# SFIT4 – a comprehensive tool to analyze atmospheric spectra measured by ground-based FTIR spectroscopy.

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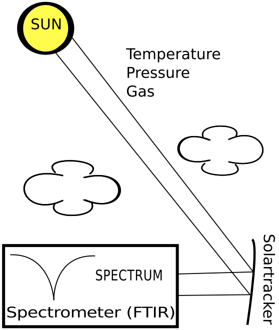
Boulder, 2019

# Introduction

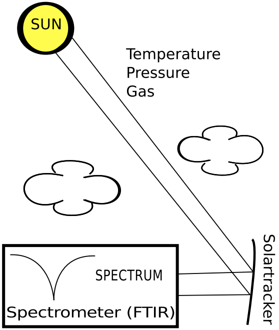
## Absorption spectroscopy




Measurements in solar or lunar absorption and emission possible

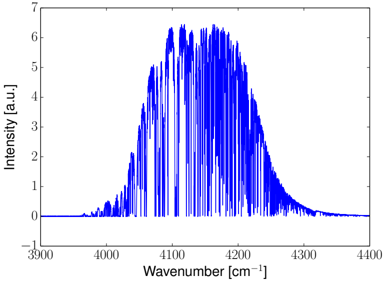
# Introduction

## Absorption spectroscopy




Measurements in solar or lunar absorption and emission possible

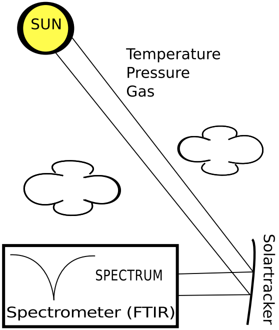
Received spectrum given by the sum of all absorption along the path of sight.




Envelope defined by band filter 3900 - 4400 $cm^{-1}$

# Introduction

## Absorption spectroscopy

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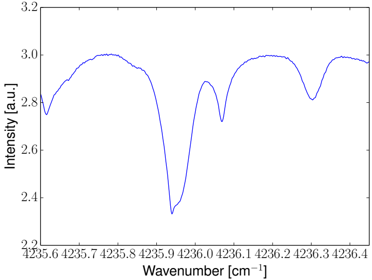
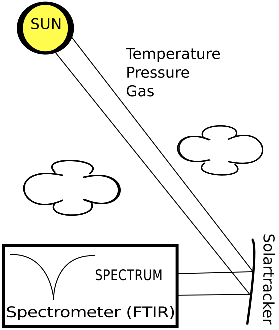



Microwindow containing a CO-line

# Introduction

## Absorption spectroscopy

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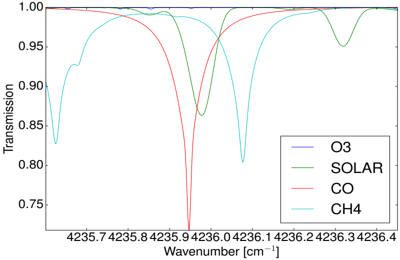
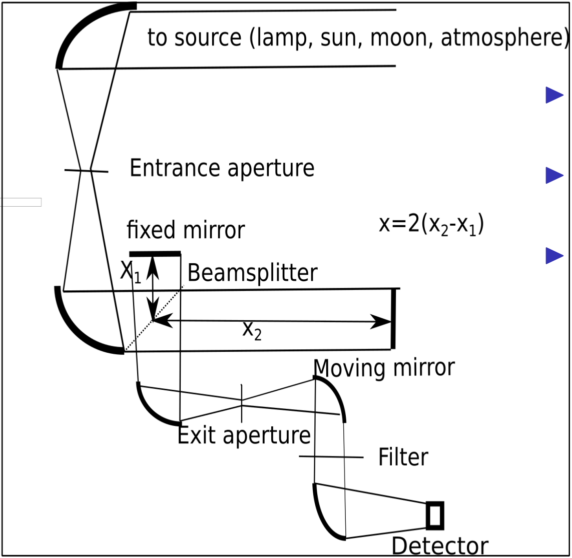



Contribution of gases and solar lines not calculated for this particular spectrum

# Introduction

## Principle of a Fourier transform spectrometer




- apertures define and restrict field of view
- aperture influences resolution
- filter restricts wavelength sensitivity

# Contents

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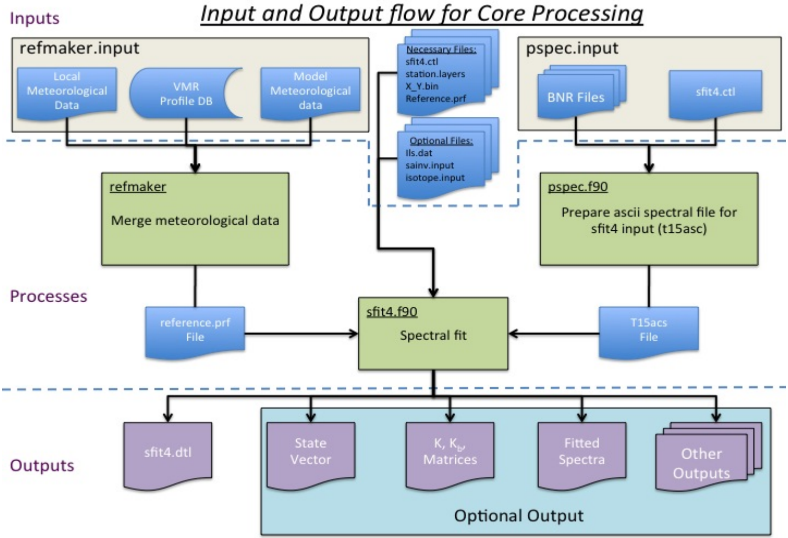
Inputs
Input and Output flow for Core Processing
refmaker.input
Local Meteorological Data
VMR Profile DB
Model Meteorological data
Necessary Files:
sfit4.ctl
station.layers
X_Y.bin
Reference.prf
Optional Files:
lls.dat
sainv.input
isotope.input
pspec.input
BNR Files
sfit4.ctl
refmaker
Merge meteorological data
pspec.f90
Prepare ascii spectral file for sfit4 input (t15asc)
Processes
reference.prf File
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Other Outputs
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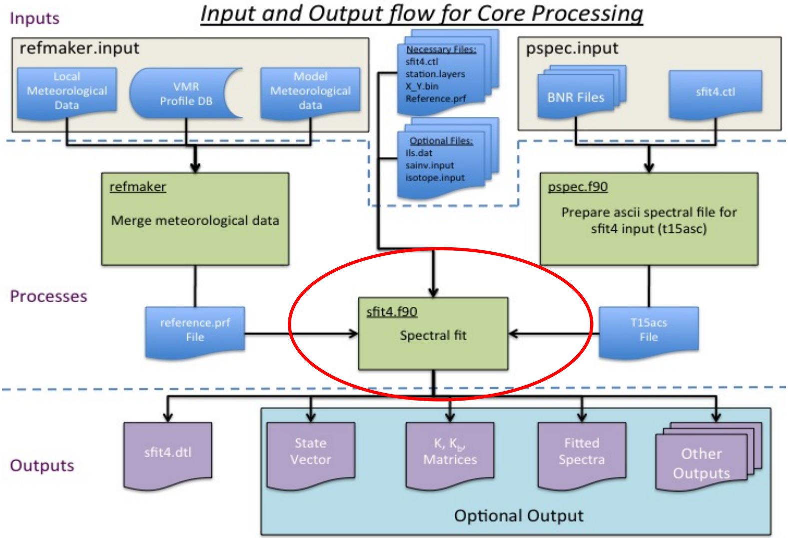
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# Overview of sfit4 package

GEOPHYSICAL RESEARCH LETTERS, VOL. 7, NO. 7, PAGES 489-492, JULY 1980

STRATOSPHERIC $NO_2$ AND $H_2O$ MI..NG RATIO PROFILES FROM HIGH RESOLUTION INFRARED SOLAR SPECTRA USING NONLINEAR LEAST SQUARES

E. Niple, W. G. Mankin

National Center for Atmospheric Research, Boulder, Colorado 80307

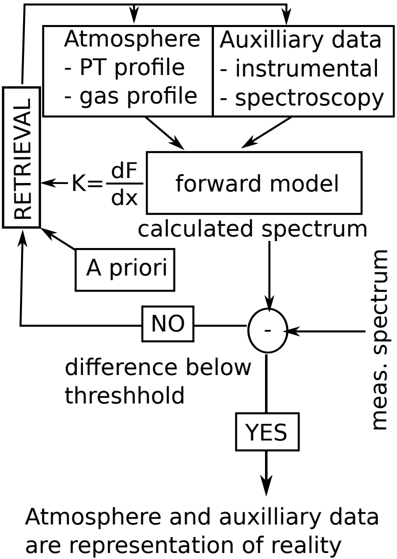
and

A. Goldman, D. G. Murcray and F. J. Murcray

Department of Physics, University of Denver, Denver, Colorado 80208

- sfit development started in the early 90ies
- aim: fast and small code to be less dependent on large computers
- first version of sfit2 ready in 1998
- SFIT4 started in 2010, first official version in 2014
- cooperation of many groups operating FTIR: NCAR Boulder, U Toronto, BIRA Brussels and U Bremen

# Overview of SFIT4




- FORWARD MODEL $F$:

$$y \; - \; \text{spectrum}$$
$$x_g \; - \; \text{atmospheric state}$$
$$x_b \; - \; \text{auxiliary parameters}$$
$$\epsilon \; - \; \text{noise on spectrum}$$
$$y = F(x_g, x_b) + \epsilon$$

- RETRIEVAL: recipe to modify $x_g$ and $x_b$
  - METHODS:
    - optimal estimation
    - Tikhonov-Phillips-regularization
  - CAVEAT: A PRIORI information necessary due to lack of information in spectrum

# Radiative transfer model

$$y \quad - \quad \text{spectrum}$$

$$x_g \quad - \quad \text{atmospheric state} \qquad x_b - \text{auxiliary parameters}$$

$$y = F(\underbrace{x}_{=(x_g,x_b)}) + \epsilon$$

- for atmosphere:
  - line-by-line model using the Voigt line shape
  - raytracing described by LBLATM
  - solar line parameters by Frank Hase
  - spectroscopic data from data bases, e.g. HITRAN
- for instruments:
  - line-shape effects: apodization function, phase shift, field-of-view
  - frequency shift of instrument
  - zero offsets due to non-linearity of detector

# Radiative transfer model

$$\begin{aligned} y &- \text{spectrum} \\ x_g &- \text{atmospheric state} \qquad x_b - \text{auxiliary parameters} \\ y &= F(\underbrace{x}_{=(x_g,x_b)}) + \epsilon \end{aligned}$$

statevector $x$ contains <u>everything</u> which could(!) be retrieved

$$x = (\underbrace{x_{z=1,\dots,n}^{\text{VMR gas 1}}, x_{z=1,\dots,n}^{\text{VMR gas 2}}, \cdots,}_{x_g,\text{atmosphere}}, \underbrace{\nu_{\text{F-AXIS SHIFT}}, \nu_{\text{SOLAR SHIFT}}, \cdots}_{x_b,\text{aux. parameters}})$$

$x_g$ is normalized or logarithmic for numerical reasons, i.e.

$$x_g = x_{\text{Atmosphere}}/x_A \qquad \text{or} \qquad x_g = \log(x_{\text{Atmosphere}})$$

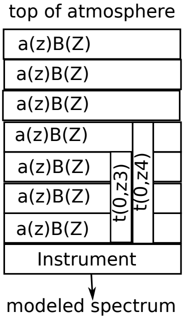
# Radiative transfer model

## Atmospheric model

### Radiance calculated by

$$I = B(\infty)\exp(-\tau(0,\infty)) + \int_0^\infty \underbrace{\alpha(z')B(z')}_{\text{Emission of layer z}} \exp(-\tau(0,z'))dz'$$

$$\tau(0,z) = \int_0^z \alpha(z')dz' \qquad \alpha(z) = \sum_{l=1}^{N} x_{a,l}(z)\alpha_l(z)$$




B(z) Planck function

Emission by Kirchhoff's law

$$e(\nu) = \alpha(\nu, P, T)B(\nu, T)$$

Transmission $\in [0, 1]$

$$T(0,z) = \exp(-\tau(0,z))$$

# Radiative transfer model

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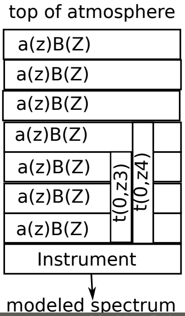


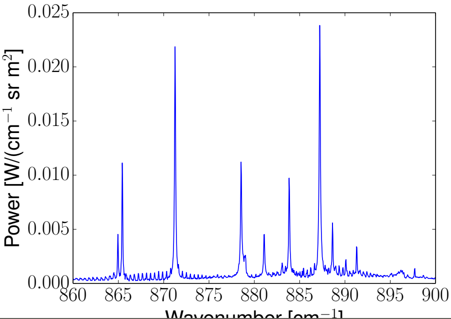

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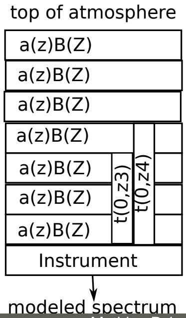


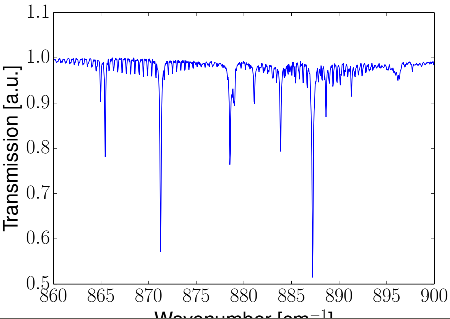

# Radiative transfer model

## The absorption cross section

- The frequency dependent absorption cross section can be written as

$$\alpha(\nu) = S(\nu_0, T)L(\nu_0, \nu, n, P, T) \quad (1)$$

with $S$ the transition intensity or source strength and $L$ the line shape normalized to 1.
- $S$ is the intensity of the line observed
- $L$ contains the effects of the environment upon the observed molecule.

# Radiative transfer model

## The absorption cross section – The intensity $S$

- Intensity for transistion from state $i$ to state $j$, $S_{ij}$ is a quantity dependent on the transition and temperature

$$S_{ij} = C \frac{\mu_{ij}^2}{TQ(T)} \left( e^{-\frac{E_j}{k_B T}} - e^{-\frac{E_i}{k_B T}} \right)$$

- HITRAN contains intensity at 296K, the energy of the lower and the higher state
- partition function $Q(t)$ calculated using TIPS method (part of HITRAN).
- extrapolation of intensity to arbitrary temperatures

$$S(T) = S(T_0) \frac{T_0 Q(T_0)}{TQ(T)} \exp \left[ \frac{E_i + E_j}{2K_B T_0} \left( 1 - \frac{T_0}{T} \right) \right]$$

# Radiative transfer model

## The absorption cross section – the line shape $L$

Active molecules: Molecules causing emission or absorption

Perturbers: or buffering gas or bath, molecules not absorbing

Translational effects

- caused by the (thermal) movement of the molecules
- Velocity distribution is Maxwell Boltzmann if not disturbed
- Line shape described by a Gauss function $L_G$

Collisional effects

- Caused by interactions of molecules
- Dephasing of radiation -> limiting correlation between different times
- line shape described by a Lorentz function $L_L$

Voigt function $$L_V(\nu) = L_G \star L_L$$

# Radiative transfer model

## The absorption cross section – the line shape *L*

Active molecules: Molecules causing emission or absorption

Perturber ...es not absorbing

Translationa... ...ffects

- caused ... by interactions of movem... ...es molecu... ...ing of radiation -> ... correlation
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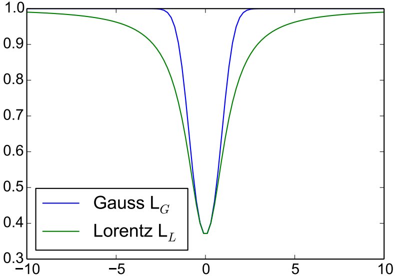



Voigt function $L_V(\nu) = L_G \star L_L$

# Radiative transfer model

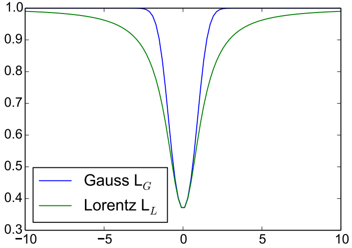
## The absorption cross section – the line shape $L$

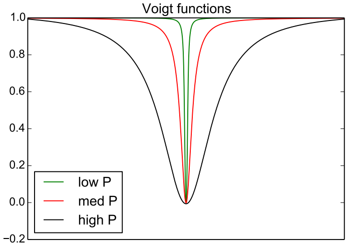
- Line width of Lorentz function increases proportional to pressure. Consequence of uncertainty relation

$$\Delta E \Delta t \leq \hbar$$

- Width of Gaussian part is roughly constant in altitude but proportional to frequency

NOTE: Altitude information is only available as long as the Lorentz part dominates



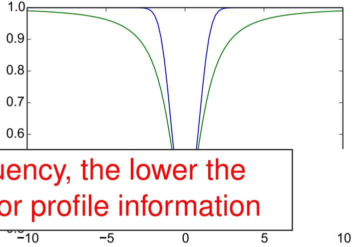



# Radiative transfer model

## The absorption cross section – the line shape *L*

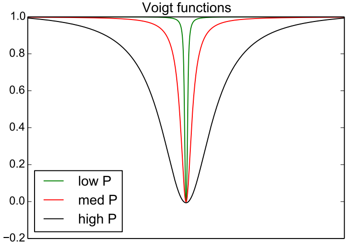
- Line width of Lorentz function increases proportional to pressure. Consequence of uncertainty

$\Delta E \Delta t \geq \hbar$




the higher the frequency, the lower the maximum altitude for profile information

- Width of Gaussian part is roughly constant in altitude but proportional to frequency




NOTE: Altitude information is only available as long as the Lorentz part dominates

# Radiative transfer model

## Calculation of the K matrix

For the retrieval and sensitivity study we need the first derivative, the so-called Jacobian of the forward model, also called the weighting function matrix $K$

Remember: $x = (x_g, x_b)$

$$
\begin{aligned}
y &= F(x) \\
K_{g,b} &:= \left.\frac{\partial F}{\partial x_{g,b}}\right|_{x^0_{g,b}}
\end{aligned}
$$

Using the K matrix, the forward model can be linearized:

$$
\begin{aligned}
F(x) &= F(x_0) + K(x_0)(x - x_0) + O\left((x - x_0)^2\right) \\
\text{using} \quad & \tilde{y} = y - y_0 \\
& \tilde{x} = x - x_0 \\
\rightsquigarrow \tilde{y} &= K\tilde{x}
\end{aligned}
$$

# Radiative transfer model

## Calculation of the K matrix

Two approaches:

1. Perturbation: for each row of the K matrix:

$$K_i = \frac{F(x + \Delta x) - F(x)}{\Delta x}$$

   -> order $N^2$

2. Semi analytic K-matrix calculation, exploits the fact that the transmission in of a layer only changes if the VMR underneath this layer changes. The spectrum and the K-matrix are calculated in two runs from TOA to the ground $\rightsquigarrow$ order $N$

# Inversion of the RTM (RETRIEVAL)

Inversion of RTM $F$ is an ill-posed problem

- In the presence of noise, information content of spectra in nadir/zenith geometry is limited, not more than a few bit
- influence of noise grows exponentially
- but: for numerical reasons, atmospheric bins should be small

$\rightsquigarrow$ number of layers higher than information content
$\rightsquigarrow$ regularization is needed

In SFIT4 two methods are implemented

- Optimal estimation (in the version of Rodgers, 2000)
- Tikhonov-Phillips-Regularization (various authors)

# Inversion of the RTM (RETRIEVAL)

## Inversion using Bayes theorem

p(y|x) - conditional probability distribution

$$\begin{aligned} p(x|y)p(y) &= p(y|x)p(x) \qquad \text{Bayes theorem} \\ \rightsquigarrow p(x|y) &= \frac{p(y|x)p(x)}{p(y)} \end{aligned}$$

We choose all probabilities to be Gaussian
Why?

- product of two Gaussian functions is Gaussian
  $\rightsquigarrow p(x|y)$ is Gaussian
- mode = mean
  $\rightsquigarrow \int p(y)$ does not need to be known

# Inversion of the RTM (RETRIEVAL)

## Inversion using Bayes theorem

$$
\begin{aligned}
p(y|x) &= C_L \exp(-(y - F(x))^T S_\epsilon^{-1}(y - F(x))) \\
p(x) &= C_A \exp(-(x - x_A)^T S_A^{-1}(x - x_A)) \\
\rightsquigarrow p(x|y) &= C \exp(-(x - \hat{x})^T S^{-1}(x - \hat{x}))
\end{aligned}
$$

getting the mode (=mean) by finding the extrema of the argument:

$$
\hat{x} = \arg\min(\underbrace{(y - F(x))^T S_\epsilon^{-1}(y - F(x)) + (x - x_A)^T S_A^{-1}(x - x_A)}_{\text{cost function}})
$$

$$
\begin{aligned}
\hat{x} &= x_A + (S_A^{-1} + K^T S_\epsilon^{-1} K)^{-1}[K^T S_\epsilon^{-1}(y - K x_A)] \\
S^{-1} &= K^T S_\epsilon^{-1} K + S_A^{-1}
\end{aligned}
$$

# Inversion of the RTM (RETRIEVAL)

Inversion using Tikhonov-Phillips-Regularization by minimizing:

$$\hat{x} = \arg\min(\underbrace{||P(y - F(x))||}_{\text{data misfit}} + \lambda \underbrace{||R(x - x_A)||}_{\text{Regularization}})$$

$\lambda$ – regularization strength

Solution by

$$\hat{x} = x_A + (R^{-2} + K^T P^{-2} K)^{-1} [K^T P^{-2} (y - K x_A)]$$

$\rightsquigarrow$ equivalent to optimal estimation with $R^2 = S_A$ and $P^2 = S_\epsilon$

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$\rightsquigarrow$ equivalent to optimal estimation with $R^2 = S_A$ and $P^2 = S_\epsilon$
NOTE: Optimal Estimation and
Tikhonov-Phillips-Regularization both have Gaussian statistics

# Inversion of the RTM

## non-linear forward models

Two iteration methods implemented:

1. Gauss-Newton iteration
   - weakly non-linear models
   - iteration only successful if started near the solution

$$x_{i+1} = x_A + (S_A^{-1} + K_i^T S_\epsilon^{-1} K_i)^{-1} K_i^T S_\epsilon^{-1} (y - F(x_i)) + K_i(x_i - x_A)$$

2. Levenberg-Marquardt iteration
   - moderatly non-linear models
   - compromise of Gauss-Newton (quick but unstable) and steepest descend iteration (slow but stable)

$$x_{i+1} = x_A + ((1+\gamma) S_A^{-1} + K_i^T S_\epsilon^{-1} K_i)^{-1} K_i^T S_\epsilon^{-1} [(y - F(x_i)) + K_i(x_i - x_A)]$$

$\gamma$ is the weighting between Gauss-Newton and steepest descent. $\gamma$ decreases when iteration successful (cost function gets lower), else is increased

$\rightsquigarrow$ $\gamma$ start with a high value and is continually decreased

# Retrieval analysis

## The averaging kernel matrix

One of the most important quantities beside the result is the sensitivity of the retrieval, or the avarging kernels A:

$$
\begin{aligned}
A &:= \frac{\partial \hat{x}}{\partial x} \\
&= \frac{\partial \hat{x}}{\partial F}\frac{\partial F}{\partial x}
\end{aligned}
$$

comparing with and identifying $y = Kx$:

$$
\begin{aligned}
\hat{x} &= x_A + (S_A^{-1} + K^T S_\epsilon^{-1} K)^{-1} K^T S_\epsilon^{-1} (y - Kx_A) \\
\hat{x} &= x_A + \underbrace{(S_A^{-1} + K^T S_\epsilon^{-1} K)^{-1} K^T S_\epsilon^{-1}}_{=D} K(x - x_A)
\end{aligned}
$$

we find a linarisation of the retrieval using $A = DK$:

$$
\boxed{\hat{x} = x_A + A(x - x_A) = (I - A)x_A + Ax}
$$

# Retrieval analysis

- Can the measured spectrum be modeled?
- Is the result sensible?
- Correlation of retrieved quantities
- Error/Sensitivity of retrieved quantities

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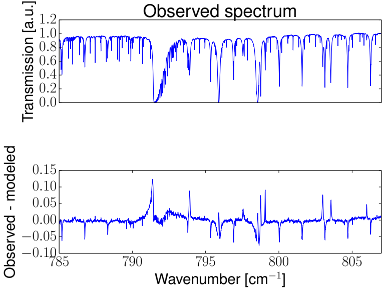
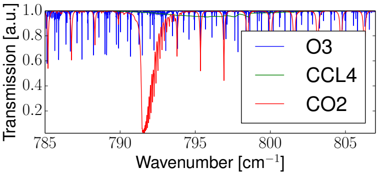



- artifacts in spectrum?
  - origin?
  - is the failure in modeling relevant?



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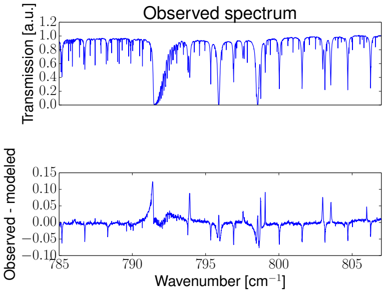


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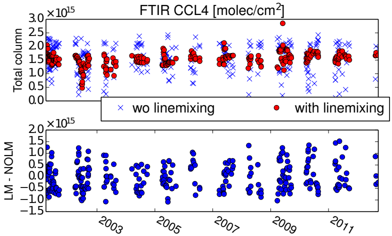

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- Can the measured spectrum be modeled?
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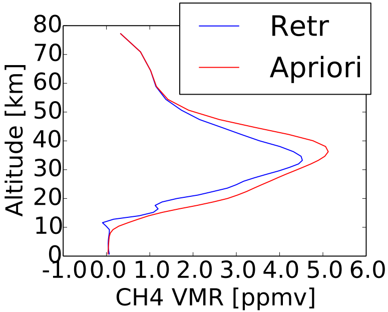
- result different from a priori?
- structure of the retrieved result ok?
- error of the retrieval sensible?



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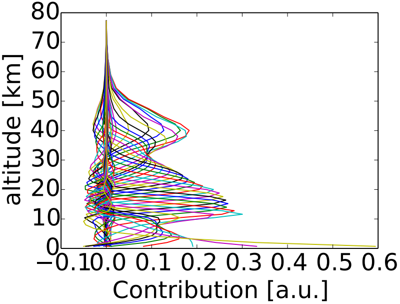
- the correlation of different entries of the state vector is given by the AVK matrix



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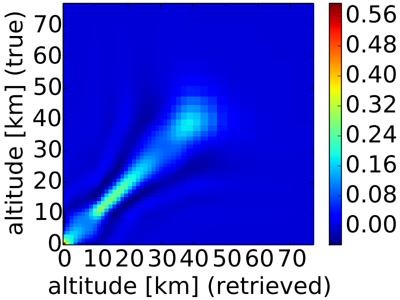
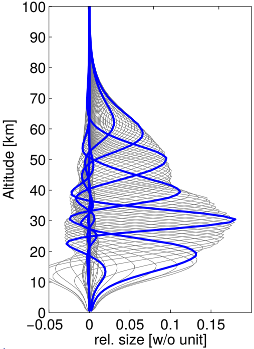
- Error/Sensitivity of retrieved quantities

- the correlation of different entries of the state vector is given by the AVK matrix



# Retrieval analysis

- Can the measured spectrum be modeled?
- Is the result sensible?
- Correlation of retrieved quantities
- Error/Sensitivity of retrieved quantities




- Ozone measurements using a millimeterwave instrument
- Measurements independent of weather and light
- Altitude range about 20 - 60 km altitude

# Retrieval analysis

- Can the measured spectrum be modeled?
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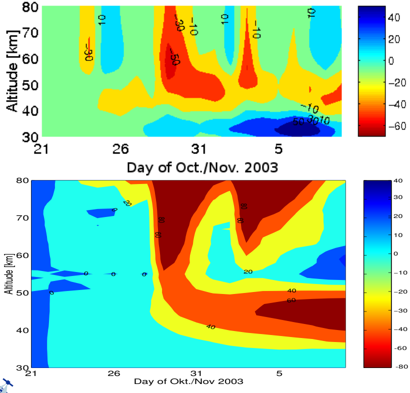
- Correlation of retrieved quantities
- Error/Sensitivity of retrieved quantities

Change of Ozone VMR in %




Upper panel: measurements of Ozone VMR during a solar proton event

Lower panel: modelling of the same event using a chemical transport model and realistic ion fluxes

# Retrieval analysis

- Can the measured spectrum be modeled?
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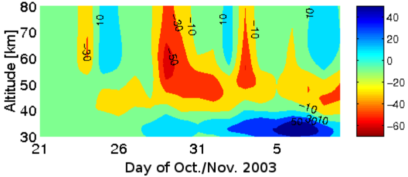
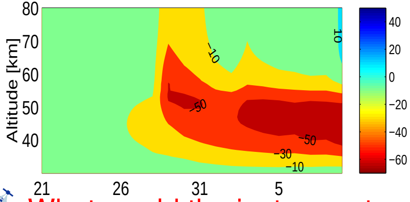
Change of Ozone VMR in %




Upper panel: measurements of Ozone VMR during a solar proton event




Lower panel: the model has been reculatulated using the measurement model

What would the instrument see, if the model would be true?

# Retrieval analysis

- Can the measured spectrum be modeled?
- Is the result sensible?
- Correlation of retrieved quantities
- Error/Sensitivity of retrieved quantities

$$
\begin{aligned}
\hat{x} - x &= (A - I)(x - x_A) && \text{Smoothing error} \\
&+ G_y \epsilon && \text{Retrieval noise} \\
&+ G_y \Delta F(x, b, \hat{b}) && \text{Forward model error} \\
&+ G_y K_b (b - \hat{b}) && \text{model parameter error}
\end{aligned}
$$

compare Rodgers (2000)

# Error calculation

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smoothing error only accessible when covariance of real ensemble is known.

retrieval noise caused by noise on spectrum.

Error due to use of wrong forward model. Difficult to assess if true forward model is not known.

FW model parameter error $K_b$ matrices are calculated in SFIT4 for $b$, can be used for sensitivity studies or error calculation, if error of quantities $b$ is known.

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: caused by noise on spectrum.

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FW model parameter error
: $K_b$ matrices are calculated in SFIT4 for $b$, can be used for sensitivity studies or error calculation, if error of quantities $b$ is known.

# Error calculation

$$\begin{aligned} \hat{x} - x &= (A - I)(x - x_A) && \text{Smoothing error} \\ &+ G_y \epsilon && \text{Retrieval noise} \\ &+ G_y \Delta F(x, b, \hat{b}) && \text{Forward model error} \\ &+ G_y K_b (b - \hat{b}) && \text{model parameter error} \end{aligned}$$

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