The Gradient Fast Line-by-Line Model

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Introduction

For the past decade the Meteorological Service of Canada (MSC) has been using the fast line-by-line radiative transfer model (FLBL) to generate accurate transmission/radiance databases from representative atmosphere databases 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.

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 a fast forward model. 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

The mono-chromatic radiative transfer equation describing the top of the atmosphere (TOA) radiance received by a satellite from a surface, assuming a non-scattering plane-parallel atmosphere and neglecting the reflected downwelling flux and solar terms, is the sum of two terms; the attenuated upward surface emission, $\Re_s$, and the sum of the attenuated upward atmospheric emissions, $\Re_a$; ie,

$$\Re = \Re_s + \Re_a = \varepsilon(\tilde{v}) B(T_s \tilde{v}) \Im(\theta, p_s, \tilde{v}) + \int_o^{p_s} B(p, \tilde{v}) \, d\Im(\theta, p, \tilde{v}) \qquad (1)$$

where p is the pressure, θ is the zenith angle defining the upward surface to TOA path, B is the

Planck function, $\Im$ is the p to TOA transmittance, and ε is the surface emissivity. The subscript 's' denotes a surface which can be a topographical or cloud top surface. $\Im$, B, ε and r are functions of wavenumber, $\tilde{\upsilon}$.

Equation 1 can be written in numerical form as:

$$\Re \ = \ \varepsilon_s(\tilde{v}) \, B_s(\tilde{v}) \, \Im_s(\theta, \tilde{v}) \ + \ \sum_{j=0}^{s} \bar{B}_j(\tilde{v}) \, (\Im_{j-1}(\theta, \tilde{v}) - \Im_j(\theta, \tilde{v})) \qquad (2)$$

where $\ \Im_j(\theta, \tilde{v}) \ = \ e^{-\sum_{i=1}^{j} \chi_i(\theta, \tilde{v})} \ $ and χ_i is the optical thickness of the ith layer.

Equation 2 is solved by dividing the atmosphere up into N layers containing N_g absorbers. The layer is indexed by the upper boundary of the layer, hence the number of levels equals the number of layers. Layer 1 has no upper boundary. It represents the semi-infinite layer above TOA. Each layer (see Fig. 1) is defined by its boundary values, p_{k-1}, p_k , T_{k-1}, T_k , $c_{k-1,\ell}$ and $c_{k,\ell}$, ($c_{k,\ell}$ is the volume mixing ratio of absorber, ℓ) and its mean layer properties, $\bar{p}_{k,\ell}, \bar{T}_{k,\ell}, u_{k,\ell}$, the mean layer pressure, temperature and absorber amount with respect to absorber ℓ. The mean layer values are defined as:

$$\bar{p}_{k\ell} = \frac{\int p_{k\ell} \, du_{k\ell}}{\int du_{k\ell}} \ , \quad \bar{T}_{k\ell} = \frac{\int T_{k\ell} \, du_{k\ell}}{\int du_{k\ell}} \qquad (3a)$$

$$\bar{c}_{k\ell} = \frac{\int c_{k\ell} \, du_{k\ell}}{\int du_{k\ell}} \ , \quad u_{k\ell} = L \frac{T_o}{P_o} \int \frac{c_{k\ell} T_k}{P_k} \, dz \quad (3b)$$

The mean layer values are evaluated by assuming that Lnp, T and c vary linearly with z and integrating across the layer. The mean layer values are used to evaluate optical thicknesses.

Fig. 1: Schematic of a 3 gas atmosphere model with a single layer highlighted.

The most accurate method of evaluating Eqn 2 is by use of a line-by-line radiative transfer model (LBL). The LBL signifies that the absorption coefficient is determined from basic physics, that is —the shape of the spectral lines, their positions and overlaps with other spectral lines, are explicitly accounted for. This physics is contained in the absorption coefficient component of the optical depth.

The layer optical depth is the sum of the product of the spectral line absorption coefficient, k, and the
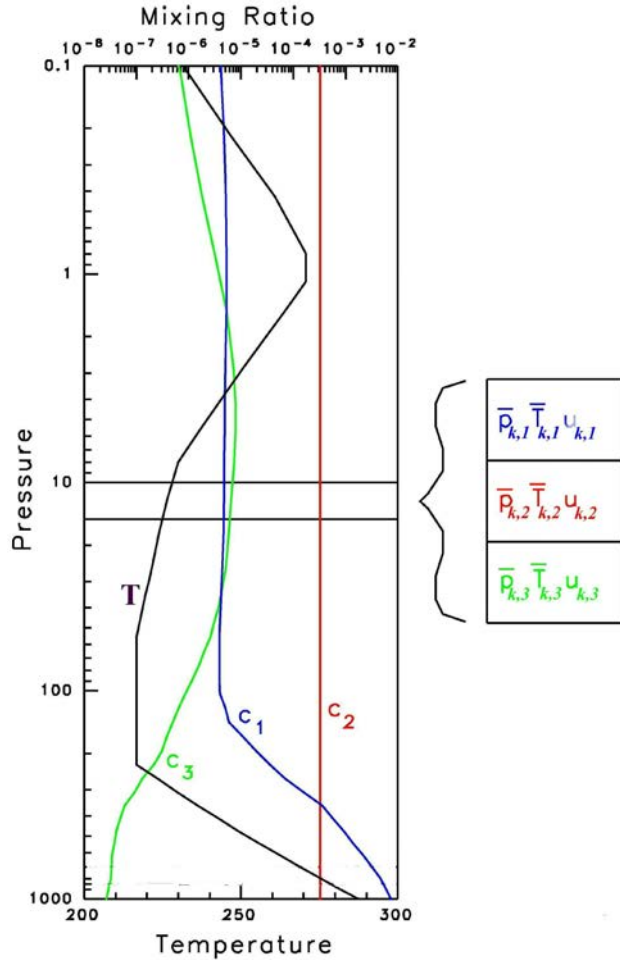
absorber amount, u, for each absorbing component within the layer, plus any continuum contributions, $\chi_{continuum}$;that is—

$$\chi_k(\theta, \tilde{v}) = \sum_{\ell=1}^{N_g} k_{k\ell}(\bar{p}_k, \bar{T}_k, u_{k\ell}, \tilde{v})\, u_{k\ell} + \chi_{k\ell}^{continuum}(\theta, \tilde{v}) \qquad (4)$$

The absorption coefficient at a specified wavenumber is built up by the summation of contributions from neighbouring lines, hence the term "line-by-line". This summation is defined as,

$$k_{k\ell}(\tilde{v}) = \sum_{m=1}^{N_{lines}} S_{k\ell m}(\tilde{v}, \bar{T}_{k\ell})\, f(\tilde{v} - \tilde{v}_{ok\ell m}, \bar{p}_{k\ell}, \bar{T}_{k\ell}, u_{k\ell}) \qquad (5)$$

where S is the spectral line strength at $\tilde{v}_{ok}$ and f is its shape function.

Potentially thousands of lines may be required to build a single point in an optical depth spectrum. Consequently, LBL calculations are relatively slow due to the many sums required to evaluate the absorption coefficients.

In order to speed up LBL calculations sufficiently for use as a research tool, a faster LBL, the FLBL, was developed (Turner, 1995). In this model, the time consuming "line-by-line" part was replaced with high resolution absorption coefficient lookup tables (k-tables), thereby transferring the CPU intensive Eqn 5 to a "once-only" off-line operation. A side benefit of this replacement is the vast simplification of the LBL code which in turn allows the code to be easily tailored to specific projects.

K-tables as a function of absorber, pressure, temperature and wavenumber have been created using a conventional LBL and HITRAN data (Rothman et al, 2003). Each table can be thought of as a collection of tables, one table per wavenumber. Consequently the spectral resolution of the FLBL is the resolution of the tables. Each table contains $k(\tilde{v})$ on a defined set of pressures and temperatures. The required $k(\tilde{v}, p, T)$ is found using a bi-cubic interpolation routine. In principle the tables should have a absorber amount dependancy however the dependence is sufficiently weak in the atmosphere that it can be ignored[1]. This simplification allows k and u to be treated independently with little loss in accuracy.

Once the spectra have been produced, simulated satellite radiances are formed by convolving the spectrum with the instrument response functions.

The Gradient FLBL (GFLBL)

One method of obtaining a Jacobian profile is by using a brute force method. This entails perturbing each level by $+/-\delta\eta$, calculating the resulting radiance and numerically differentiating; ie,

$$\frac{\partial \Re}{\partial \eta_k} = \frac{\Re(\eta_k + \delta\eta) - \Re(\eta_k - \delta\eta)}{2\delta\eta} \qquad (6)$$

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[1] Water vapour is an exception, however it can be separated into two components that are independent of absorber amount (Turner, 1995)

With this method a complete Jacobian profile would require 2*N separate FLBL executions. In practise the FLBL is not executed 2*N times independently, but uses a specialized version (BFFLBL) to do the perturbations and differencing internally for an entire profile. This version can only perturb one variable at a time, hence separate runs are required to generate a temperature or a volume mixing ratio Jacobian profile. This process is very time consuming. In addition, some experimentation is needed to determine a suitable value for the perturbation.

In order to make finding the gradient more efficient and accurate, Eqn 2 is differentiated analytically with respect to the profile temperatures and volume mixing ratios at each prescribed level.

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

$$
\bar{B}_p \mathfrak{S}_p \frac{\partial \chi_p}{\partial \eta_p} + \bar{B}_{p+1} \mathfrak{S}_{p+1} \frac{\partial \chi_{p+1}}{\partial \eta_p} - \left(\frac{\partial \chi_{p+1}}{\partial \eta_p} + \frac{\partial \chi_p}{\partial \eta_p} \right) \sum_{k=p+2}^{n} \Re_k^a \tag{7}
$$

where $\quad A_p = \frac{c_2 \, e^{c_2 \tilde{v}/T_p}}{c_1 \, \tilde{v}^2 \, T_p^2}$, $\quad \bar{A}_p = \frac{c_2 \, e^{c_2 \tilde{v}/\bar{T}_p}}{c_1 \, \tilde{v}^2 \, \bar{T}_p^2}$.

The optical depth derivatives are

$$
\frac{\partial \chi_{p+1}}{\partial \eta_p} = \sum_{l=1}^{N_g} \left(k_{p+1,l} \frac{\partial u_{p+1,l}}{\partial \eta_p} + u_{p+1,l} \frac{\partial k_{p+1,l}}{\partial \eta_p} \right) \quad \text{and} \quad \frac{\partial \chi_p}{\partial \eta_p} = \sum_{l=1}^{N_g} \left(k_{pl} \frac{\partial u_{pl}}{\partial \eta_p} + u_{pl} \frac{\partial k_{pl}}{\partial \eta_p} \right) \tag{8}
$$

The absorption coefficient is evaluated using the layer's mean values, $\bar{p}$ and $\bar{T}$, thus their derivatives with respect to the levels η must be known. Noting that $\bar{p}$ and $\bar{T}$ are dependent on all adjacent level values (see Eqn 3), then:

$$
\frac{\partial k_{p+1,l}}{\partial \eta_p} = \left(\frac{\partial k_{p+1,l}}{\partial \bar{p}_{p+1,l}} \frac{\partial \bar{p}_{p+1,l}}{\partial \eta_p} + \frac{\partial k_{p+1,l}}{\partial \bar{T}_{p+1,l}} \frac{\partial \bar{T}_{p+1,l}}{\partial \eta_p} + \frac{\partial k_{p+1,l}}{\partial \bar{c}_{p+1,l}} \frac{\partial \bar{c}_{p+1,l}}{\partial \eta_p} \right) \quad \text{and} \quad \frac{\partial k_{pl}}{\partial \eta_p} = \left(\frac{\partial k_{pl}}{\partial \bar{p}_{pl}} \frac{\partial \bar{p}_{pl}}{\partial \eta_p} + \frac{\partial k_{pl}}{\partial \bar{T}_{pl}} \frac{\partial \bar{T}_{pl}}{\partial \eta_p} + \frac{\partial k_{pl}}{\partial \bar{c}_{pl}} \frac{\partial \bar{c}_{pl}}{\partial \eta_p} \right)
$$

The derivatives $\dfrac{\partial k_{pl}}{\partial \bar{p}_{pl}}$ and $\dfrac{\partial k_{pl}}{\partial \bar{T}_{pl}}$ are evaluated from the look-up table simultaneously with k since the bi-cubic interpolation coefficients can also be used to evaluate the derivatives. Since k_{pl} is assumed to be independent of absorber amount, $\dfrac{\partial k_{pl}}{\partial \bar{c}_{pl}} = 0$.

The current GFLBL code generates;
1) TOA transmittance profiles for each individual gas, the total (all absorbers), the so-called uniformly mixed gases (UMG), and water vapour plus UMG;
2) the Planck-weighted equivalents of item 1,
3) the attenuated p_k to TOA surface emission assuming $\epsilon_k=1$
4) the attenuated p_k to TOA atmospheric emissions
5) the derivative of item 3 (k = s) with respect to p_p, T_p, and c_{pl}.
6) the derivative of item 4 (k = s) with respect to p_p, T_p, and c_{pl}.
The attenuated surface radiances, item 3, is a set of radiances that assumes a surface exists at all

levels. This is useful for considering "black" clouds at level k. Items 5 and 6 are kept separate in order to avoid executing the GFLBL for different values of surface emissivity (assuming ϵ is constant across the response function).

Comparison Between BFFLBL and GFLBL

The BFFLBL and GFLBL models were compared by calculating the temperature, water vapour and ozone Jacobians for 20 AIRS channels. The channels and 53 profiles selected are taken from a recent inter-comparison of radiative transfer models for simulating AIRS radiances (Saunders, 2005, URL 2003). The temperature perturbation and volume mixing ratio perturbation used by the BFFLBL is $\pm\frac{1}{2}$K and $\pm5\%$ of the vmr respectively.

A sample of the Jacobian comparisons is shown in figure 2. In general, the two compare very well, however occasionally the BFFLBL curves can be noisy. The noise, as yet, has never appeared in any temperature Jacobian curves but does occasionally appear in volume mixing ratio Jacobians. This noise is likely due to numerics.

In addition the GFLBL compared moderately well against other models the aforementioned inter-comparison.

Finally, on a LINUX workstation (i686 under RedHat8) the amount of CPU consumed for GFLBL is measured in seconds, whereas to obtain the same volume of results the BFFLBL consumes is measured in hours. Typically the BFLBL consumes 700 times more CPU time.
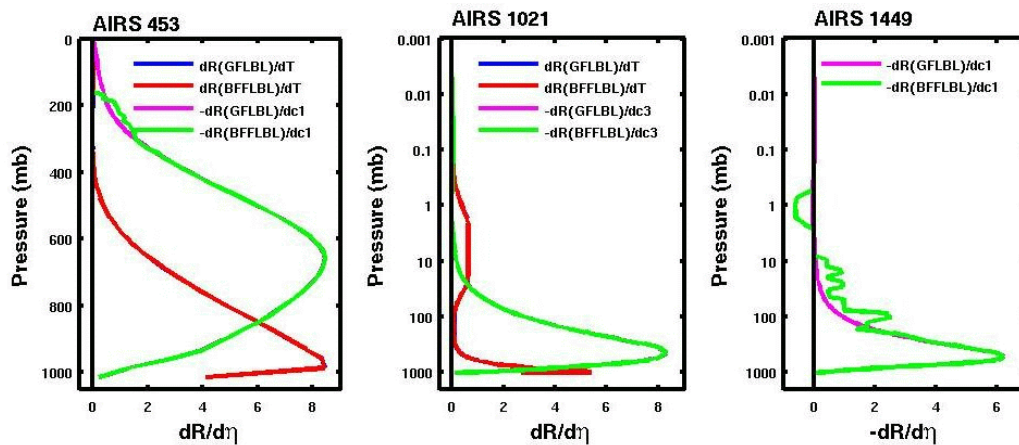

Fig. 2: Comparison of the GFLBL and BFFLBL temperature, H_2O vmr and O_3 vmr Jacobian profiles for 3 AIRS channels assuming profile 52 of the ECMWF set.

Applications

In general the gradient version of fast forward models are, by design, incapable of producing Jacobian profiles of each of the individual absorbers imbedded in the model. Consequently they cannot be used to access the sensitivity of these absorbers to perturbations in the atmosphere. The GFLBL can be used to obtain the Jacobian profile for each absorber used by the model. Because of its speed, it can produce Jacobian profiles for many different atmospheres in a reasonable amount of time. For example, Fig. 3 is a plot of the temperature and eight volume mixing ratios sensitivities for seven AIRS channels around 2386(cm[-1]) based on the 53 IC2003 inter-comparison profiles. The sensitivity is an estimate of the change in brightness temperature for a change in temperature, ΔT, or change in volume mixing ratio as a percentage at some level; ie,

$$S(T_k) \ = \ \Delta T \ \frac{\partial BT}{\partial T_k} \qquad \text{or} \qquad S(c_{k\ell}) \ = \ a \ c_{k\ell} \ \frac{\partial BT}{\partial c_{k\ell}} \tag{9}$$
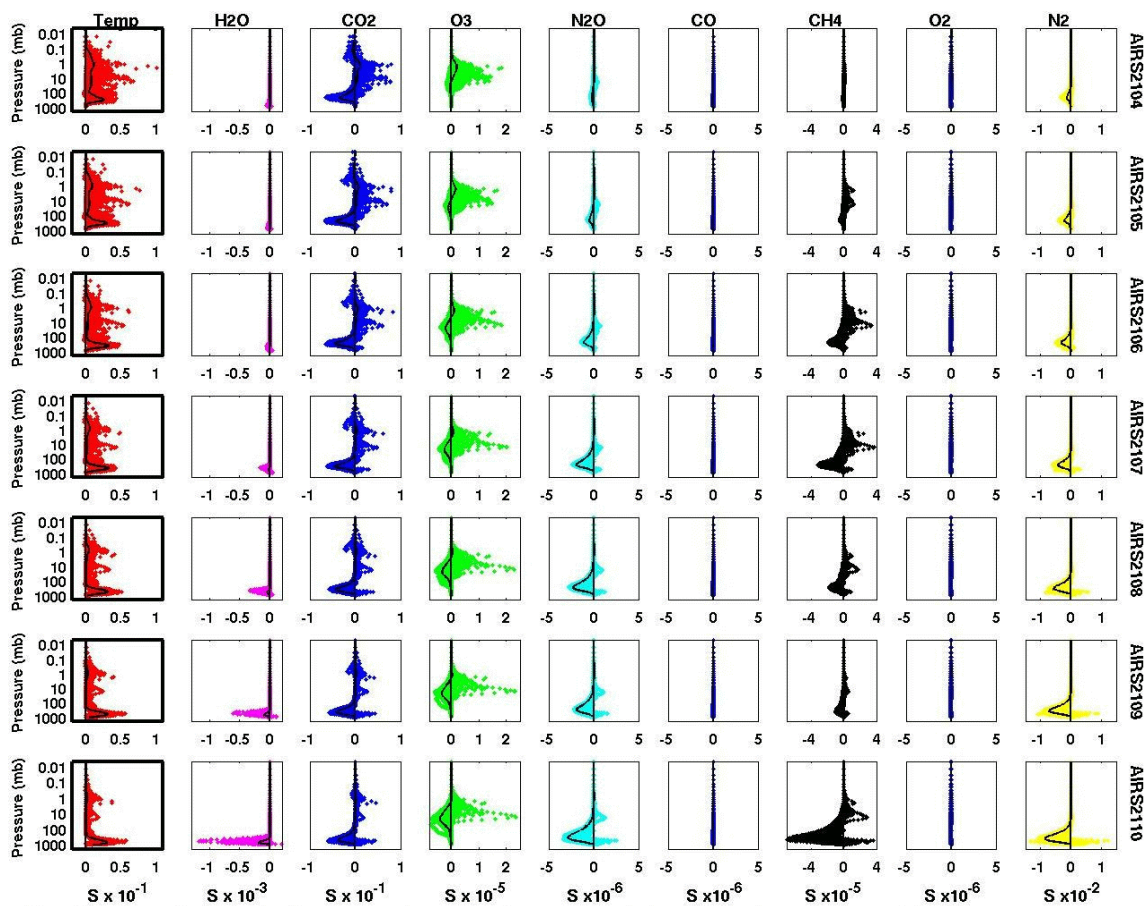
where T = 1K and a = .1 (10%)

Fig. 3: Plot of the sensitivity of a group of AIRS channels to a 1K or 10% change in temperature or vmr for 53 atmospheres. The solid black line is for profile 52.

As can be seen in Fig. 3, these channels are most sensitive to temperature and CO_2, and to a small extent H_2O. There is a strong sensitivity to N_2, however 10% changes in N_2 are highly unlikely. The sensitivity to H_2O increases with channel. Usually one gauges the suitability of a channel by considering only the profiles for a couple of a atmospheres. However, with a larger group of profiles one can see that the average atmosphere doesn't necessarily coincide with an average sensitivity. In fact there is significant variation in both the temperature and CO_2 profiles around the mean profiles at heights where the average shows no significant values.

Another use of the GFLBL is to validate re-mapping algorithms. For example, one cannot directly compare a Jacobian profile calculated on a set of M-levels with a calculation on a set of N-levels by simple interpolation since the Jacobian calculation at a specific level is implicitly dependent on the thicknesses of the layers adjacent to the level.

One method to remap a Jacobian profile from M to N levels is by weighting the M-Jacobian profile with its adjacent layers, interpolating the result to N-levels and then weighting it with the new adjacent layers, that is—

$$J_i^* = \frac{J_i^M}{\beta} \begin{cases} \beta = (p_2^M - p_1^M), & i = 1 \\ \beta = (p_{i+1}^M - p_{i-1}^M), & i = 2, M-1 \\ \beta = (p_M^M - p_{M-1}^M), & i = M \end{cases} \text{ and } J_j^N = J_j^* \beta \begin{cases} \beta = (p_2^N - p_1^N), & j = 1 \\ \beta = (p_{j+1}^N - p_{j-1}^N), & j = 2, N-1 \\ \beta = (p_N^N - N_{N-1}^N), & j = N \end{cases}$$

where J_i^* is interpolated onto J_j^* via linear interpolation.

To see how well this algorithm performs, the temperature Jacobian profile for a few channels was evaluated on five versions of the same atmosphere. Each atmosphere is an interpolation of the original atmosphere, from 25 levels to 6, 12, 25, 50 and 98 levels. For this example the top and bottom levels of the five atmospheres were fixed to the same pressure. The other levels are spaced such that the number of molecules per layer slowly decreases with height.

The Jacobians of these five atmospheres were then remapped to the other four atmospheres for a total of 25 possible re-mappings. Figure 4 compares these re-mappings with the "truth" as evaluated by the GFLBL for two AIRS channels. In general this method works fairly well for cases when M is greater than N. However the location and number of levels are factors that must be considered. It should also be noted that this method does not work equally well for all channels as demonstrated in Fig. 4 where the method does a better job in AIRS 1090 than in AIRS 1766.
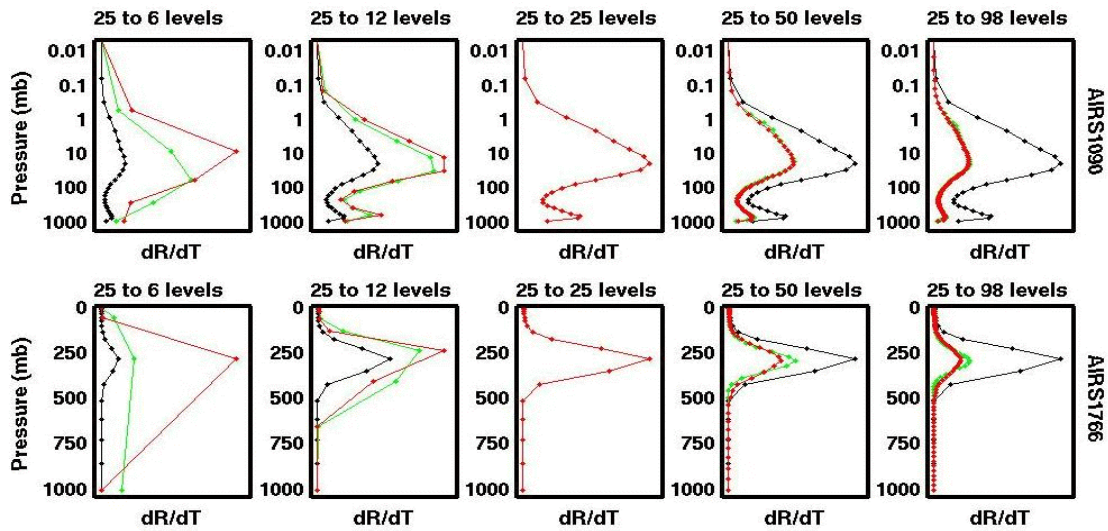
Fig 4: Remapping of a M-level Jacobian (—) to a N-level Jacobian (—) using the weighted adjacent layers method. The results are compared with the GFLBL (—)results.

Another method of remapping a Jacobian profile from M to N levels is to use the adjoint code of a forward linear interpolation routine. Figure 5 illustrates the adjoint method using the same setup as was used for figure4.
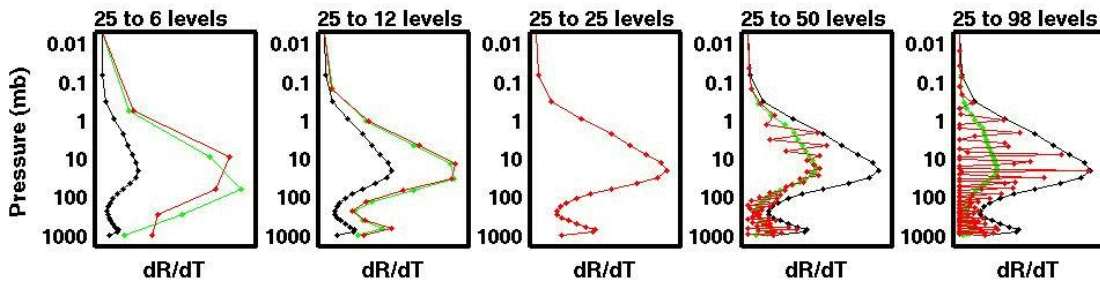

Fig 5: Remapping of a M-level Jacobian (—) to a N-level Jacobian (—) using the adjoint method. The results are compared with the GFLBL (—)results. Profile 52 and AIRS 1090 are considered for this example.

The adjoint method works fine when the re-mapping steps down from M to N levels. Unfortunately a significant amount of noise is introduced one is stepping up.   This method is used to transfer the radiance Jacobians from a 43 level model to a 28 level model in MSC's NWP model, thus when the number of NWP levels is raised, either a new method has to be adopted or the number of radiation levels increased.

Conclusions

A gradient version of the FLBL has been developed that is relatively quick and accurate. Its intent is to complement the FLBL as a research tool for examining Jacobians, sensitivities and anything else that is related to the gradient of the radiative transfer equation. It has been used to demonstrate

problems in the remapping of Jacobian profiles when mapping from a few levels to many levels using the adjoint method.

In its current form it the GFLBL does not consider the reflected down-welling flux term or the solar term in a non-scattering atmosphere, although the most recent version of the FLBL can. The next version of the GFLBL will be incorporating one or both of these. In addition the model will extended to include spherical geometry in order to handle limb sounding.

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