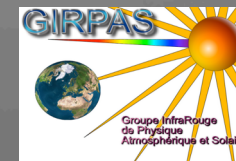


# SFit2 Updates for 2010

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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<sub>3</sub>CH from H08 and previous pseudolines as CH<sub>3</sub>CNPL
  - 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 CO<sub>2</sub> 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/ $\mu$ window + code to support it
  - Support for cross-section data

# 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/H<sub>2</sub>O; 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/H<sub>2</sub>O 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<sup>-1</sup> sr cmr<sup>2</sup>)
- 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
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 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: bininput, 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                03
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