SFit2 Updates for 2010

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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 CH_3CH from H08 and previous pseudolines as CH_3CNPL
  - 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
- SIMUL v117: TIPS / HITRAN 08, Faster!

V4.00 *progressing*

- Largely work of Mathias Palm
  - Log scaling of vmr by gas
  - Include emission of atmosphere & source (moon)
  - Analytic derivatives for vmrs
  - Levenberg-Marquardt iterative scheme
  - This is combined with v394lp…
- In development
  - New raytracing module (from lblrtm v9.8)
    - This will be a subroutine leading to temperature retrievals
  - Line mixing for CO2 Q-Branches (from J-M Hartman (Philippe))
  - Speed dependent Voigt (from C Boone)
  - New tagged - variable input format (with reader & writer)
  - Retrieval of a function of VMR
  - Arbitrary SZA/µwindow + code to support it
  - Support for cross-section data

Log scaling of Retrieval Gases

- New flag in binput to switch on or off
- vmr $\longrightarrow$ ln(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 cmr^2)
- Switch: - spectrum normalized

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
chi_2_y  =  2.0671E+00                    cost for spectrum
chi2     =  3.0438E+00                    cost sum
chi2_old =  3.4307E+00                    cost of last successful iteration
d chi_2  =  3.8689E-01                    change in cost (decrease is positive)
gamma    = 1.0e3                          actual value of gamma
```

- Chi_2_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.

V 4.00 *continued*

What do the changes mean?

- More versatile, faster!
- Remove explicit isotope separation
- New inputs: binput, fastcode, t15asc, vmr profiles
  - Some new coding for you
  - Ease for new users
  - Zypher2 future's is unknown?
- Support code
  - Preping spectra
  - Simple scripts for running – not quite batch processing

- Users Meeting Planned

```
# General I/O Files
input.file.mass_paths           fasc.ms
input.file.press_temp           fasc.pt
input.file.mix_ratios           fasc.mix
input.file.ascii_spec           t15asc
input.drct.HITRAN_linelist       /data2/cfgl_orig/
input.file.solar_linelist       /data2/solar5/090525.dat

output.file.detail              detail
output.file.spectra             pbpfile
output.file.summary             summary
output.file.statevec            statevec
output.file.K                   K.out
output.file.Sa                  Sa.out
output.file.simul               0

# Definition for retrieval gases
ret.gas.N                       4
input.flag.isotope              .TRUE.
input.file.isotope              isotope.inp

gas.1.name                  O3
gas.1.flag.ret              1
gas.1.scale                 1.0
gas.1.flag.cov              4
gas.1.ilcor.width           4.000
gas.1.ilcor.minZ            0.610
gas.1.ilcor.maxZ            100.000

# Retrieval parameter
rt.lm.flag                   .TRUE.
rt.lm.gamma_start            100000.000
rt.lm.gamma_dec              10.000
rt.lm.gamma_inc              10.000
rt.lm.stop                   0.500

rt.ftflg.wavenumber_shift    1
rt.prior.wavenumber_shift    0.000
rt.sigma.wavenumber_shift    0.100
```

1. Section of New (B)Input (on left)

Grouped by :
#General I/O files
#Retrieval Gases
#Retrieval parameters
#Band Parameters
#Forward Model Parameters

2. Atmosphere Model Input
Also new tagged format

3. a Priori profiles
No change

4. Spectra
Same ‘t15asc’ but tagged with time and SZA

- end