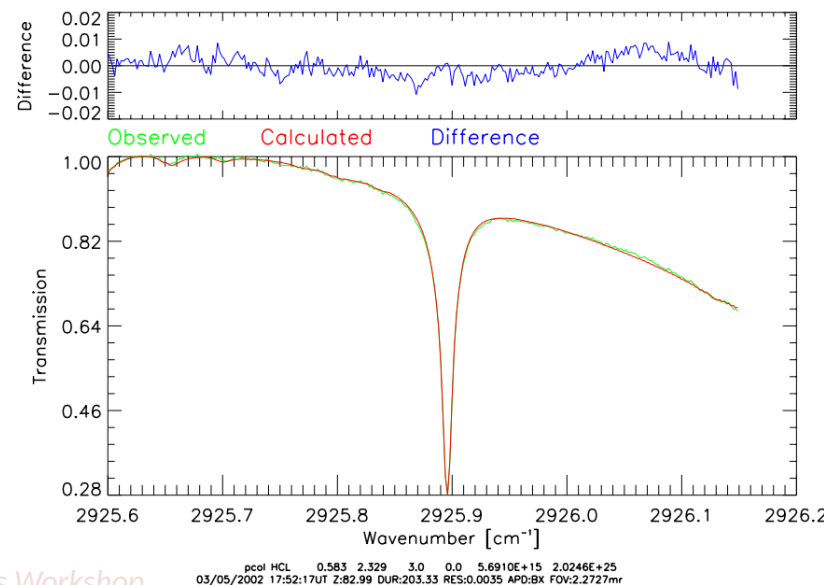
2925 / 84.62 / 250cm

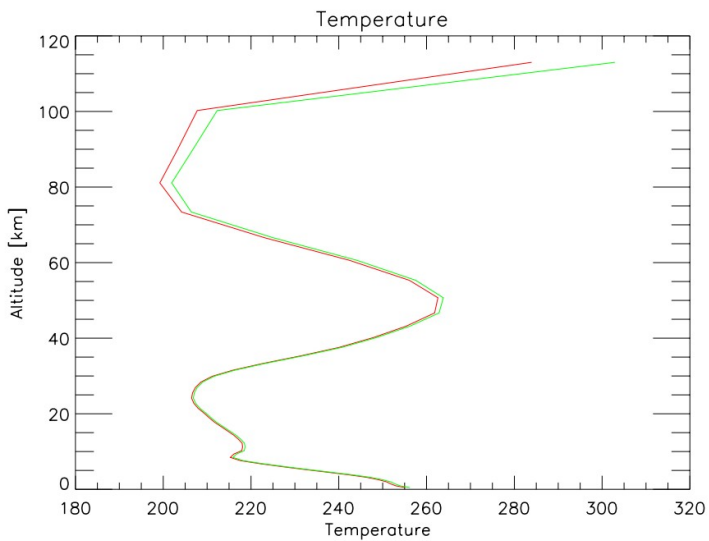
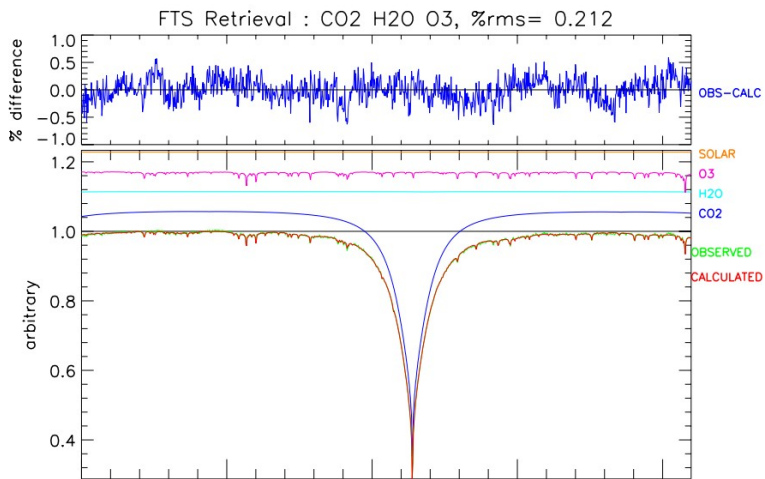
2925 / 83.11 / 250cm

2944 / 82.99 / 100cm

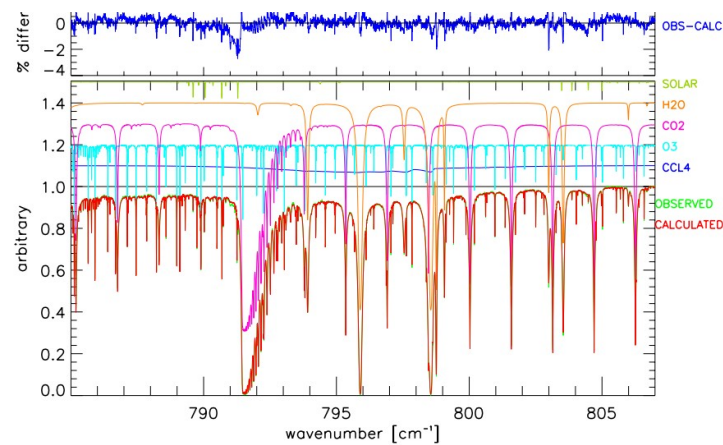
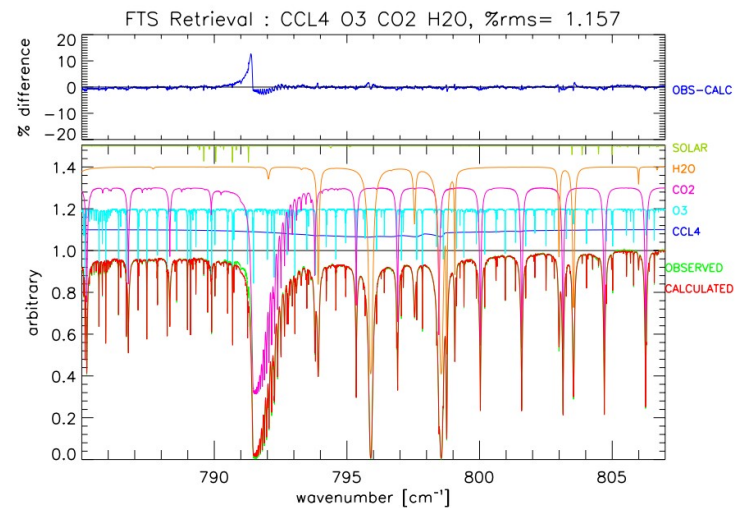
Single retrieval from 3 spectra with different SZA
and resolutions. *

*all spectra from one μ w must have same
resolution & point spacing.

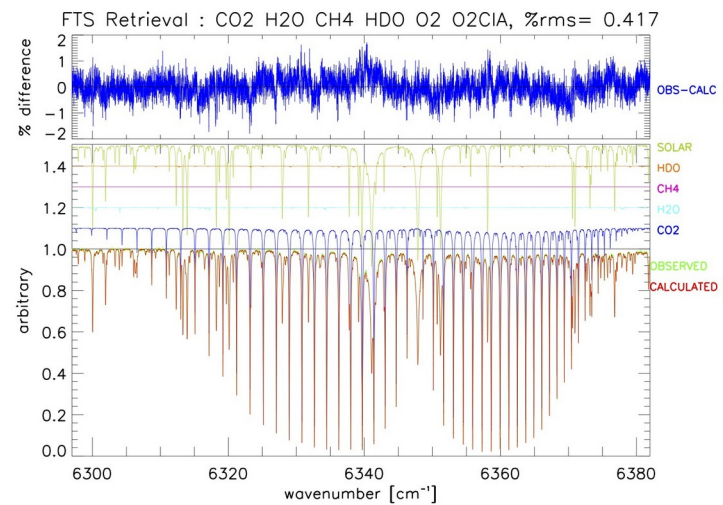
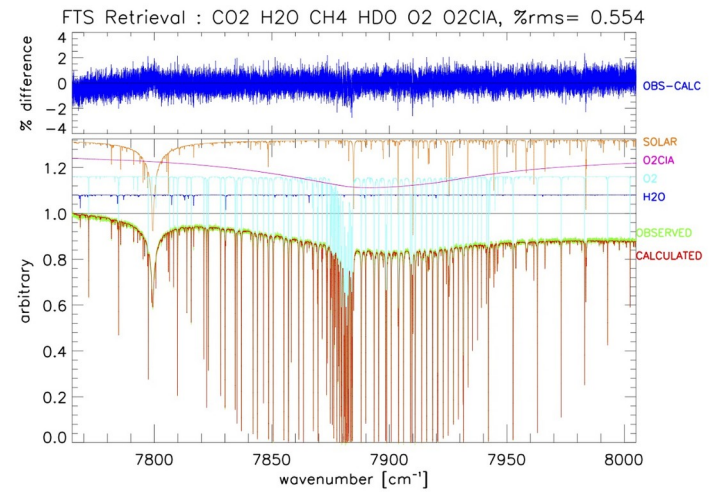
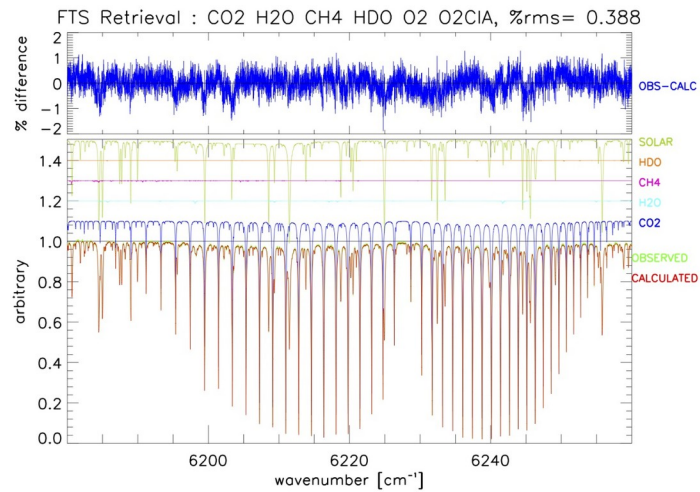




Work in progress
Retrieval of temperature profile from
single CO₂ absorption feature



Line Mixing required for CCl₄
Only CO₂ so far



Simultaneous fit CO2, CO2 & O2

Bialystok, Poland

Status

- Current version d0.9.2.1 with several testcases available :
 - ftp://acd.ucar.edu//user/jamesw/IRWG_NORS_EW/sfit4/delta
- Input / output files & formats complete
- Derivatives of several retrieval / model parameters calculated for error analysis (K_b)
- Temperature retrieval in process
- Testing / bug fixes in process
- Suite of testcases for IRWG windows in process
- Python based spectral processing environment in process
 - *A hot topic next week!*
- Some (but not complete) documentation available

end

Latest Release Version SFIT2 V3.94

- SFIT2 v394 delivered Winter '09
 - Primarily HITRAN 08 & molecular database
- But also
 - Perturbation ability: Added flags to make small changes in
 - line intensity
 - Air broadened halfwidth
 - Use CH₃CH from H08 and previous pseudolines as CH₃CNPL
 - Bug fixes eg writing second Sa off diag elements
 - Intensity scaling in isotope substitution
 - Output Sa.complete, Parm.out, Prfs.out
 - Better use of matrix intrinsics
- Lapack version available 3.94LP
 - Matrix inversion
 - direct output: AK & AK Eigenvectors, Smoothing error

Log scaling of Retrieval Gases

- New flag in binput to switch on or off
- $\text{vmr} \rightarrow \ln(\text{vmr})$
- Output (K-matrices and AVK) changed accordingly
- Schneider and Hase (2009) for more information
- Retrieval of ratio (e.g. HDO/H₂O; Schneider et. al., 2006) only possible via extra SA matrix, not checked yet...

Schneider, M.; Hase, F. & Blumenstock, T. Ground-based remote sensing of HDO/H₂O ratio profiles: introduction and validation of an innovative retrieval approach Atmos. Chem. Phys., 2006, 6, 4705-4722

Schneider, M. & Hase, F. Ground-based FTIR water vapour profile analyses Atmos. Meas. Tech., 2009, 2, 609 - 619

Emission modelling

- New switch emission modelling off or on
- Input Temperature of blackbody radiation at TOA
- Switch: E – emission, M - for reflection of sunlight on moon)
- Switch: Units Watt/(cm⁻¹ sr cmr²)
- Switch: - spectrum normalized

V 4.00 *continued*

What do the changes mean?

- More versatile, faster!
- New inputs: bininput, fastcode, t15asc
 - Some new coding for you
 - Ease for new users
 - Zyper2 future's is unknown?
- Support code
 - Preping spectra
 - Simple scripts for running – not quite batch processing
- Users Meeting Planned

Levenberg-Marquardt Iteration Scheme

- New flags in binput:
- Switch: for Gauss-Newton iteration or Levenberg-Marquardt iteration-scheme
- Value of start for gamma
- Value for decrease of gamma if successful
- Value for increase of gamma if not successful
- Value to break off if cost does not decrease more than 0.5

Sample Output:

```
ITER= 8 RMS(%)= 0.0718869 NVAR=117 NFIT= 311
chi2_x    = 9.7670E-01          cost for state vector
chi2_y    = 2.0671E+00          cost for spectrum
chi2      = 3.0438E+00          cost sum
chi2_old  = 3.4307E+00          cost of last successful iteration
d chi2    = 3.8689E-01          change in cost (decrease is positive)
gamma     = 1.0e3               actual value of gamma
```

• Chi2_y is set up in a way, that it is 1 if the noise given (in binput) is the same as spectral noise and residual is perfect.

map of Input & output files ... needs to be cleaned up

! --- SET DEFAULT FILENAMES

TFILE(08) = 'pbpfile'

! --- ISOTOPE SEPARATION FILE

TFILE(09) = 'isotope.input'

TFILE(15) = 't15asc'

TFILE(16) = 'detail'

! --- STATEVEC

TFILE(18) = 'statevec'

! --- SET MIXOUTPUT FILENAME AS STATE VECTOR FILENAME + .MXF

TFILE(17) = TRIM(TFILE(18))/' '.mxf

! --- SAVED SYNTHETIC SPECTRUM

TFILE(19) = 'synspec.out'

! --- SUMMARY

TFILE(20) = 'summary'

! --- SET PARTIAL COLUMN OUTPUT FILENAME AS STATE VECTOR FILENAME + .PRC

TFILE(22) = TRIM(TFILE(18))/' '.prc

! --- EMPIRICAL MODULATION FUNCTION

TFILE(23) = 'ils.dat'

! --- EMPIRICAL PHASE FUNCTION

TFILE(24) = 'ils.dat'

! --- CHANNEL OUTPUT

TFILE(30) = 'chnspec.data1'

TFILE(40) = 'chnspec.data2'

! --- SET SHORT FILENAME AS SUMMARY FILENAME + .ST

TFILE(31) = TRIM(TFILE(20))/' '.st

! --- DEFAULT FIRST RETRIEVAL GAS SA OUTPUT FILENAME

! --- OUTPUT DEPENDS ON NAME SA .NORM, .VMR, .PCOL

TFILE(61) = 'Sa.norm'

! --- DEFAULT SAINV INPUT FILENAME

TFILE(62) = 'Sainv.input'

! --- DEFAULT COMPLETE SA OUTPUT FILENAME

TFILE(63) = 'Sa.complete'

! --- DEFAULT K,SE,SA MATRICES OUTPUT FILENAME

TFILE(66) = 'K.out'

! --- SE OUTPUT

TFILE(67) = 'Se.out'

! --- DEFAULT K TRANSPOSED FILENAME

TFILE(68) = 'KT.out'

! --- LEVENBERG-MARQUARDT DETAILS

TFILE(70) = 'detail.opt'

! --- LAYERING SCHEME - OUTPUT FROM WACCM PROFILES

TFILE(71) = 'station.layers'

! --- REFERENCE VMR PROFILES

TFILE(72) = 'reference.prf'

! --- RAYTRACE DETAILED OUTPUT AKA TAPE6

TFILE(73) = 'raytrace.out'

TFILE(74) = 'raytrace.pt'

TFILE(75) = 'raytrace.ms'

TFILE(76) = 'raytrace.mix'

TFILE(77) = 'raytrace.sa'

TFILE(78) = 'raytrace.pnch'

! --- RESERVED FOR GASOUT NAME CHANGES - SEE FRWDMDL.F90

!TFILE(80)

TFILE(81) = 'AK.out'

TFILE(82) = 'SM.out'

TFILE(83) = 'SS.out'

TFILE(84) = 'A-S.out'

TFILE(85) = 'AEIGEN.out'

TFILE(88) = 'PRFS.out'

TFILE(89) = 'Parm.out'

TFILE(91) = 'Spec.out'

General

```
file.stalayers      = station.layers
file.refprofile     = reference.prf
file.spectrum       = tl5asc.4
file.eap_dat        = ils.dat
file.epps_dat       = ils.dat
file.sa_matrix      = sa.input
file.isotope        = isotope.input
file.solarlines     = ../line1ist/solar/120621/solar.dat
file.line1ist       = ./02723.690800-02930.039200.hbin
```

(Very new) sfit4.ct1

General I/O files

Definition for retrieval gases

```
gas.layers          =          47
gas                 = HCL CH4 O3 HDO N2O NO2
gas.HCL.ifoff       =          1
gas.HCL.zwid        =          3.000
gas.HCL.zmin        =          0.225
gas.HCL.zmax        =        120.000
gas.HCL.logstate    =          F
gas.HCL.ifprf       =          T
gas.HCL.sigma       =
  0.62398  0.33613  0.33382  0.22898  0.14726
  0.14435  0.14265  0.14204  0.14226  0.14383
  0.14538  0.14531  0.14490  0.14430  0.14320
  0.14272  0.14354  0.14652  0.15191  0.15851
  0.16395  0.16691  0.17080  0.17993  0.19615
  0.21887  0.24784  0.27969  0.30479  0.32309
  0.34501  0.37861  0.42903  0.50225  0.58601
  0.62527  0.61862  0.63071  0.73872  0.92782
  1.08104  1.19786  1.28879  1.35951  1.42124
  1.46301  1.48165
gas.CH4.ifprf       =          F
gas.CH4.sigma       =
  1.00000  1.00000
```

Retrieval Gases

Forward model parameters

```
fw.delnu            =          0.10000
fw.lshapemodel      =          0
fw.linemixing       =          T
fw.linemixing.gas   = CO2
fw.solar            =          T
fw.solar.shift      =        0.00000
fw.ifps             =          F
fw.ieap             =          4
fw.neap             =          0
fw.iepps            =          4
fw.nephs            =          0
fw.emission         =          F
fw.ifiso            =          T
fw.write_k          =          T
fw.write_gasfiles   =          T
fw.write_gasfiles.type =          1
```

Forward Model Parameters

IRWG/NORS Error Analysis Workshop,
NCAR, January 2013

Retrieval parameter

```

rt                =          T
rt.write_sa       =          F
rt.lm             =          F
rt.lm.gamma_start =      100000.
rt.lm.gamma_dec   =       10.0
rt.lm.gamma_inc   =       10.0
rt.convergence    =       0.1
rt.tolerance      =       0.05
rt.max_iteration  =       15
rt.wshift         =       2
rt.wshift.apriori =     0.000
rt.wshift.sa      =     0.100
rt.slope          =          T
rt.slope.apriori  =     0.000
rt.slope.sa       =     0.100
rt.solar          =          T
rt.solar.apriori  =     1.000
rt.solar.sa       =     0.500
rt.ifdiff         =          T
rt.temperature    =          F
rt.raytonly       =          F

```

Retrieval parameters

Microwindows and their parameters

```

band              =    1 2
band.1.nu_start   =      2727.730
band.1.nu_stop    =      2727.830
band.1.zshift     =          0
band.1.zshift.apriori =     0.000
band.1.zshift.sa  =     0.200
band.1.beam       =          0
band.1.dn         =     0.800E-03
band.1.wavfac     =          1.000
band.1.pmax       =      257.143
band.1.omega      =       2.273
band.1.iap        =          0
band.1.snr        =      200.000
band.1.gasb       = HCL    03    HD0

```

```

band.2.nu_start   =      2775.700
band.2.nu_stop    =      2775.800
band.2.zshift     =          0
band.2.zshift.apriori =     0.000
band.2.zshift.sa  =     0.200
band.2.beam       =          0
band.2.dn         =     0.800E-03
band.2.wavfac     =          1.000
band.2.pmax       =      257.143
band.2.omega      =       2.273
band.2.iap        =          0
band.2.snr        =      200.000
band.2.gasb       = HCL    03    N20

```

Band Parameters