

The Gradient Fast Line-by-Line Model

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Introduction

For the past decade the Meteorological Service of Canada has been using the fast line-by-line radiative transfer model (FLBL) to generate accurate transmission/radiance databases from representative atmosphere data-bases for the purpose of validation, and for generating coefficients for fast forward models, such as MSCFAST (Garand, 1999). The FLBL is also used as a research tool. For example; the examination of the approximations used by forward models to identify systematic errors and to indicate potential methods of improvement (eg Turner, 2004, Turner,2000).

Many organizations have developed tangent linear adjoint models for data assimilation. In order to validate the adjoint models, the gradient of the radiative transfer model (or jacobian) is required. In the past a brute force method is used to calculate a Jacobian with the FLBL. In the case of a top of the atmosphere (TOA) radiance, this entails perturbing each variable in the radiative transfer equation, in turn, by some amount and recalculating the radiance. The original and perturbed radiances are then numerically differenced to obtain the derivative with to the perturbed variable. This is a time consuming process since it requires the FLBL to be executed each time a variable is perturbed. In addition, there are errors inherent to numerical differentiation.

It would be advantageous to have a more accurate and faster gradient model than the brute force

method as a research tool. An analytical differentiation of the FLBL model was performed, which lead to a much faster and less error prone gradient model. The Gradient FLBL, GFLBL, is considerably faster than the brute force FLBL model and as such could be used effectively for validating the gradient and tangent linear adjoint of fast forward models. The following is a brief review of the FLBL radiative transfer model followed on by the introduction of the gradient GFLBL and some simple applications.

The Fast Line-by-line Layer-by-layer Model (FLBL)

- ♠ FLBL uses ♣ generation of transmittance/radiance databases for generating fast forward model coefficients; eg MSCFAST (Garand et al, 1999)
- ♣ fast forward model validation (Saunders et al, 2005, Tumer et al, 2001, Soden et al,2000)
- ♣ identifying systematic errors in fast forward models (Tumer 2004, Turner 2000)
- ♣ calculation of Jacobians, $\frac{d\mathfrak{S}}{d\vec{x}}$, $\frac{d\mathfrak{R}}{d\vec{x}}$, $\frac{dB_T}{d\vec{x}}$, ... using brute force methods

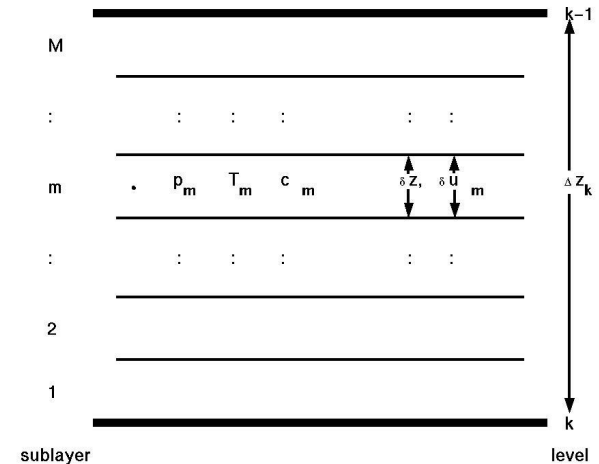
♠ FLBL solves the numerical form of radiative transfer model for a nadir viewing satellite; that is—

$$\mathfrak{R} = \varepsilon_s(\tilde{\nu}) B_s(\tilde{\nu}) \mathfrak{S}_s(\theta, \tilde{\nu}) + \sum_{j=0}^s \bar{B}_j(\tilde{\nu}) (\mathfrak{S}_{j-1}(\theta, \tilde{\nu}) - \mathfrak{S}_j(\theta, \tilde{\nu})) \quad (1)$$

where $\mathfrak{S}_j(\theta, \tilde{\nu}) = e^{-\sum_{i=1}^j \chi_i(\theta, \tilde{\nu})}$, χ_i is the optical thickness of the i^{th} layer.

Atmospheric Model

- ♠ divide atmosphere into N layers/levels with N_G absorbers (user defined)
- ♠ user supplies atmospheric profile on z, p, T and \vec{c} (km, mb, K & vmr)
- ♠ the atmospheric profile levels define the radiation vertical integration levels
- ♠ FLBL operates on the z-coordinate internally



- ♠ k^{th} layer ♣ boundaries, $p_{k-1}, p_k, T_{k-1}, T_k, c_{k-1,\ell}, c_{k,\ell}$.

♣ properties
$$\bar{p}_{kl} = \frac{\int p_{kl} du_{kl}}{\int du_{kl}}, \quad \bar{T}_{kl} = \frac{\int T_{kl} du_{kl}}{\int du_{kl}}, \quad \bar{c}_{kl} = \frac{\int c_{kl} du_{kl}}{\int du_{kl}}, \quad u_{kl} = L \frac{T_o}{P_o} \int \frac{c_{kl} T_k}{P_k} dz$$

- ♠ in evaluating the mean layer properties ♣ a layer is subdivided into N_{sub} layers of equal δz
 ♣ logp, T and \vec{c} are assumed to be linear in z over the layer
- ♠ all calculations below use all, or part of the 53 atmospheres defined for a recent inter-comparison (URL01, 2003, Saunders et al 2005)

Optical Depth Model

- ♠ layer optical depth is the sum of the contributions from spectral lines and continua due to all absorbers

$$\chi_k(\theta, \tilde{\nu}) = \sum_{\ell=1}^{N_g} k_{k\ell}(\bar{p}_k, \bar{T}_k, u_{k\ell}, \tilde{\nu}) u_{k\ell} + \chi_{k\ell}^{continuum}(\theta, \tilde{\nu})$$

- ♠ absorption coefficient at $\tilde{\nu}$ for gas ℓ is built up by summing the contributions from neighbouring lines, (see fig below) hence the term “line-by-line”; that is—

$$k_{k\ell}(\bar{p}_k, \bar{T}_k, u_{k\ell}, \tilde{\nu}) = \sum_{m=1}^{N_{lines}} S_{k\ell m}(\tilde{\nu}, \bar{T}_{k\ell}) f(\tilde{\nu} - \tilde{\nu}_{ok\ell m}, \bar{p}_{k\ell}, \bar{T}_{k\ell}, u_{k\ell})$$

- ♣ S is the spectral line strength at $\tilde{\nu}_{ok\ell}$ and f is its shape function
- ♠ potentially tens of thousands of lines used to build $k_{k\ell}(\tilde{\nu})$, consequently, LBLs are relatively slow due to the large summations required
- ♠ LBL speed up by replacing the time consuming calculation of k by absorption coefficient look up tables (Turner, 1995)
- ♠ tables of $k(\tilde{\nu}, \bar{p}, \bar{T})$ are created using MSC’s conventional LBL and HITRAN (Rothman et al, 2003)
- ♠ FLBL is ♣ about 60 to 80 times faster than conventional LBL
 - ♣ results are generally with 1.5% of an LBL for integrations greater than $.25(\text{cm}^{-1})$

The Gradient FLBL (GFLBL)

- ♠ in the past, a Jacobian profile was calculated by a brute force method
 - ♣ entails perturbing each level, in turn, by $\pm\delta\eta$, calculating the perturbed radiance and then numerically differentiating; ie,

$$\frac{\partial \mathfrak{R}}{\partial \eta_k} = \frac{\mathfrak{R}(\eta_k + \delta\eta) - \mathfrak{R}(\eta_k - \delta\eta)}{2\delta\eta}$$

- ♠ method requires $2*n$ separate FLBL executions to complete one Jacobian profile
 - ♣ in practise a specialized FLBL program (BFFLBL) perturbs at all levels and differences internally
 - ♣ process is very time consuming
 - ♣ some experimentation is needed to determine a suitable value for the perturbation
- ♠ a more accurate and efficient way is to differentiate Eqn. (1) analytically
 - ♣ Note that derivatives with respect to a level are inherently related to the adjacent layers

$$\frac{\partial \mathfrak{R}}{\partial \eta_p} = \mathfrak{R}^s \left[A_s B_s \frac{\partial T_s}{\partial \eta_p} - \frac{\partial \chi_{p+1}}{\partial \eta_p} - \frac{\partial \chi_p}{\partial \eta_p} + \frac{1}{\varepsilon_s} \frac{\partial \varepsilon_s}{\partial \eta_p} \right] + \mathfrak{R}_p^a \bar{B}_p \bar{A}_p \frac{\partial \bar{T}_p}{\partial \eta_p} + \mathfrak{R}_{p+1}^a \left(\bar{B}_{p+1} \bar{A}_{p+1} \frac{\partial \bar{T}_{p+1}}{\partial \eta_p} - \frac{\partial \chi_p}{\partial \eta_p} \right) +$$

$$\bar{B}_p \mathfrak{S}_p \frac{\partial \chi_p}{\partial \eta_p} + \bar{B}_{p+1} \mathfrak{S}_{p+1} \frac{\partial \chi_{p+1}}{\partial \eta_p} - \left(\frac{\partial \chi_{p+1}}{\partial \eta_p} + \frac{\partial \chi_p}{\partial \eta_p} \right) \sum_{k=p+2}^n \mathfrak{R}_k^a$$

$$\clubsuit \quad A_p = \frac{c_2 e^{c_2 \bar{\nu}/T_p}}{c_1 \bar{\nu}^2 T_p^2} \quad \text{and} \quad \bar{A}_p = \frac{c_2 e^{c_2 \bar{\nu}/\bar{T}_p}}{c_1 \bar{\nu}^2 \bar{T}_p^2}$$

$$\clubsuit \quad \frac{\partial \chi_{p+1}}{\partial \eta_p} = \sum_{\ell=1}^{N_g} \left(k_{p+1,\ell} \frac{\partial u_{p+1,\ell}}{\partial \eta_p} + u_{p+1,\ell} \frac{\partial k_{p+1,\ell}}{\partial \eta_p} \right) \quad \text{and} \quad \frac{\partial \chi_p}{\partial \eta_p} = \sum_{\ell=1}^{N_g} \left(k_{p\ell} \frac{\partial u_{p\ell}}{\partial \eta_p} + u_{p\ell} \frac{\partial k_{p\ell}}{\partial \eta_p} \right)$$

♠ expanding $\frac{\partial k}{\partial \eta}$ with respect to the layer values

$$\frac{\partial k_{p+1,\ell}}{\partial \eta_p} = \left(\frac{\partial k_{p+1,\ell}}{\partial \bar{p}_{p+1,\ell}} \frac{\partial \bar{p}_{p+1,\ell}}{\partial \eta_p} + \frac{\partial k_{p+1,\ell}}{\partial \bar{T}_{p+1,\ell}} \frac{\partial \bar{T}_{p+1,\ell}}{\partial \eta_p} + \frac{\partial k_{p+1,\ell}}{\partial \bar{c}_{p+1,\ell}} \frac{\partial \bar{c}_{p+1,\ell}}{\partial \eta_p} \right) \quad \& \quad \frac{\partial k_{p\ell}}{\partial \eta_p} = \left(\frac{\partial k_{p\ell}}{\partial \bar{p}_{p\ell}} \frac{\partial \bar{p}_{p\ell}}{\partial \eta_p} + \frac{\partial k_{p\ell}}{\partial \bar{T}_{p\ell}} \frac{\partial \bar{T}_{p\ell}}{\partial \eta_p} + \frac{\partial k_{p\ell}}{\partial \bar{c}_{p\ell}} \frac{\partial \bar{c}_{p\ell}}{\partial \eta_p} \right)$$

♣ $\frac{\partial k_{p\ell}}{\partial \bar{p}_{p\ell}}$ and $\frac{\partial k_{p\ell}}{\partial \bar{T}_{p\ell}}$ are evaluated from the lookup k-table simultaneously with $k(\tilde{\nu})$ using the same bi-cubic interpolation coefficients

♠ currently the GFLBL code generates

♣ \mathfrak{S}_k for all individual absorbers, $\mathfrak{S}_k(\text{UMG})$, $\mathfrak{S}_k(\text{UMG}+\text{H}_2\text{O})$ & $\mathfrak{S}_k(\text{ALL})$, for all k

♣ Planck-weighted \mathfrak{S}_k all individual absorbers, for all k

♣ \mathfrak{R}_k^a assuming $\varepsilon = 1$ (surface assumed to be on all levels), for all k

♣ \mathfrak{R}_k^s attenuated p_k to TOA atmospheric emissions, for all k

♣ $\frac{\partial \mathfrak{R}_n^a}{\partial \eta_p}$ & $\frac{\partial \mathfrak{R}_n^s}{\partial \eta_p}$ for all p, $\eta = p, T, \bar{c}$

♠ all the above values are convoluted with specified response functions

Comparison Between BFFLBL and GFLBL

- ♠ compare the T, H₂O and O₃ jacobians for 20 AIRS channels and profile 52 (see Fig 1)
 - ♣ use the same channels & profiles as used in recent inter-comparison (Saunders, et al 2005)
 - ♣ BFFLBL temperature and volume mixing ratio perturbations are $\pm 1/2$ K and $\pm 5\%$ of c
 - ♣ GFLBL curves are smooth and compare well with the BFFLBL
 - ♣ some of the BFLBL vmr Jacobian curves are noisy, appears to be numerics

- ♠ on a LINUX workstation (i686 under RedHat8)
 - ♣ GFLBL is measured in CPU seconds
 - ♣ BFFLBL is measured in CPU hours
 - ♣ typically the BFFLBL consumes 700 times more CPU time than the GFLBL

- ♠ GFLBL compares acceptably against other models (Saunders et al, 2005)
(see poster by Saunders)

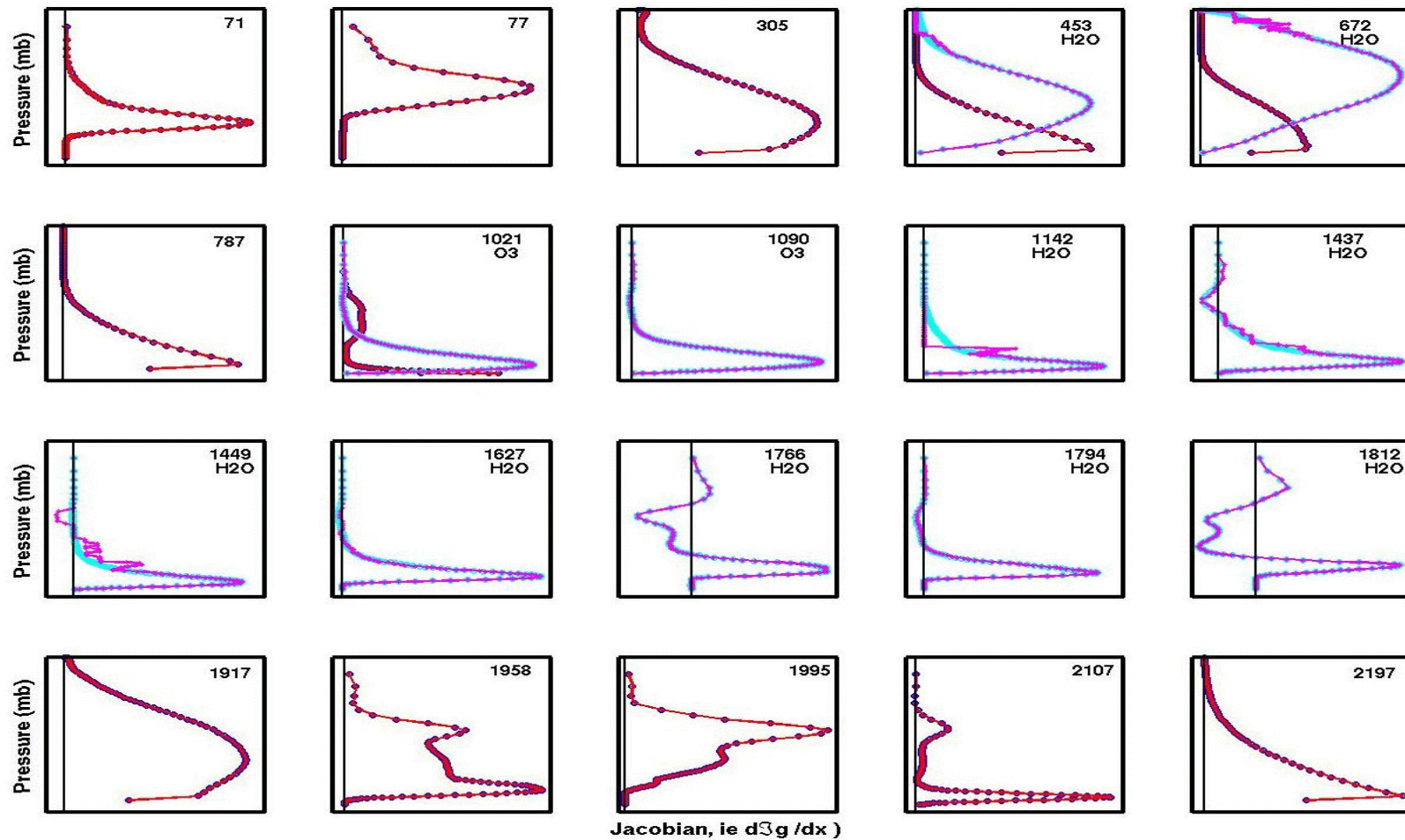


Fig. 1: Comparison of the GFLBL and BFFLBL temperature, H₂O and O₃ Jacobians for profile 52
 Temperature Jacobian, ● BFFLBL ● GFLBL
 VMR Jacobian, ● BFFLBL ● GFLBL (absorber indicated in box)

Applications

- ♠ production of the Sensitivity of a channel to changes in temperature and absorber amount
- ♣ S is the change in TOA BT for a change in T or c at a particular level; typically plotted as a profile

$$S(T_k) = \Delta T \frac{\partial BT}{\partial T_k} \quad \text{or} \quad S(c_{k\ell}) = \Delta c_\ell \frac{\partial BT}{\partial c_{k\ell}}$$

- ♣ Fig 2 is an example of visualizing which spectral (or channel) regions are most sensitive to a variable and at what altitudes for a given atmospheric profile
 - ◆ this example is for the 2180 to 2275(cm^{-1}) where the 4.5 μ band of N_2O resides
 - ◆ sensitivity to a change of 1K or a change of 10% in vmr are plotted
 - ◆ this region is particularly sensitive to temperature, N_2O & CO_2 , and slightly to H_2O & CO
- ♣ Fig 3 is an example of visualizing the variability of sensitivity profiles to a multitude of profiles
 - ◆ 7 AIRS channels from 2104 to 2110 (2383.3 to 2389.1 (cm^{-1}))
 - ◆ temperature, CO_2 , N_2 and H_2O dominate, although one would not expect N_2 to vary by 10%
- ♠ GFLBL can be used to test algorithms involving radiance derivatives
 - ♣ Fig 4. Illustrates the results of using the adjoint code of a linear interpolator to transform the Jacobian from an atmosphere from M levels to one with N levels. A straight-forward interpolation is invalid as the Jacobian depends on the thickness of the adjacent layers.
 - ◆ AIRS 1090 and profile 52 is used for this example
 - ◆ reference profile (M-levels) has 25 levels and for the destination profile, $N=6, 12, 25, 50$ & 98
 - ◆ for this example the top and bottom levels are fixed to the same pressure
 - ◆ GFLBL used to calculate “truth” for all models

- ◆ results indicate that ♥ for $N \lesssim M$ the re-mappings are acceptable
 - ♥ for $N > M$ a fair bit of noise is introduced
- ◆ currently the MSC remaps the radiation Jacobians from the 43 RTTOVS levels to the operational NWP model's 28 levels using the adjoint code to the linear interpolation routine, however the NWP model levels are to be increased to 58 levels. Fig 4 indicates that the adjoint code needs to be reworked or the number of radiation levels used raised

Future Work

- ♠ broaden the GFLBL to include
 - ♣ the reflected down-welling term
 - ♣ the reflected solar term (non-scattering)
 - ♣ spherical geometry (for limb-scanning)

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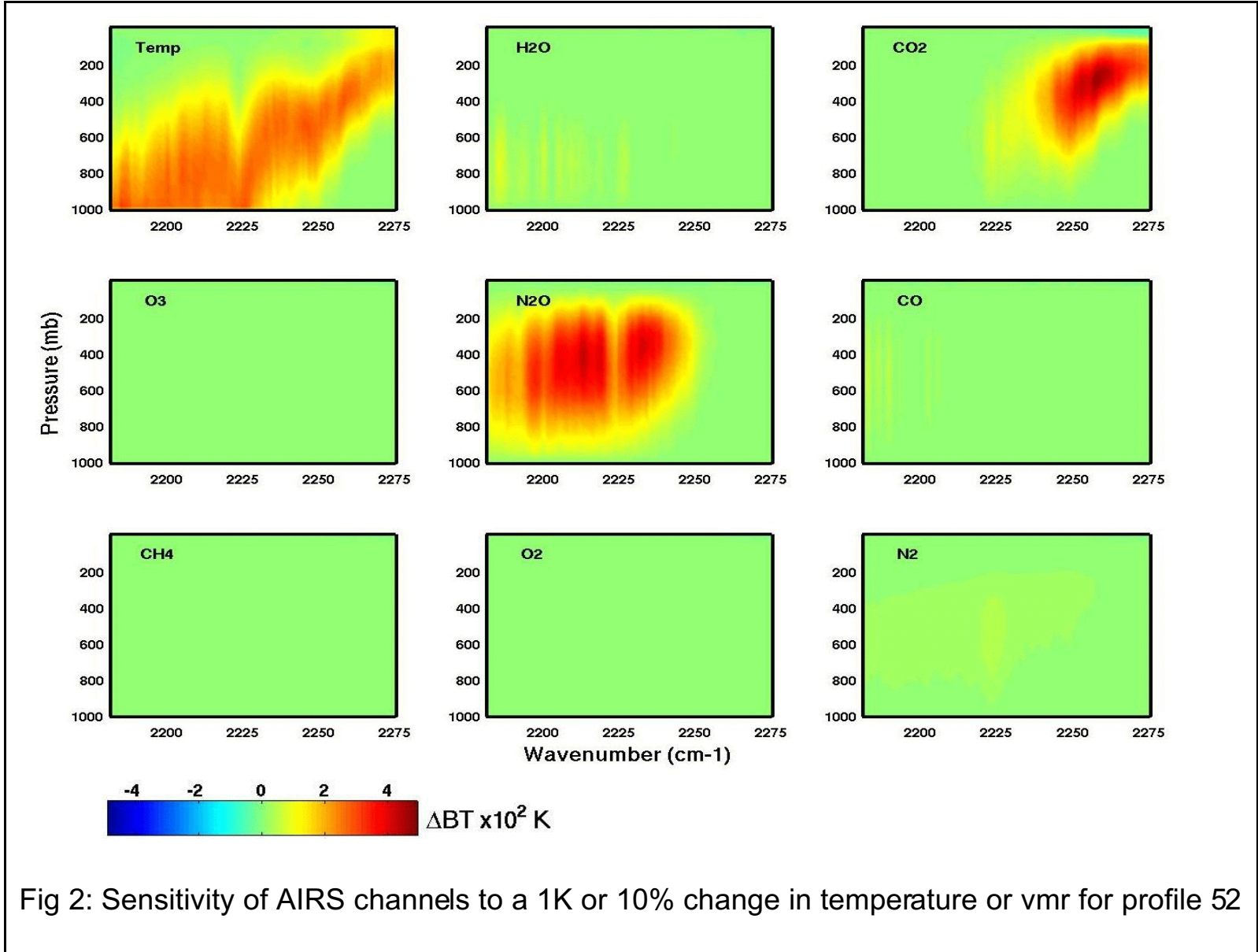


Fig 2: Sensitivity of AIRS channels to a 1K or 10% change in temperature or vmr for profile 52

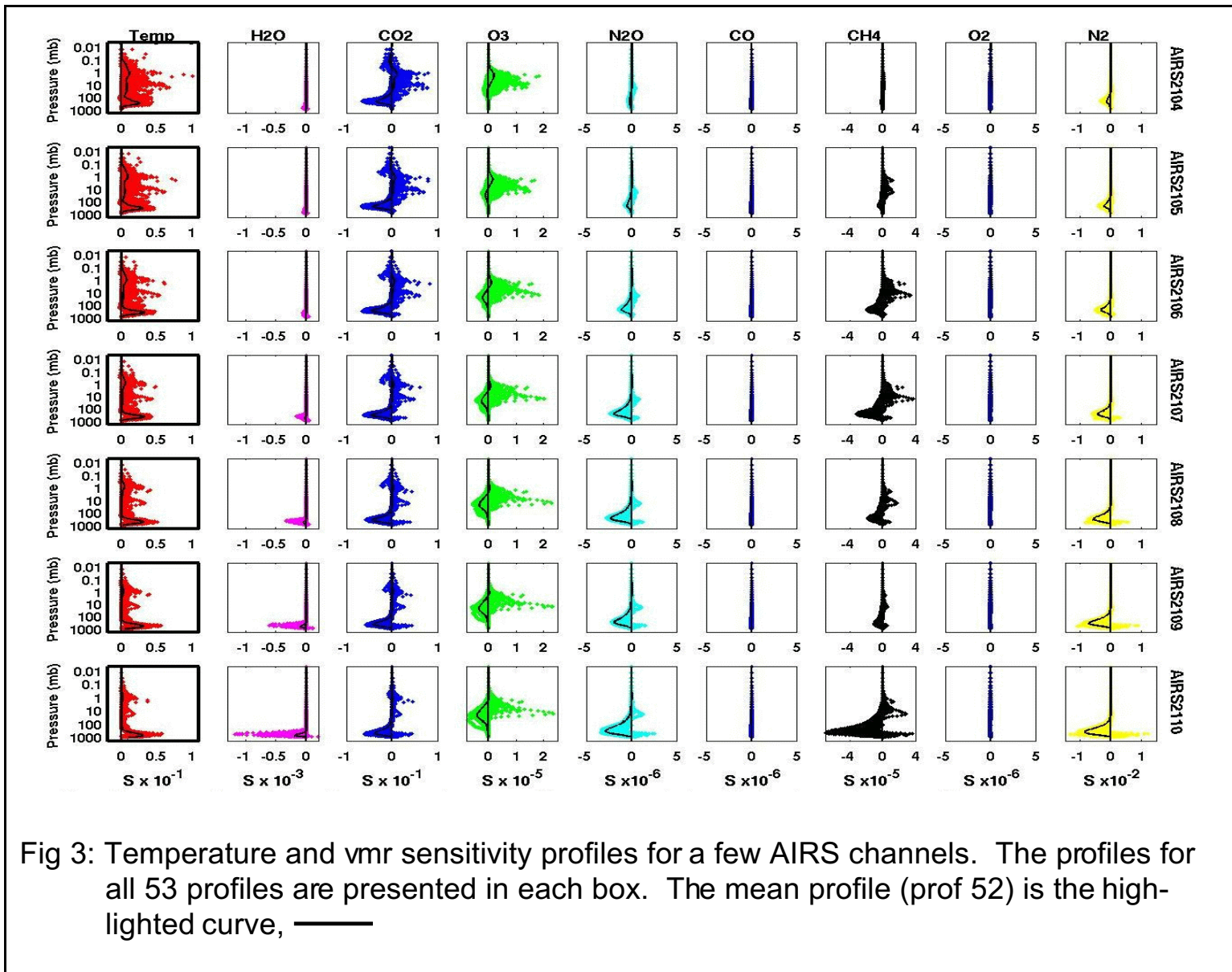
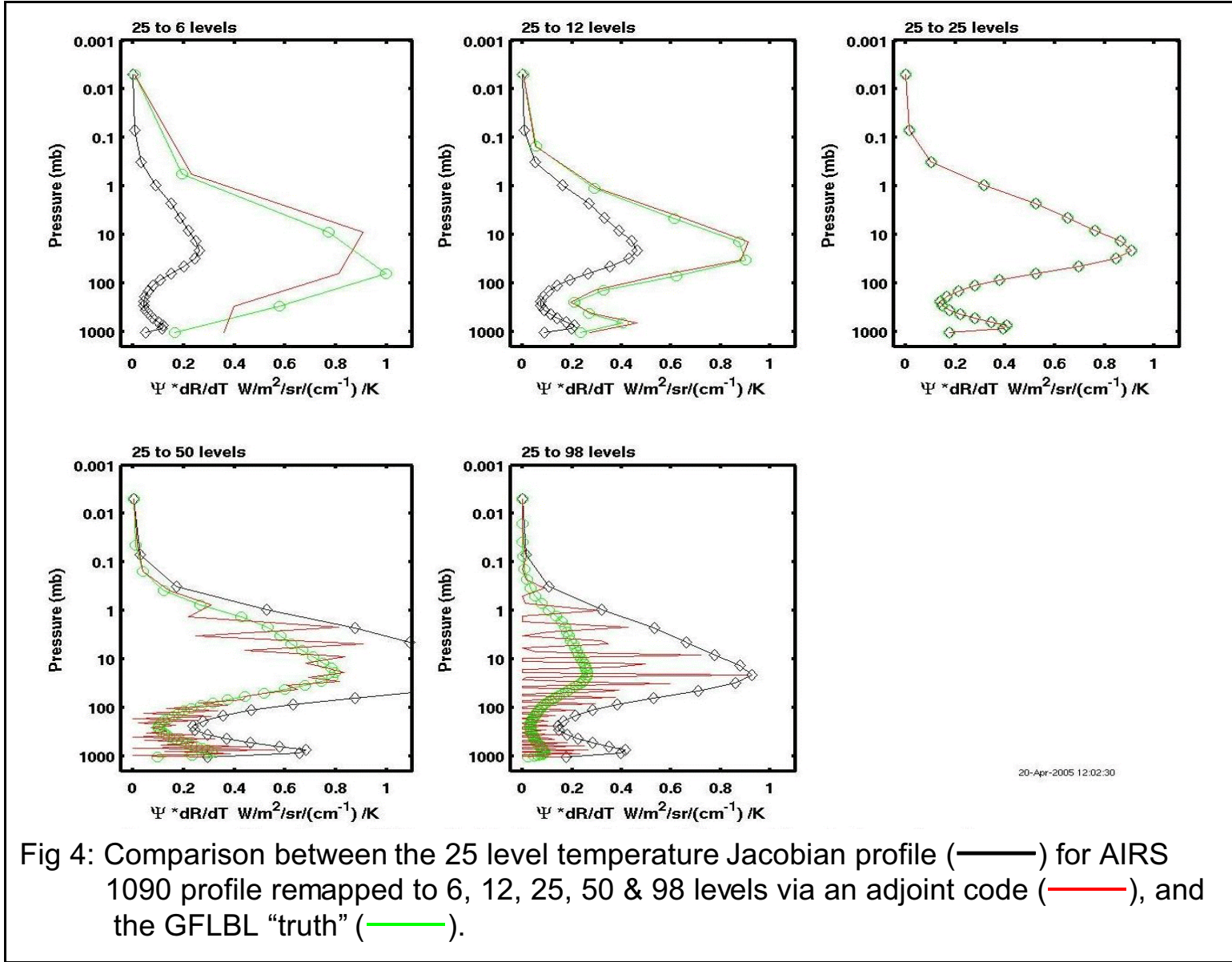


Fig 3: Temperature and vmr sensitivity profiles for a few AIRS channels. The profiles for all 53 profiles are presented in each box. The mean profile (prof 52) is the high-lighted curve, **——**



International TOVS Study Conference, 14th, ITSC-14, Beijing, China, 25-31 May 2005.
Madison, WI, University of Wisconsin-Madison, Space Science and Engineering Center,
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