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Linearization of the Interaction Principle: Analytic Jacobians in the "Radiant" Model

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Abstract

In this paper we present a new linearization of the Radiant radiative transfer model. Radiant uses discrete ordinates for solving the radiative transfer equation in a multiply-scattering anisotropic medium with solar and thermal sources, but employs the adding method (interaction principle) for the stacking of reflection and transmission matrices in a multilayer atmosphere. For the linearization, we show that the entire radiation field is analytically differentiable with respect to any surface or atmospheric parameter for which we require Jacobians (derivatives of the radiance field). Derivatives of the discrete ordinate solutions are based on existing methods developed for the LIDORT radiative transfer models. Linearization of the interaction principle is completely new and constitutes the major theme of the paper. We discuss the application of the Radiant model and its linearization in the Level 2 algorithm for the retrieval of columns of carbon dioxide as the main target of the Orbital Carbon Observatory (OCO) mission.

Keywords: Radiative transfer; Discrete ordinates; Doubling-adding; Pseudo-spherical; Linearization; OCO mission; Carbon dioxide retrieval.

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1. Introduction

1.1. Background to radiative transfer linearization

It is well known that there are many methods to solve for the radiation field in a multilayer multiply-scattering anisotropic medium with solar and thermal sources. Techniques include the discrete ordinate approach originally pursued by Chandrasekhar [1], the doubling-adding method, finite difference methods, spherical harmonics, invariant imbedding, Gauss-Seidel iteration, successive orders of scattering, Monte-Carlo methods and others; for a review of radiative transfer (RT) solution methods, see for example [2]. Of these methods, a survey of the literature reveals that the discrete ordinate and the doubling-adding methods are the most widely used. The well-known discrete ordinate DISORT model [3] has became a standard in the atmospheric science community. Another discrete ordinate code is LIDORT [4]; this model was designed to generate radiances and analytic Jacobians and is fully linearized. In this paper, we will employ the linearized LIDORT formulation for the discrete ordinate part of the Radiant model. The doubling-adding technique is also known as matrix-operator theory or discrete space theory; the formalism is based around the interaction principle of layer adding. Doubling refers to the generation of global reflection and transmittance matrices and source vectors for two identical layers; adding refers to the interaction principle applied to two layers with differing optical properties. Discrete ordinate and doubling-adding methods are closely related; for a discussion, see for example [5].

For the retrieval of atmospheric and other geophysical quantities from space using nonlinear iterative fitting methods, it is a requirement for the forward model to not only generate simulated radiances but also radiance derivatives (variously called Jacobians or weighting functions or sensitivity functions) with respect to the state vector retrieval parameters. Analytic derivatives are straightforward to generate in radiative transfer transmittance models for infrared and microwave retrievals based on line absorption. However, RT modeling with scattered light is much more complex and, until fairly recently, radiance derivatives were generated by cumbersome finite-difference methods. The RT calculation of accurate analytic Jacobians in scattering models has been addressed recently in a number of papers. These include the family of discrete ordinate codes LIDORT [4, 6, 7, 8] with linearization based on complete analytic differentiation of the full multilayer discrete ordinate soluution, the LIRA model [9, 10, 11] with linearization based on adjoint perturbation methods, the GOMETRAN models [12, 13, 14] with derivatives determined by perturbation analysis, and others (e.g. the work of Ustinov [15]).

The Radiant model [16, 17, 18] was designed to take advantage of the two main methods of radiative transfer solution in a multiply-scattering multilayer atmosphere. As such, Radiant is a hybrid model consisting of two parts. The first part uses the discrete ordinate approach to generate the homogeneous and particular solutions (due to the solar scattering and/or thermal sources) of the radiative transfer equation (RTE) on a layer-by-layer basis. The second part uses the adding method for the stacking of reflection and transmission matrices and source function vectors in order to find the radiance fields corresponding to whole-atmosphere reflectances and transmittances at top of atmosphere (TOA) and bottom of atmosphere (BOA). In this work we present a complete linearization of the Radiant model; we demonstrate that the radiation field is analytically differentiable with respect to any atmospheric or surface property for which a Jacobian is required. For the discrete ordinate part of Radiant, the linearization work is based closely on that used in the LIDORT model [4, 8]. The linearization of the adding principle is completely new.

1.2. The Radiant model in the OCO mission

Radiant is the radiative transfer model selected for the Orbiting Carbon Observatory (OCO) Level 2 algorithm to retrieve column-weighted CO_2 from a remote sensing platform [19, 20]. The aim of the mission is to retrieve total CO_2 to an accuracy 1 part per million on regional scales in order to provide accurate input for the determination of carbon fluxes on a global basis (see for example [21]). The OCO mission is scheduled for a 2008 launch and will be synchronized ahead of the EOS A-train in a 705 km polar orbit. The OCO instrument comprises 3 high-resolution spectrometers measuring earthshine backscatter in the O_2 A band, the weak CO_2 band at 1.61 μm and the strong CO_2 band at 2.06 μm. There are three science modes of operation: the nadir viewing mode (over most surfaces), the glint mode for glancing incidence over sunlit oceans, and the target mode (stare capability). In nominal nadir-viewing mode, the spatial footprint is approximately 1.25 x 2.3 km. The inverse problem will be based on classical optimal estimation methods [22], while the forward model part of the retrieval requires a full scattering radiative transfer treatment. For more details on the OCO mission, see [20].

The OCO forward model requirements have influenced the Radiant model development. Since OCO will measure at high solar zenith angles, it is necessary for Radiant to treat solar beam attenuation in a curved spherical-shell atmosphere (scattering is still treated as plane-parallel). This is the commonly-used pseudo-spherical (PS) approximation [23]. Here we follow the average secant PS formulation as in the LIDORT models [4]. For the glint and target modes, satellite viewing angles may reach up to 75° from nadir, and it then becomes necessary to treat source function integration along the line-of-sight for a curved atmosphere [14, 24, 25]. As with DISORT and LIDORT, Radiant uses the Nakajima-Tanaka TMS single-scatter correction [26] to derive more accurate radiance fields. Given the wide variety of land surfaces sampled, the Radiant model has also been given a full BRDF surface reflectance capability based on the formulations in DISORT [27] and (for the derivation of analytic weighting functions with respect to surface properties) LIDORT [8].

There is also a spectral binning procedure in the OCO L2 algorithm which pre-calculates and stores classified sets of reflection and transmission matrices. The integration of spectral binning in Radiant is a considerable task that is outside the scope of the present work; more details will be presented in a forthcoming paper [28].

1.3. Scope of the paper

The first two sections are devoted to the discrete ordinate part of Radiant. Section 2 sets up the radiative transfer equation (RTE), defines inputs of basic optical properties and their derivatives, and gives a summary of the pseudo-spherical approximation. Section 3 discusses homogeneous and particular solutions for the RTE in each layer and summarizes the generation of analytic derivatives for these solutions. These two sections are based closely on the

LIDORT formalism; we summarize results without giving detailed proofs. In section 4, we establish the link between the discrete ordinate solutions and the adding formalism by derivation of the reflection and transmission function matrices and solar source function vectors for each atmospheric layer from the discrete ordinate solutions of section 3. In addition we derive analytic derivatives of these quantities with respect to atmospheric variables. This material is unfamiliar (especially the linearization aspects) and we have gone into more detail here.

In section 5, we describe the interaction principle or adding mechanism to build whole-atmosphere reflection and transmission matrices and source vectors through the repeated addition of layer quantities. We apply the boundary conditions and solve for the radiance field at the top and bottom of the atmosphere (TOA and BOA). Although this material is familiar, we have given a detailed exposition as a prelude to the new part of the paper in section 6. Here we present a complete analytic differentiation of the whole adding operation, and we demonstrate how analytic weighting functions may be derived from this operation. Section 7 contains a digest of additional implementations in Radiant (in particular the BRDF specifications and the single scatter corrections), and some notes on the verification of the model. In the conclusion, we remark on future developments for the forthcoming OCO application.

2. Basic Equations and Definitions

2.1. Radiative transfer equations

All scattering processes are treated for a plane-parallel medium, but we allow for curved path attenuation of the solar beam before scattering (this is the pseudo-spherical approximation). Single scattering albedos and phase functions are independent of height in a given atmospheric layer. The atmosphere is regarded as a collection (or stack) of optically uniform layers; we use optical thickness x (measured from the top of a layer) as the vertical coordinate.

We first consider the RTE for a single layer. The intensity is expanded as a Fourier cosine series in the relative azimuth $\phi - \phi_0$. Using the expansion of the phase function in terms of Legendre polynomials in the cosine of the scatter angle, plus the addition theorem for Legendre polynomials, the azimuthal dependence of the phase function can also be expressed as a cosine series in relative azimuth. The azimuth separation follows immediately, and we obtain the following equation for each Fourier component $I^m(x, \mu)$ of the intensity:

$$\mu \frac{dI^m(x,\mu)}{dx} = I^m(x,\mu) - \int_{-1}^{1} \Pi^m(\mu,\mu')I^m(x,\mu')d\mu' - \frac{F_\odot}{2\pi}\epsilon_{m0}\Pi^m(\mu,-\mu_0)\hat{T}e^{-x\lambda}, \tag{1}$$

where μ is the polar angle cosine. The last term in Eq. (1) is the solar source: $F_\odot$ is the solar extraterrestrial flux, and λ and $\hat{T}$ are the average secant and initial transmittance (to the layer top) of the solar beam in the pseudo-spherical approximation (we define these quantities below in section 2.3). The phase function quantities Π^m are defined in terms of normalized associated Legendre polynomials $P_l^m(\mu)$ and coefficients β_l (the phase function Legendre expansion coefficients multiplied by $2l+1$)) through:

$$\Pi^m(\mu,\mu') = \frac{1}{2}\omega \sum_{l=m}^{2N-1} \beta_l P_l^m(\mu) P_l^m(\mu'). \tag{2}$$

The integral in Eq. (1) is the multiple scatter contribution. To obtain discrete ordinate solutions, we replace this term with a summation using a "double Gauss" quadrature scheme defined for the two polar angle half-spaces. Each quadrature has N points, with abscissae and weights $\{\mu_i, a_i\}, i = 1,\ldots,N$ in the positive half-space and $\{-\mu_i, a_i\}, i = 1,\ldots,N$ for the negative half-space. The RTE is then replaced by the discrete ordinate form:

$$\mu_i \frac{dI^m(x,\mu_i)}{dx} = I^m(x,\mu_i) - \sum_{j=\pm 1}^{j=\pm N} a_j \Pi^m(\mu_i,\mu_j) I^m(x,\mu_j) - \frac{F_\odot}{2\pi}\epsilon_{m0}\Pi^m(\mu_i,-\mu_0)\hat{T}e^{-\lambda x}. \tag{3}$$

2.2. *Optical property inputs*

For a given layer n, the input optical properties are the total layer single scattering albedo ω_n, the layer optical thickness (for extinction) Δ_n and the total layer phase function Legendre expansion coefficients β_{ln}. From Eq. (3), it is the combination $\phi_{ln} \equiv \omega_n \beta_{ln}$ that occurs in the RTE. Apart from specification of the surface reflectance, the set of inputs $\{\omega_n, \Delta_n, \beta_{ln}\}$ is sufficient to solve for the radiance field in a multilayer multiply-scattering atmosphere.

For the additional output of an *analytic* weighting function with respect to an atmospheric variable ξ_n in layer n, we require analytic derivatives of the basic optical property inputs with respect to ξ_n. Defining the linearization operator $\mathcal{L}_n \equiv \frac{\partial}{\partial \xi_n}$, then the additional inputs to the linearized model are $\mathcal{L}_n[\omega_n]$, $\gamma_n \equiv \mathcal{L}_n[\Delta_n]$ and $\mathcal{L}_n[\beta_{ln}]$. In the sequel, we will use the combination $\psi_{ln} \equiv \mathcal{L}[\phi_{ln}] = \mathcal{L}[\omega_n \beta_{ln}]$. These derivative inputs are the end points in the chain rule differentiation of the radiance field.

2.3. Pseudo-spherical formulation

In terms of a vertical optical thickness grid Δ_n for $n = 1, \ldots N_a$ (where N_a is the total number of layers in the model atmosphere), the attenuation of the solar beam at any point within layer n is given by $\hat{T}(x) = \hat{T}_n e^{-\lambda_n x}$ where $\hat{T}_n$ is the transmittance of the solar beam to the top of the layer and λ_n the average secant for that layer. In a curved atmosphere, we use the geometrical *Chapman factors* $\{f_{n,k}\}$: these are the slant path geometrical distances traversed through each of the layers k, $k = 1, \ldots, n$ divided by the corresponding vertical distances. In a plane parallel atmosphere, $f_{n,k} = \frac{1}{\mu_0}$ (a constant), where μ_0 is the solar zenith angle cosine. From the definition of attenuation, it follows that $\hat{T}_n = \hat{T}_{n-1} e^{-\lambda_{n-1}\Delta_{n-1}}$ for attenuation to the top of layer n, and hence for $n > 1$ the initial transmittance and average secant can be expressed as

$$\hat{T}_n = \exp\left[-\sum_{k=1}^{n-1} f_{n-1,k}\Delta_k\right]; \tag{4}$$

$$\lambda_n = \frac{\sum_{k=1}^{n} f_{n,k}\Delta_k - \sum_{k=1}^{n-1} f_{n-1,k}\Delta_k}{\Delta_n}, \tag{5}$$

with $\hat{T}_n = 1$ and $\lambda_n = f_{n,n}$ for $n = 1$.

Linearization of the pair $\left\{\hat{T}_n, \lambda_n\right\}$ is straightforward, and requires knowledge only of input quantities $\gamma_n = \mathcal{L}_n[\Delta_n]$. $\mathcal{L}_k[\hat{T}_n]$ will refer to a linearization of $\hat{T}_n$ due to variation of a quantity in a layer $k < n$. Since the solar beam is attenuated through the atmosphere to layer n, variations in layers $k < n$ will contribute in the differentiation of $\hat{T}_n$, and layers $k \leq n$ will contribute in the differentiation of λ_n. For $n > 1$ and $k < n$, we find

$$\mathcal{L}_k[\hat{T}_n] = -\gamma_k f_{n-1,k} \hat{T}_n, \tag{6}$$

and $\mathcal{L}_n[\hat{T}_n] = 0$ for $n = 1$. For the average secant linearization $\mathcal{L}_k[\lambda_n]$, we have:

$$\mathcal{L}_k[\lambda_n] = \quad \frac{(f_{n,k} - f_{n-1,k})\gamma_k}{\Delta_n} \quad (n > 1, k < n); \tag{7}$$

$$\mathcal{L}_n[\lambda_n] = \qquad \frac{(f_{n,n} - \lambda_n)\gamma_n}{\Delta_n} \quad (n > 1). \tag{8}$$

and $L_n[\lambda_n] = 0$ for $n = 1$. In the plane parallel case, $\mathcal{L}_k[\lambda_n] = 0$ for every n, k since $\lambda_n = 1/\mu_0$.

Slant path lengths may be easily computed for a shell atmosphere with no refraction; we require only knowledge of the level altitudes and the earth radius. In this case, the solar zenith cosine is μ_0 at all levels. In a refractive atmosphere, we use Snell's law and refractive bending through a finely-layered atmosphere; pressure and temperature profiles are now required as input. In the refracting case, the solar zenith angle changes slightly through the atmosphere from its TOA value of θ_0: the ray tracing yields SZA values all levels, and we define representative solar zenith cosines $\tilde{\mu}_n$ for each layer n as the average of the layer boundary values (see [4] for more details on this point).

3. Basic RTE solutions and linearizations

This section is concerned with discrete ordinate solutions to the RTE in an optically uniform layer. The theory may be found in a number of places in the literature [4, 5, 16].

3.1. Homogeneous solutions

To get solutions of the homogeneous version of Eq. (3), we substitute $I_j \sim X_j e^{-\nu x}$ for $j = \pm 1, \ldots, \pm N$. By using the sum and difference vectors $\vartheta_j = X_j + X_{-j}$ and $\varsigma_j = X_j - X_{-j}$ for $j = 1, \ldots, N$, Eq. (3) is reduced to an N-rank eigenproblem with eigenvalues ν_α^2 and eigenvectors ς_α:

$$\left(\mathbf{\Gamma} - \nu_\alpha^2 \mathbf{E}\right) \varsigma_\alpha = 0, \quad \text{where} \quad \mathbf{\Gamma} = (\zeta - \eta)(\zeta + \eta); \tag{9}$$

$$\zeta_{ij} = \left(\Pi_{ij}^{+} w_j - \delta_{ij}\right) / \mu_i \quad \text{and} \quad \eta_{ij} = -\Pi_{ij}^{-} w_j / \mu_i. \tag{10}$$

The eigenvalues $\pm\nu_\alpha$ occur in pairs. In the above equations, $\alpha = 1, \ldots, N$, $\mathbf{E}$ is the identity matrix and the elements $\Pi_{ij}^{\pm} = \Pi^{\pm}(\mu_i, \pm\mu_j)$ are given by Eq. (2) evaluated at quadrature polar angle cosines. The sum vector ϑ_α satisfies the auxiliary equation:

$$\nu_\alpha \vartheta_{i\alpha} = \sum_{j=1}^{N} (\zeta_{ij} + \eta_{ij}) \varsigma_{j\alpha}. \tag{11}$$

Equations (9) and (11) are sufficient to determine the solution of the homogeneous equations. The eigenproblem in (9) can be solved reliably using standard numerical routines. We define the eigenvectors ς_α to have unit length. We also define N-vectors $\mathbf{X}_\alpha^{\pm}$ such that $X_{j\alpha}^{\pm} = \frac{1}{2}(\varsigma_{j\alpha} \pm \vartheta_{j\alpha})$, where $j = 1, \ldots, N$. These solution vectors are then combined as the columns of matrices of solutions $\mathbf{Y}_\pm$ which we will require for linearizing the transmission and reflection matrices in section 4. We collect eigenstream layer transmittances $\exp[-\nu_\alpha\Delta]$ as diagonal elements of the matrix $\mathbf{\Lambda} = \mathrm{diag}[\mathrm{e}^{-\nu_1\Delta}, \ldots, \mathrm{e}^{-\nu_\mathrm{N}\Delta}]$.

We now turn to the linearization of the above process. The layer index n is implicit in this section. From the definition of $\Pi^\pm_{ij}$, we can define the linearizations

$$\mathcal{L}_n[\Pi^\pm_{ij}] = \frac{1}{2}\sum_{l=m}^{2N-1} \psi_{ln} P^m_l(\pm\mu_i) P^m_l(\mu_j), \tag{12}$$

and the linearizations $\mathcal{L}[\zeta]$ and $\mathcal{L}[\eta]$ then follow from Eq. (10); $\mathcal{L}[\mathbf{\Gamma}]$ then follows from the definition in Eq. (9). Differentiation of the eigenproblem in (9) yields:

$$(\mathbf{\Gamma} - \nu^2_\alpha \mathbf{E})\mathcal{L}[\varsigma_\alpha] = 2\nu_\alpha \mathcal{L}[\nu_\alpha]\varsigma_\alpha - \mathcal{L}[\mathbf{\Gamma}]\varsigma_\alpha. \tag{13}$$

For each α, this linear system has $N+1$ unknowns $\mathcal{L}[\nu_\alpha]$ (a scalar) and $\mathcal{L}[\varsigma_\alpha]$ (an N-vector).. An additional constraint comes from the unit normalization condition imposed on the eigenvectors: since $\varsigma_\alpha \cdot \varsigma_\alpha = 1$ (a vector product), then $\mathcal{L}[\varsigma_\alpha] \cdot \varsigma_\alpha = 0$. This constraint combined with (13) is sufficient to solve the $N+1$ linear system (see [6] for more detail). From these results, it is easy to write down the linearizations of the solution vectors $\mathbf{X}^\pm_\alpha$ and hence the matrices $\mathbf{Z}_\pm = \mathcal{L}[\mathbf{Y}_\pm]$ required for linearization of the transmission and reflection matrices in section 4. We will also need linearizations of the layer transmittances $\exp[-\nu_\alpha\Delta]$:

$$\mathcal{L}[e^{-\nu_\alpha\Delta_n}] = -(\mathcal{L}[\nu_\alpha]\Delta_n + \nu_\alpha\gamma_n)e^{-\nu_\alpha\Delta_n}. \tag{14}$$

We collect these linearizations in the diagonal matrix $\mathbf{H} = \mathcal{L}[\mathbf{\Lambda}]$.

3.2. Particular solutions

To get the particular integral corresponding to solar forcing, we try a solution of the form $I_j^{\pm} \sim B_{jn}^{\pm} \hat{T}_n \exp(-x\lambda_n)$ in Eq. (3) (now we retain the layer indexing explicitly). This eliminates the optical depth dependence and we are left with a linear system of order $2N$. The reduction in order follows from the use of sum and difference vectors $\mathbf{K}_n^* = \mathbf{B}_n^+ - \mathbf{B}_n^-$, $\mathbf{J}_n^* = \mathbf{B}_n^+ + \mathbf{B}_n^-$, $\mathbf{D}_n^* = \mathbf{A}_n^+ - \mathbf{A}_n^-$ and $\mathbf{S}_n^* = \mathbf{A}_n^+ + \mathbf{A}_n^-$, where $A_n^{\pm}(\mu_i) = \frac{F_{\odot}}{2\pi} (2 - \delta_{m0}) \Pi_n(\pm\mu_i, -\tilde{\mu}_n)$ and the Π matrix is defined in the usual way. We eliminate $\mathbf{J}_n^*$ in favor of $\mathbf{K}_n^*$ to get

$$\left(\mathbf{\Gamma}_n - \mathbf{E}\lambda_n^2\right) \mathbf{K}_n^* = -\left(\zeta_n - \eta_n\right) \mathbf{D}_n^* - \lambda_n \mathbf{S}_n^* \tag{15}$$

for the difference vector $\mathbf{K}_n^*$. $\mathbf{\Gamma}_n$ is the eigenmatrix in (9) and $\mathbf{E}$ is again the identity matrix. This linear system of order N is solved numerically by LU decomposition. The sum vector $\mathbf{J}_n^*$ is found from the auxiliary equation

$$\lambda_n \mathbf{J}_n^* = \left(\zeta_n + \eta_n\right) \mathbf{K}_n^* + \mathbf{D}_n^*. \tag{16}$$

This is enough to establish the solutions for $\mathbf{B}_n^{\pm}$. In section 4, we will use the vector quantities $\mathbf{F}_n^{\pm} \equiv \mathbf{B}_n^{\pm} \hat{T}_n$ (solar source solution vectors scaled by the initial transmittances) and the scalar average secant transmittances $Q_n \equiv \exp[-\lambda_n \Delta_n]$.

For the linearization, we allow variations in layers k above or equal to layer n. The original particular solution was determined from the linear system (15). The application of the linearization operator $\mathcal{L}_k$ will result in the same linear system, but with a different (perturbed) source vector on the right hand side. We note first that $\mathcal{L}_k[\Gamma_n] = 0$ for $k \neq n$, since Γ_n only depends on the optical property combination $\phi_{ln} = \omega_n \beta_{ln}$ in layer n. This is also true for ζ and

η and vectors $\mathbf{A}_n^{\pm}$ defined above: for $k \neq n$, we have $\mathcal{L}_k[\zeta_n]$, $\mathcal{L}_k[\eta_n]$, and $\mathcal{L}_k[\mathbf{A}_n^{\pm}] = 0$ and for $k = n$, these can be written down easily in terms of the optical property linearizations ψ_{ln}. This means that the linearizations $\mathcal{L}_k[\mathbf{S}_n^*]$ and $\mathcal{L}_k[\mathbf{D}_n^*]$ are defined only for $k = n$. The linearization of Eq. (15) is then

$$\left(\mathbf{\Gamma}_n - \mathbf{E}\lambda_n^2\right) \mathcal{L}_k\left[\mathbf{K}_n^*\right] = \delta_{nk}\mathbf{\Omega}_n - \mathbf{S}_n^* \mathcal{L}_k\left[\lambda_n\right], \tag{17}$$

where we have defined the following auxiliary quantity:

$$\mathbf{\Omega}_n = -\mathcal{L}_n\left[\zeta_n - \eta_n\right]\mathbf{D}_n^* - \left(\zeta_n - \eta_n\right)\mathcal{L}_n\left[\mathbf{D}_n^*\right] - \lambda_n \mathcal{L}_n\left[\mathbf{S}_n^*\right] - \mathcal{L}_n\left[\mathbf{\Gamma}_n\right]\mathbf{K}_n^*. \tag{18}$$

This establishes $\mathcal{L}_k[\mathbf{K}_n^*]$; we can then linearize the auxiliary relation Eq. (16) to get $\mathcal{L}_k[\mathbf{J}_n^*]$. Finally, we combine these two sum and difference linearizations to get the result for $\mathcal{L}_k[\mathbf{B}_n^{\pm}]$. In section 4, we also use vector quantities $\mathbf{G}_{kn}^{\pm} \equiv \mathcal{L}_k[\mathbf{F}_n^{\pm}]$, which are established from product differentiation of $\mathbf{B}_n^{\pm}\hat{T}_n$. The linearized whole layer transmittance scalar is given by

$$\Theta_{kn} \equiv \mathcal{L}_k[Q_n] = -(\mathcal{L}_k[\lambda_n]\Delta_n + \delta_{kn}\lambda_n\gamma_n)Q_n. \tag{19}$$

This finishes the set-up and linearization of the basic RTE solution.

4. Layer reflection, transmission and source functions

We start with the general discrete ordinate solution in a given layer:

$$I_i^{\pm} = \sum_{\alpha=1}^{N} \left\{ L_\alpha X_{i\alpha}^{\pm} \mathrm{e}^{-\nu_\alpha x} + M_\alpha X_{i\alpha}^{\mp} \mathrm{e}^{-\nu_\alpha (\Delta - x)} \right\} + F_i^{\pm} \mathrm{e}^{-\lambda x}, \tag{20}$$

where $i, \alpha = 1, \dots N$, and $X_{i\alpha}^{\pm}$ and ν_α are the discrete ordinate solutions vectors and separation constants (eigenvalues), respectively; $F_i^{\pm}$ is the particular integral source vector for the solar beam. Δ is the whole layer optical thickness. We recall the following notation (boldface entries for vectors and matrices): $\mathbf{\Lambda} = \delta_{i\alpha} \mathrm{e}^{-\Delta \nu_\alpha}$; $\mathbf{Y}_{\pm} = X_{i\alpha}^{\pm}$; $Q = \mathrm{e}^{-\Delta\lambda}$; $\mathbf{F}^{\pm} = F_i^{\pm}$.

In Eq. (20), $\mathbf{L}$ and $\mathbf{M}$ are vectors of integration constants. In the DISORT and LIDORT discrete ordinate models, these vectors are established for all layers in the atmosphere by application of boundary conditions at the top and bottom of the atmosphere and continuity conditions across intermediate layer interfaces. This is the boundary value problem for a multi-layer atmosphere; for a description, see [4] for example.

4.1. Elimination of integration constants

In Radiant, we take a different path towards boundary value determination. From Eq. (20), we rewrite the upwelling and downwelling intensities at the layer boundaries as:

$$\mathbf{I}^{\uparrow}(0) = \quad \mathbf{Y}_{+}\mathbf{L} + \mathbf{Y}_{-}\boldsymbol{\Lambda}\mathbf{M} + \mathbf{F}^{+}; \tag{21}$$

$$\mathbf{I}^{\downarrow}(0) = \quad \mathbf{Y}_{-}\mathbf{L} + \mathbf{Y}_{+}\boldsymbol{\Lambda}\mathbf{M} + \mathbf{F}^{-}; \tag{22}$$

$$\mathbf{I}^{\uparrow}(\Delta) = \quad \mathbf{Y}_{+}\boldsymbol{\Lambda}\mathbf{L} + \mathbf{Y}_{-}\mathbf{M} + \mathbf{F}^{+}Q; \tag{23}$$

$$\mathbf{I}^{\downarrow}(\Delta) = \quad \mathbf{Y}_{-}\boldsymbol{\Lambda}\mathbf{L} + \mathbf{Y}_{+}\mathbf{M} + \mathbf{F}^{-}Q. \tag{24}$$

The first two equations in this set are for optical thickness $x = 0$ at layer top; the second two equations apply for $x = \Delta$ at the lower boundary. The layer index n is understood.

The object is to eliminate $\mathbf{L}$ and $\mathbf{M}$ from two of these four equations in order to find two relations between the four intensity vectors, and hence to establish the layer reflection and transmission matrices $\mathbf{r}^{\pm}$ and $\mathbf{t}^{\pm}$ and layer source vectors $\mathbf{s}^{\pm}$. We multiply Eqs. (22) and (23) by $\mathbf{Y}_{-}^{-1}$ and eliminate $\mathbf{L}$ in favor of $\mathbf{M}$. The result is:

$$\mathbf{M} = \mathbf{D}^{-1}\left\{\mathbf{I}^{\uparrow}(\Delta) - \mathbf{C}\mathbf{I}^{\downarrow}(0) + \mathbf{C}\mathbf{F}^{-} - \mathbf{F}^{+}Q\right\}, \tag{25}$$

where we have defined the auxiliary matrices:

$$\mathbf{C} \equiv \quad \mathbf{Y}_{+}\boldsymbol{\Lambda}\mathbf{Y}_{-}^{-1}; \tag{26}$$

$$\mathbf{D} \equiv \quad \mathbf{Y}_{-}[\mathbf{E} - (\mathbf{Y}_{-}^{-1}\mathbf{Y}_{+}\boldsymbol{\Lambda})^{2}]. \tag{27}$$

A similar operation can be performed to eliminate $\mathbf{M}$ in favor of $\mathbf{L}$:

$$\mathbf{L} = \mathbf{D}^{-1}\left\{\mathbf{I}^{\downarrow}(0) - \mathbf{C}\mathbf{I}^{\uparrow}(\Delta) + \mathbf{C}\mathbf{F}^{+}Q - \mathbf{F}^{-}\right\}. \tag{28}$$

We now substitute these last results into Eqs. (21) and (24) to get:

$$\mathbf{I}^{\downarrow}(\Delta) = \quad \mathbf{t}^{-}\mathbf{I}^{\downarrow}(0) + \mathbf{r}^{+}\mathbf{I}^{\uparrow}(\Delta) + \mathbf{s}^{-}; \tag{29}$$

$$\mathbf{I}^{\uparrow}(0) = \quad \mathbf{t}^{+}\mathbf{I}^{\uparrow}(\Delta) + \mathbf{r}^{-}\mathbf{I}^{\downarrow}(0) + \mathbf{s}^{+}, \tag{30}$$

from which we can now read off the desired results:

$$\mathbf{t}^{-} = \mathbf{t}^{+} = \mathbf{t} = \quad \mathbf{Y}_{-}\mathbf{\Lambda}\mathbf{D}^{-1} - \mathbf{Y}_{+}\mathbf{D}^{-1}\mathbf{C}; \tag{31}$$

$$\mathbf{r}^{-} = \mathbf{r}^{+} = \mathbf{r} = \quad \mathbf{Y}_{+}\mathbf{D}^{-1} - \mathbf{Y}_{-}\mathbf{\Lambda}\mathbf{D}^{-1}\mathbf{C}; \tag{32}$$

$$\mathbf{s}^{+} = \quad \mathbf{F}^{+} - \mathbf{t}\mathbf{F}^{+}Q - \mathbf{r}\mathbf{F}^{-}. \tag{33}$$

$$\mathbf{s}^{-} = \quad \mathbf{F}^{-}Q - \mathbf{t}\mathbf{F}^{-} - \mathbf{r}\mathbf{F}^{+}Q; \tag{34}$$

It can be shown that the expressions for $\mathbf{r}$ and $\mathbf{t}$ can be re-cast in the forms:

$$\mathbf{t} = \quad \mathbf{a}\mathbf{D}^{-1}; \tag{35}$$

$$\mathbf{r} = \quad \mathbf{b}\mathbf{D}^{-1}; \tag{36}$$

where

$$\mathbf{a} \equiv \quad (\mathbf{Y}_{-} - \mathbf{Y}_{+}\mathbf{Y}_{-}^{-1}\mathbf{Y}_{+})\mathbf{\Lambda}; \tag{37}$$

$$\mathbf{b} \equiv \quad \mathbf{Y}_{-}\mathbf{\Lambda}\mathbf{c} - \mathbf{Y}_{+}; \tag{38}$$

$$\mathbf{c} \equiv \quad \mathbf{Y}_{-}^{-1}\mathbf{Y}_{+}\mathbf{\Lambda};. \tag{39}$$

and $\mathbf{D}$ is given in Eq. (27). This form is used in Radiant to improve numerical efficiency by requiring fewer matrix manipulations.

4.2. *Linearizing the* $\mathbf{r}$ *and* $\mathbf{t}$ *matrices*

For a given layer, r and t matrix derivatives will depend only on quantities varying in that layer, so we continue to suppress layer index n in this subsection. The following quantities have already been established from the linearization of the homogeneous solutions: $\mathbf{Z}_{\pm} = \mathcal{L}_n[\mathbf{Y}_{\pm}]$ and $\mathbf{H} = \mathcal{L}_n[\mathbf{\Lambda}]$. We proceed to apply chain-rule differentiation to establish the linearizations $\mathbf{u} \equiv \mathcal{L}[\mathbf{r}]$ and $\mathbf{v} \equiv \mathcal{L}[\mathbf{t}]$. We first linearize the auxiliary matrices $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ and $\mathbf{D}$ defined in the previous subsection, along with two additional matrices $\mathbf{e}$ and $\mathbf{f}$ defined as $\mathbf{e} = \mathbf{E} - \mathbf{c}^2$ (where $\mathbf{E}$ is the identity matrix) and $\mathbf{f} = \mathbf{Y}_-^{-1}\mathbf{Y}_+$. Upon differentiating, we obtain

$$\mathcal{L}[\mathbf{a}] = (\mathbf{Z}_- - \mathbf{Z}_+\mathbf{f} - \mathbf{Y}_+\mathcal{L}[\mathbf{f}])\mathbf{\Lambda} + (\mathbf{Y}_- - \mathbf{Y}_+\mathbf{f})\mathbf{H}; \tag{40}$$

$$\mathcal{L}[\mathbf{b}] = \mathbf{Z}_-\mathbf{\Lambda}\mathbf{c} + \mathbf{Y}_-(\mathbf{H}\mathbf{c} + \mathbf{\Lambda}\mathcal{L}[\mathbf{c}]) - \mathbf{Z}_+; \tag{41}$$

$$\mathcal{L}[\mathbf{c}] = \mathbf{Y}_-^{-1}\left\{\mathbf{Z}_+\mathbf{\Lambda} + \mathbf{Y}_+\mathbf{H} - \mathbf{Z}_-\mathbf{c}\right\}; \tag{42}$$

$$\mathcal{L}[\mathbf{D}] = \mathbf{Z}_-\mathbf{e} + \mathbf{Y}_-\mathcal{L}[\mathbf{e}]; \tag{43}$$

$$\mathcal{L}[\mathbf{e}] = -\mathcal{L}[\mathbf{c}]\mathbf{c} - \mathbf{c}\mathcal{L}[\mathbf{c}]; \tag{44}$$

$$\mathcal{L}[\mathbf{f}] = \mathbf{Y}_-^{-1}(-\mathbf{Z}_-\mathbf{f} + \mathbf{Z}_+). \tag{45}$$

Finally, we return to the matrix definitions of $\mathbf{t}$ and $\mathbf{r}$ in Eqs. (35) and (36). Upon differentiating and using the definitions of $\mathbf{t}$, $\mathbf{r}$, $\mathbf{D}$, $\mathcal{L}[\mathbf{a}]$, $\mathcal{L}[\mathbf{b}]$, and $\mathcal{L}[\mathbf{D}]$, the complete linearization of the transmission and reflection matrices can be expressed as

$$\mathbf{v} = \left\{\mathcal{L}[\mathbf{a}] - \mathbf{t}\mathcal{L}[\mathbf{D}]\right\}\mathbf{D}^{-1}; \tag{46}$$

$$\mathbf{u} = \left\{\mathcal{L}[\mathbf{b}] - \mathbf{r}\mathcal{L}[\mathbf{D}]\right\}\mathbf{D}^{-1}. \tag{47}$$

It is worth noting again that these two linearizations are only defined for the layer in which a quantity is varying, that is, $\mathcal{L}_k[\mathbf{r}_n] = \mathcal{L}_k[\mathbf{t}_n] = 0$ for $k \neq n$.

4.3. *Linearizing the* $\mathbf{s}_n^\pm$ *vectors*

For the source terms due to solar forcing, we reintroduce the layer index n for which linearizations are required, and use layer index k for those layers which are responsible for the linearizations. From Section 3.3, we know that the scalar Q_n has linearizations from layers $k \leq n$, and the same applies to the source function vectors $\mathbf{F}_n^\pm$. We have already defined the linearizations $\mathbf{G}_{kn}^\pm = \mathcal{L}_k[\mathbf{F}_n^\pm]$ (vectors) and $\Theta_{kn} = \mathcal{L}_k[Q_n]$ (scalars). Continuing, we also know $\mathbf{u}_n$ and $\mathbf{v}_n$ from the preceding analysis. We can now apply straightforward chain rule differentiation to the definitions for $\mathbf{s}_n^\pm$ in Eqs. (33) and (34). The results for $\mathbf{w}_{kn}^\pm \equiv \mathcal{L}_k[\mathbf{s}_n^\pm]$ are:

$$\mathbf{w}_{kn}^+ = \mathbf{G}_{kn}^+ - \mathbf{t}_n \left\{ \mathbf{G}_{kn}^+ Q_n + \mathbf{F}_n^+ \Theta_{kn} \right\} - \delta_{kn} \mathbf{v}_n \mathbf{F}_n^+ Q_n - \mathbf{r}_n \mathbf{G}_{kn}^- - \delta_{kn} \mathbf{u}_n \mathbf{F}_n^-, \tag{48}$$

$$\mathbf{w}_{kn}^- = \mathbf{G}_{kn}^- Q_n - \mathbf{F}_n^- \Theta_{kn} - \mathbf{r}_n \left\{ \mathbf{G}_{kn}^+ Q_n + \mathbf{F}_n^+ \Theta_{kn} \right\} - \delta_{kn} \mathbf{u}_n \mathbf{F}_n^+ Q_n - \mathbf{t}_n \mathbf{G}_{kn}^- - \delta_{kn} \mathbf{v}_n \mathbf{F}_n^-. \tag{49}$$

This completes the linearization of transmission and reflection matrices and source vectors.

5. The Interaction Principle

Now we turn to the stacking of layers (known variously as the adding method, the interaction principle or matrix operator theory). Although the adding method is hardly new, we will take some care over the mathematical exposition, as this will be important for the linearization that follows in section 6. Symbols $\mathbf{r}_n$ and $\mathbf{t}_n$ indicate *layer* reflection and transmittance matrices, and $\mathbf{s}_n^{\pm}$ *layer* source function vectors. We use symbols $\mathbf{R}_n^{\pm}$ and $\mathbf{T}_n^{\pm}$ for the reflection and transmittance matrices appropriate to a *stack* of n layers, and $\mathbf{S}_n^{\pm}$ for the corresponding stack source function vectors. Given such a stack of size $n-1$ for which $\mathbf{R}_{n-1}^{\pm}$, $\mathbf{T}_{n-1}^{\pm}$ and $\mathbf{S}_{n-1}^{\pm}$ have already been established, we then wish to add the next layer n to the stack. New stack variables $\mathbf{R}_n^{\pm}$, $\mathbf{T}_n^{\pm}$ and $\mathbf{S}_n^{\pm}$ are based on the existing stack and on the addition of layer quantities $\mathbf{r}_n$, $\mathbf{t}_n$ and $\mathbf{s}_n^{\pm}$. The interaction principle accomplishes this task.

5.1. Adding Layers

We write $\mathbf{I}_n^{\uparrow}$ and $\mathbf{I}_n^{\downarrow}$ for the upwelling and downwelling radiance fields at the lower boundary of layer n ($\mathbf{I}_0$ is the TOA field). For the existing stack of $n-1$ layers:

$$\mathbf{I}_{n-1}^{\downarrow} = \quad \mathbf{T}_{n-1}^{-}\mathbf{I}_0^{\downarrow} + \mathbf{R}_{n-1}^{+}\mathbf{I}_{n-1}^{\uparrow} + \mathbf{S}_{n-1}^{-}; \tag{50}$$

$$\mathbf{I}_0^{\uparrow} = \quad \mathbf{T}_{n-1}^{+}\mathbf{I}_{n-1}^{\uparrow} + \mathbf{R}_{n-1}^{-}\mathbf{I}_0^{\downarrow} + \mathbf{S}_{n-1}^{+}, \tag{51}$$

while for the new layer n, we have:

$$\mathbf{I}_n^{\downarrow} = \mathbf{t}_n\mathbf{I}_{n-1}^{\downarrow} + \mathbf{r}_n\mathbf{I}_n^{\uparrow} + \mathbf{s}_n^{-}; \tag{52}$$

$$\mathbf{I}_{n-1}^{\uparrow} = \mathbf{t}_n\mathbf{I}_n^{\uparrow} + \mathbf{r}_n\mathbf{I}_{n-1}^{\downarrow} + \mathbf{s}_n^{+}, \tag{53}$$

For a stack of n layers obtained by combining these sets of equations, we define new stack variables through:

$$\mathbf{I}_n^{\downarrow} = \mathbf{T}_n^{-}\mathbf{I}_0^{\downarrow} + \mathbf{R}_n^{+}\mathbf{I}_n^{\uparrow} + \mathbf{S}_n^{-}; \tag{54}$$

$$\mathbf{I}_0^{\uparrow} = \mathbf{T}_n^{+}\mathbf{I}_n^{\uparrow} + \mathbf{R}_n^{-}\mathbf{I}_0^{\downarrow} + \mathbf{S}_n^{+}. \tag{55}$$

To establish the new stack variables, Eq. (53) is first inserted into Eq. (50), to eliminate $\mathbf{I}_{n-1}^{\uparrow}$ and thus obtain the following equation for $\mathbf{I}_{n-1}^{\downarrow}$:

$$\mathbf{I}_{n-1}^{\downarrow} = \mathbf{P}_n^{-}\left\{\mathbf{T}_{n-1}^{-}\mathbf{I}_0^{\downarrow} + \mathbf{R}_{n-1}^{+}\mathbf{t}_n\mathbf{I}_n^{\uparrow} + \mathbf{R}_{n-1}^{+}\mathbf{s}_n^{+} + \mathbf{S}_{n-1}^{-}\right\}. \tag{56}$$

We have defined the auxiliary matrix:

$$\mathbf{P}_n^{-} = \left(\mathbf{E} - \mathbf{R}_{n-1}^{+}\mathbf{r}_n\right)^{-1}, \tag{57}$$

where $\mathbf{E}$ is again the identity matrix. For the downward adding, the auxiliary equation Eq. (56) is inserted into Eq. (52) to express $\mathbf{I}_n^{\downarrow}$ in terms of $\mathbf{I}_0^{\downarrow}$ and $\mathbf{I}_n^{\uparrow}$. Similarly for the upward adding, auxiliary equation Eq. (56) is inserted into Eq. (53). Comparing the results with the definitions in Eqs. (54) and (55), we find:

$$\mathbf{T}_n^{-} = \mathbf{t}_n\mathbf{P}_n^{-}\mathbf{T}_{n-1}^{-}; \tag{58}$$

$$\mathbf{R}_n^{-} = \mathbf{R}_{n-1}^{-} + \mathbf{T}_{n-1}^{+}\mathbf{P}_n^{+}\mathbf{r}_n\mathbf{T}_{n-1}^{-}; \tag{59}$$

$$\mathbf{S}_n^{-} = \mathbf{s}_n^{-} + \mathbf{t}_n\mathbf{P}_n^{-}(\mathbf{R}_{n-1}^{+}\mathbf{s}_n^{+} + \mathbf{S}_{n-1}^{-}). \tag{60}$$

for the downwelling interaction and

$$\mathbf{T}_n^+ = \mathbf{T}_{n-1}^+\mathbf{P}_n^+\mathbf{t}_n; \tag{61}$$

$$\mathbf{R}_n^+ = \mathbf{r}_n + \mathbf{t}_n\mathbf{P}_n^-\mathbf{R}_{n-1}^+\mathbf{t}_n; \tag{62}$$

$$\mathbf{S}_n^+ = \mathbf{S}_{n-1}^+ + \mathbf{T}_{n-1}^+\mathbf{P}_n^+(\mathbf{r}_n\mathbf{S}_{n-1}^- + \mathbf{s}_n^+), \tag{63}$$

for the upwelling interaction. Here, we have defined another auxiliary matrix:

$$\mathbf{P}_n^+ = (\mathbf{E} - \mathbf{r}_n\mathbf{R}_{n-1}^+)^{-1}. \tag{64}$$

The interaction principle is expressed through these two sets Eqs. (58)-(60) and (61)-(63). There is no stack above the first layer; therefore, for $n = 1$ we have:

$$\mathbf{T}_1^\pm = \mathbf{t}_1; \quad \mathbf{R}_1^\pm = \mathbf{r}_1; \quad \mathbf{S}_1^\pm = \mathbf{s}_1^\pm. \tag{65}$$

The adding process is depicted in Figure (1).

INSERT FIGURE 1 here.

5.2. TOA and BOA output

If the atmosphere has a total of N_a layers, the adding operation is repeated until reflection and transmission matrices and source vectors are obtained for the whole atmosphere, and the TOA upwelling field and the BOA downwelling field are given through:

$$\mathbf{I}_{N_a}^\downarrow = \mathbf{T}_{N_a}^-\mathbf{I}_0^\downarrow + \mathbf{R}_{N_a}^+\mathbf{I}_{N_a}^\uparrow + \mathbf{S}_{N_a}^-; \tag{66}$$

$$\mathbf{I}_0^\uparrow = \mathbf{T}_{N_a}^+\mathbf{I}_{N_a}^\uparrow + \mathbf{R}_{N_a}^-\mathbf{I}_0^\downarrow + \mathbf{S}_{N_a}^+. \tag{67}$$

Suitable boundary conditions are then applied to set the TOA and BOA fields. At the surface, we have a reflectance condition:

$$\mathbf{I}^{\uparrow}_{N_a} = \mathbf{R}_G \mathbf{I}^{\downarrow}_{N_a} + \mathbf{I}^{\uparrow}_{D}, \tag{68}$$

where $\mathbf{R}_G$ is a surface reflectance matrix and $\mathbf{I}^{\uparrow}_{D}$ is the reflected direct-beam field at BOA. For a Lambertian surface, the matrix $\mathbf{R}_G$ has elements $(R_G)_{ij} = 2\rho\delta_{0m}\mu_j a_j$ for Lambertian albedo ρ and discrete ordinate streams and weights μ_j and a_j respectively. Assuming a TOA boundary condition $\mathbf{I}^{\downarrow}_{0} = 0$ (no downwelling diffuse radiance at the top of the atmosphere), Eq. (68) is then substituted in Eq. (66), to obtain the following for the BOA downwelling field:

$$\mathbf{I}^{\downarrow}_{N_a} = \left(\mathbf{E} - \mathbf{R}^{+}_{N_a}\mathbf{R}_G\right)^{-1}\left\{\mathbf{S}^{-}_{N_a} + \mathbf{R}^{+}_{N_a}\mathbf{I}^{\uparrow}_{D}\right\}. \tag{69}$$

This is then substituted in Eq. (68) which is in turn substituted into Eq. (67) to obtain the TOA upwelling field.

6. Linearization of the adding method

6.1. Linearization setup and rules

We wish now to linearize the complete set of stack equations from section 5. Layer index k indicates the *active layer* containing one or more atmospheric variables for which we desire to define weighting functions, and layer index n is used for the addition of *stacking layers* in the interaction principle. In section 4, we wrote down matrix expressions for layer quantities $\mathbf{r}_k$, $\mathbf{t}_k$ and $\mathbf{s}_k^{\pm}$ in terms of the RTE solutions. We also derived their derivatives $\mathbf{u}_k \equiv \mathcal{L}_k[\mathbf{r}_k]$, $\mathbf{v}_k \equiv \mathcal{L}_k[\mathbf{t}_k]$ and $\mathbf{w}_{kn}^{\pm} \equiv \mathcal{L}_k[\mathbf{s}_n^{\pm}] \;\forall\; n \geq k$.

We use the following symbols to denote stack linearization: $\mathbf{U}_{kn}^{\pm} \equiv \mathcal{L}_k[\mathbf{R}_n^{\pm}]$; $\mathbf{V}_{kn}^{\pm} \equiv \mathcal{L}_k[\mathbf{T}_n^{\pm}]$ and $\mathbf{W}_{kn}^{\pm} \equiv \mathcal{L}_k[\mathbf{S}_n^{\pm}]$. All stacks above k will be unchanged by any variation in layer k. Thus:

$$\mathbf{U}_{kn}^{\pm} = 0, \quad \mathbf{V}_{kn}^{\pm} = 0 \quad \text{and} \quad \mathbf{W}_{kn}^{\pm} = 0 \;\forall\, n \leq k. \tag{70}$$

Once we reach the active layer, we will pick up linearization. There are two situations to consider.

1. When the stack addition reaches active layer k, that is $k = n$, we will pick up variations $\mathbf{u}_k$, $\mathbf{v}_k$ and $\mathbf{w}_{kk}^{\pm}$ from linearizations of the layer reflection and transmission matrices and source function vectors. The linearized stack is now active, and $\mathbf{U}_{kn}^{\pm}$, $\mathbf{V}_{kn}^{\pm}$ and $\mathbf{W}_{kn}^{\pm}$ are now defined for the first time. [The special case $k = n = 1$ is considered below].

2. For layer additions below k, that is $n > k$, the linearizations picked up in the previous step

will propagate downwards to the bottom of the atmosphere, but there will be additional variations $\mathbf{w}_{kn}^{\pm}$ in the solar source terms to be included in the stacking.

To perform the linearized adding, we could proceed by adding layers one-by-one as with the normal adding process (Figure 1). However, we may achieve increased numerical efficiency by re-using various layer-associated matrices and vectors that were obtained during the computation of the basic state radiances. In addition, one may also re-use blocks consisting of *stacks* of atmospheric layers. This idea is referred to as *layer-saving* and is depicted in Figure 2, in which the third layer is active (that is, weighting function variables belong to this layer). From the figure, we observe there are two fundamental operations to perform: (1) adding an individual linearized lower layer to an unlinearized upper stack consisting of one or more layers; and (2) adding a lower stack consisting of one of more layers to the already linearized upper stack to obtain the linearized stack for the entire model atmosphere. Aside from the initial computations of necessary matrix and vector products, these two operations encompass the essence of linearized adding using the layer-saving mode.

To aid the discussion of these operations, we employ double subscripts on $\mathbf{T}^{\pm}$, $\mathbf{R}^{\pm}$, and $\mathbf{S}^{\pm}$ in order to distinguish between matrices associated with different stacks of layers. For example, $\mathbf{T}_{1,k-1}^{+}$ is the upwelling transmission matrix associated with the stack of layers 1 to $k-1$, whereas $\mathbf{T}_{k+1,n}^{+}$ is the same matrix associated with the stack of layers $k+1$ to n.

INSERT FIGURE 2 here.

6.2. Operation 1: adding a linearized lower layer to an unlinearized upper stack

In this case, we have $n = k$; therefore, linearizations $\mathbf{u}_k$, $\mathbf{v}_k$ and $\mathbf{w}^{\pm}_{kk}$ will apply for the linearized layer. In what follows next, we use the following auxiliary matrices

$$\mathbf{P}^{+}_{kk} = (\mathbf{E} - \mathbf{r}_k\mathbf{R}^{+}_{1,k-1})^{-1}, \qquad \mathbf{P}^{-}_{kk} = (\mathbf{E} - \mathbf{R}^{+}_{1,k-1}\mathbf{r}_k)^{-1}; \tag{71}$$

$$\mathcal{A}^{+}_{kk} = \mathbf{T}^{+}_{1,k-1}\mathbf{P}^{+}_{kk}, \qquad \mathcal{A}^{-}_{kk} = \mathbf{t}_k\mathbf{P}^{-}_{kk}; \tag{72}$$

$$\mathcal{B}^{+}_{kk} = \mathbf{u}_k\mathbf{R}^{+}_{1,k-1}, \qquad \mathcal{B}^{-}_{kk} = \mathbf{R}^{+}_{1,k-1}\mathbf{u}_k; \tag{73}$$

$$\mathcal{C}^{+}_{kk} = \mathbf{P}^{+}_{kk}\mathbf{t}_k, \qquad \mathcal{C}^{-}_{kk} = \mathbf{P}^{-}_{kk}\mathbf{T}^{-}_{1,k-1}; \tag{74}$$

$$\mathcal{D}^{+}_{kk} = \mathbf{P}^{-}_{kk}\mathbf{R}^{+}_{1,k-1}\mathbf{t}_k, \qquad \mathcal{D}^{-}_{kk} = \mathbf{P}^{+}_{kk}\mathbf{r}_k\mathbf{T}^{-}_{1,k-1}; \tag{75}$$

$$\mathcal{E}^{+}_{kk} = \mathbf{P}^{+}_{kk}(\mathbf{r}_k\mathbf{S}^{-}_{1,k-1} + \mathbf{s}^{+}_{k}), \qquad \mathcal{E}^{-}_{kk} = \mathbf{P}^{-}_{kk}(\mathbf{R}^{+}_{1,k-1}\mathbf{s}^{+}_{k} + \mathbf{S}^{-}_{1,k-1}). \tag{76}$$

These matrices (with the exception of $\mathcal{B}^{\pm}_{kk}$) represent matrix products that are constructed during the computation of radiances for the base atmospheric state; they are saved and re-used here in the linearized adding process. We may now apply chain-rule linearization to Eqs. (58)-(60) to obtain the downward set of linearized transmission and reflection matrices and accompanying source vector. Doing this, we get:

$$\mathbf{V}^{-}_{kk} = (\mathbf{v}_k + \mathcal{A}^{-}_{kk}\mathcal{B}^{-}_{kk})\mathcal{C}^{-}_{kk}; \tag{77}$$

$$\mathbf{U}^{-}_{kk} = \mathcal{A}^{+}_{kk}(\mathcal{B}^{+}_{kk}\mathcal{D}^{-}_{kk} + \mathbf{u}_k\mathbf{T}^{-}_{1,k-1}); \tag{78}$$

$$\mathbf{W}^{-}_{kk} = \mathbf{v}_k\mathcal{E}^{-}_{kk} + \mathcal{A}^{-}_{kk}(\mathcal{B}^{-}_{kk}\mathcal{E}^{-}_{kk} + \mathbf{R}^{+}_{1,k-1}\mathbf{w}^{+}_{kk}) + \mathbf{w}^{-}_{kk}, \tag{79}$$

for the downward stack linearizations.

Similarly, applying the chain rule to Eqs. (61)-(63) for the upward set, we get:

$$\mathbf{V}^{+}_{kk} = \mathcal{A}^{+}_{kk}(\mathcal{B}^{+}_{kk}\mathcal{C}^{+}_{kk} + \mathbf{v}_k); \tag{80}$$

$$\mathbf{U}^{+}_{kk} = \mathbf{v}_k\mathcal{D}^{+}_{kk} + \mathcal{A}^{-}_{kk}(\mathcal{B}^{-}_{kk}\mathcal{D}^{+}_{kk} + \mathbf{R}^{+}_{1,k-1}\mathbf{v}_k) + \mathbf{u}_k; \tag{81}$$

$$\mathbf{W}^{+}_{kk} = \mathcal{A}^{+}_{kk}(\mathcal{B}^{+}_{kk}\mathcal{E}^{+}_{kk} + \mathbf{u}_k\mathbf{S}^{-}_{1,k-1}) + \mathbf{w}^{+}_{kk}, \tag{82}$$

for the upward stack linearizations. The case $k = n = 1$ is special. There is no stack, and we just initialize the linearizations with:

$$\mathbf{V}^{\pm}_{11} = \mathbf{v}_1, \quad \mathbf{U}^{\pm}_{11} = \mathbf{u}_1, \ \text{ and } \ \mathbf{W}^{\pm}_{11} = \mathbf{w}^{\pm}_{11}. \tag{83}$$

6.3. *Operation 2: adding a lower stack to a linearized upper stack*

In this case, we have already picked up the stack linearization as far as layer k, as expressed through Eqs. (77)-(79) and (80)-(82). For the remaining lower stack consisting of layers $n > k$ to N_a, there is no variation of the layer reflectance and transmittance matrices $\mathbf{r}_n$ and $\mathbf{t}_n$; however, there are solar source function variations $\mathbf{w}^{\pm}_{kn} = \mathcal{L}_k[\mathbf{s}^{\pm}_n]$ which must be taken into account. As noted above, these arise because variations in layer k will propagate downwards to layers $n > k$ because of solar beam attenuation. As in the previous case, we define a set of auxiliary matrices:

$$\mathbf{P}^{+}_{kn} = (\mathbf{E} - \mathbf{R}^{-}_{k+1,n}\mathbf{R}^{+}_{1,k})^{-1}, \qquad \mathbf{P}^{-}_{kn} = (\mathbf{E} - \mathbf{R}^{+}_{1,k}\mathbf{R}^{-}_{k+1,n})^{-1}; \tag{84}$$

$$\mathcal{A}^{+}_{kn} = \mathbf{T}^{+}_{1,k}\mathbf{P}^{+}_{kn} \qquad \mathcal{A}^{-}_{kn} = \mathbf{T}^{-}_{k+1,n}\mathbf{P}^{-}_{kn}; \tag{85}$$

$$\mathcal{B}^{+}_{kn} = \mathbf{U}^{+}_{kn}\mathbf{R}^{-}_{k+1,n}, \qquad \mathcal{B}^{-}_{kn} = \mathbf{R}^{-}_{k+1,n}\mathbf{U}^{+}_{kn}; \tag{86}$$

$$\mathcal{C}^{+}_{kn} = \mathbf{P}^{+}_{kn}\mathbf{T}^{+}_{k+1,n}, \qquad \mathcal{C}^{-}_{kn} = \mathbf{P}^{-}_{kn}\mathbf{T}^{-}_{1,k}; \tag{87}$$

$$\mathcal{D}^{+}_{kn} = \mathbf{P}^{-}_{kn}\mathbf{R}^{+}_{1,k}\mathbf{T}^{+}_{k+1,n}, \qquad \mathcal{D}^{-}_{kn} = \mathbf{P}^{+}_{kn}\mathbf{R}^{-}_{k+1,n}\mathbf{T}^{-}_{1,k}; \tag{88}$$

$$\mathcal{E}^{+}_{kn} = \mathbf{P}^{+}_{kn}(\mathbf{R}^{-}_{k+1,n}\mathbf{S}^{-}_{1,k} + \mathbf{S}^{+}_{k+1,n}), \qquad \mathcal{E}^{-}_{kn} = \mathbf{P}^{-}_{kn}(\mathbf{R}^{+}_{1,k}\mathbf{S}^{+}_{k+1,n} + \mathbf{S}^{-}_{1,k}). \tag{89}$$

where the subscript n in $\mathbf{P}^{\pm}_{kn}$, $\mathcal{A}^{\pm}_{kn}$, $\mathcal{B}^{\pm}_{kn}$, $\mathcal{C}^{\pm}_{kn}$, $\mathcal{D}^{\pm}_{kn}$ and $\mathcal{E}^{\pm}_{kn}$ denotes that these quantities are associated with the stack of layers from $k+1$ to $n = N_a$. Once again, we apply chain-rule differentiation to the stacking equations and find

$$\mathbf{V}^{-}_{kn} = \mathcal{A}^{-}_{kn}(\mathcal{B}^{+}_{kn}\mathcal{C}^{-}_{kn} + \mathbf{V}^{-}_{kk}); \tag{90}$$

$$\mathbf{U}^{-}_{kn} = \mathbf{V}^{+}_{kk}\mathcal{D}^{-}_{kn} + \mathcal{A}^{+}_{kn}(\mathcal{B}^{-}_{kn}\mathcal{D}^{-}_{kn} + \mathbf{R}^{-}_{k+1,n}\mathbf{V}^{-}_{kk}); \tag{91}$$

$$\mathbf{W}^{-}_{kn} = \mathcal{A}^{-}_{kn}(\mathcal{B}^{+}_{kn}\mathcal{E}^{-}_{kn} + \mathbf{U}^{+}_{kk}\mathbf{S}^{+}_{k+1,n} + \mathbf{R}^{+}_{1,k}\mathcal{W}^{+}_{kn} + \mathbf{W}^{-}_{kk}) + \mathcal{W}^{-}_{kn}, \tag{92}$$

for the downward stack linearizations and

$$\mathbf{V}^{+}_{kn} = (\mathbf{V}^{+}_{kk} + \mathcal{A}^{+}_{kn}\mathcal{B}^{-}_{kn})\mathcal{C}^{+}_{kn}; \tag{93}$$

$$\mathbf{U}^{+}_{kn} = \mathcal{A}^{-}_{kn}(\mathcal{B}^{+}_{kn}\mathcal{D}^{+}_{kn} + \mathbf{U}^{+}_{kk}\mathbf{T}^{+}_{k+1,n}); \tag{94}$$

$$\mathbf{W}^{+}_{kn} = \mathbf{V}^{+}_{kk}\mathcal{E}^{+}_{kn} + \mathcal{A}^{+}_{kn}(\mathcal{B}^{-}_{kn}\mathcal{E}^{+}_{kn} + \mathbf{R}^{-}_{k+1,n}\mathbf{W}^{-}_{kk} + \mathcal{W}^{+}_{kn}) + \mathbf{W}^{+}_{kk}, \tag{95}$$

for the upward stack linearizations.

In these results, everything has been defined with the exception of source vectors $\mathcal{W}^-_{kn}$ and $\mathcal{W}^+_{kn}$ required in Eqs. (92) and (95). These are constructed from the bottom of the atmosphere upwards using the auxiliary matrices

$$\mathbf{P}^+_{in} = (\mathbf{E} - \mathbf{R}^-_{i+1,n}\mathbf{r}_i)^{-1}; \tag{96}$$

$$\mathbf{P}^-_{in} = (\mathbf{E} - \mathbf{r}_i\mathbf{R}^-_{i+1,n})^{-1}; \tag{97}$$

$$\mathcal{F}^+_{in} = \mathbf{t}_i\mathbf{P}^+_{in}; \tag{98}$$

$$\mathcal{F}^-_{in} = \mathbf{T}^-_{i+1,n}\mathbf{P}^-_{in}, \tag{99}$$

and the equations

$$\mathcal{W}^+_{k(i,n)} = \mathcal{F}^+_{in}(\mathbf{R}^-_{i+1,n}\mathbf{w}^-_{ki} + \mathcal{W}^+_{k(i+1,n)}) + \mathbf{w}^+_{ki}; \tag{100}$$

$$\mathcal{W}^-_{k(i,n)} = \mathcal{F}^-_{in}(\mathbf{r}_i\mathcal{W}^+_{k(i+1,n)} + \mathbf{w}^-_{ki}) + \mathcal{W}^-_{k(i+1,n)}, \tag{101}$$

where i varies from $n = N_a$ to $k+1$. Here, $\mathcal{W}^\pm_{k(i,n)} = \mathbf{w}^\pm_{ki}$ when $i = n$ initially and $\mathcal{W}^\pm_{k(k+1,n)} = \mathcal{W}^\pm_{kn}$ when $i = k+1$ is obtained.

6.4. TOA and BOA weighting functions

The stack linearization is completed when $n = N_a$ in Eqs. (90)-(92) and (93)-(95). The end result is a set of linearized reflection and transmission matrices and source vectors for the whole model atmosphere. We can then apply these results to the boundary conditions and get the desired linearizations of the TOA upwelling field and BOA downwelling field: in other words, the weighting functions.

Referring now to the downwelling field in Eq. (69), the linearization of the auxiliary matrix $\mathbf{B} = (\mathbf{E} - \mathbf{R}^{+}_{N_a}\mathbf{R}_G)^{-1}$ is given by

$$\mathcal{L}_k[\mathbf{B}] = \mathbf{B}\mathbf{U}^{+}_{k,N_a}\mathbf{R}_G\mathbf{B}. \tag{102}$$

It is then straightforward to apply chain-rule linearizations to the expressions for the BOA-downwelling and TOA-upwelling radiances and find:

$$\mathbf{K}^{\downarrow}_{k,N_a} = \mathbf{B}(\mathbf{U}^{+}_{k,N_a}\mathbf{R}_G\mathbf{I}^{\downarrow}_{N_a} + \mathbf{W}^{-}_{k,N_a}); \tag{103}$$

$$\mathbf{K}^{\uparrow}_{k,0} = \mathbf{V}^{+}_{k,N_a}\mathbf{R}_G\mathbf{I}^{\downarrow}_{N_a} + \mathbf{T}^{+}_{N_a}\mathbf{R}_G\mathbf{K}^{\downarrow}_{k,N_a} + \mathbf{W}^{+}_{k,N_a}. \tag{104}$$

where the direct field linearization has been omitted from these results.

6.5. *Albedo weighting functions*

We add here a note on the determination of weighting functions with respect to a surface variable. In this case, the only variation is with the albedo matrix $\mathbf{R}_G$, that is we assume a linearization $\mathcal{L}_h[\mathbf{R}_G]$ with respect to some surface property h (e.g. Lambertian albedo). Referring again to Eq. (69), the linearization of $\mathbf{B} = (\mathbf{E} - \mathbf{R}^{+}_{N_a}\mathbf{R}_G)^{-1}$ is now:

$$\mathcal{L}_h[\mathbf{B}] = \mathbf{B}\mathbf{R}^{+}_{N_a}\mathcal{L}_h[\mathbf{R}_G]\mathbf{B}. \tag{105}$$

There is no linearization of the atmospheric stack in this case. Applying chain-rule differentiation to the BOA-downwelling and TOA-upwelling radiances, we find:

$$\mathbf{K}^{\downarrow}_{N_a} = \mathcal{L}_h[\mathbf{B}](\mathbf{S}^{-}_{N_a} + \mathbf{R}^{+}_{N_a}\mathbf{I}^{\uparrow}_{D}) + \mathbf{B}\mathbf{R}^{+}_{N_a}\mathcal{L}_h[\mathbf{I}^{\uparrow}_{D}]; \tag{106}$$

$$\mathbf{K}^{\uparrow}_{N_a} = \mathcal{L}_h[\mathbf{R}_G]\mathbf{I}^{\downarrow}_{N_a} + \mathbf{R}_G\mathbf{K}^{\downarrow}_{N_a} + \mathcal{L}_h[\mathbf{I}^{\uparrow}_{D}]; \tag{107}$$

$$\mathbf{K}^{\uparrow}_{0} = \mathbf{T}^{+}_{N_a}\mathbf{K}^{\uparrow}_{N_a}. \tag{108}$$

This completes the derivation. Radiant has a full BRDF formulation of the surface and, in section 7, we summarize this implementation.

7. Other Radiant Issues

7.1. Additional Radiant implementations

The option of using delta-M scaling [29] is a standard feature of this and other models. This approximation is useful for sharply peaked phase functions and essentially replaces part of the phase function with a delta-function, the remaining part then showing a smoother scatter-angle dependence which can be readily treated with discrete ordinate methods. The delta-M scaling factor f for this partition arises from the constraint of phase function normalization. All optical properties are scaled by this application. For details of the standard scaling, see [5]; delta-M scaling of the linearized optical property inputs is treated in [7].

For dealing with non-Lambertian surfaces with a known BRDF specification, the formalism developed in [8] has been implemented in Radiant. BRDFs are represented as a linear sum of up to three BRDF *kernels*, where each kernel shape is taken from a semi-empirical formulation. In this sum, each kernel is multiplied by a linear coefficient, and each kernel may be dependent on a number of non-linear parameters which characterize the kernel shape function. The Lambertian kernel is isotropic. For sunglint off an ocean surface, the key BRDF kernel is the Cox-Munk Gaussian distribution of wave-facets characterized by the wind-speed. This BRDF formalism is completely differentiable with respect to both the linear kernel coefficients and the nonlinear kernel characterization factors such as the wind-speed in the Cox-Munk kernel. Some 8 kernels are listed in [8] and these have all been used in Radiant.

A separate module has been written for the *exact* single scatter solution to the RTE in the regular pseudo-spherical Radiant model; this module is fully linearized. This single scatter module is exact in the sense that all phase function information is used in the single scatter computations - the module is designed to replace the truncated form of the single scatter normally produced by Radiant. When delta-M scaling applies, only the optical thickness values are used in their delta-M scaled form. This single scatter improvement is known as the Nakajima-Tanaka (N-T) "TMS" correction [26] and it has been implemented in LIDORT (Versions 2.1 and higher) and DISORT (Version 2.0).

For wide-angle off-nadir views (sunglint mode in OCO), attenuation and single scattering along line-of-sight paths should also be treated for a curved atmosphere. This means that the N-T single scatter computation must allow for varying geometry along the viewing path. A treatment for this has been developed in the LIDORT model [25]. This will also be implemented in Radiant and is fully linearized.

7.2. Verification

We have verified Radiant by extensive comparisons against DISORT (plane-parallel) and LIDORT (pseudo-spherical case). All three models contain similar derivations of the discrete ordinate RTE solutions. The major difference is in the use of the adding method in Radiant to derive the radiance field; this replaces the linear algebra approach of the other models for the determination of integration constants. However, these approaches are alternative solutions to the boundary value problem, so one would expect comparisons to show high levels of agreement. This is indeed the case; radiance agreements between LIDORT and Radiant are better than 1 part in 10^6 (7SF) for all cases considered. Weighting functions were checked initially through the use of finite difference estimates. Further direct comparisons were made with LIDORT output, and again precision was very high - better than 1 part in 10^4 for all cases considered. All BRDF options implemented in Radiant have also been successfully tested both for the radiance and Jacobian fields.

8. Concluding Remarks

In this paper, we have derived a new linearization (analytic differentiation) of the interaction principle in multilayer radiative transfer theory. This linearization is part of the Radiant radiative transfer code, a composite discrete-ordinate adding model which has a major role in the forward part of the OCO Level 2 retrieval algorithm for the remote sensing of carbon dioxide. It is shown that the complete Radiant scattering code can be linearized, thereby providing analytic Jacobians (weighting functions) for any surface and/or atmospheric parameter that is part of the inverse problem. Radiant has additional capabilities to deal with large solar zenith angles (the pseudo-spherical approximation) and bidirectional reflectances at the surface.

With the addition of a treatment for the line-of-sight in a curved atmosphere, the Radiant development will be completed for OCO; the integration of Radiant with the binning treatment will be described in an accompanying paper [28]. OCO is actually a polarizing instrument, measuring the radiation field perpendicular to the scattering plane (that is, OCO measures $I_{\perp} = I - Q$, for Stokes vector $\mathbf{I} = [I, Q, U, V]$. It will therefore be necessary to apply a correction to the scalar field generated by Radiant. This will be done by means of a look-up table which will generate two quantities: the correction I_{vector}/I_{scalar} and the Q Stokes parameter. Aerosols (the main source of scattered light in the near infrared) are depolarizing in general so it is expected these corrections will be straightforward to classify (see for example [30]). In dealing with polarization, it is necessary to have a full vector RT model to deal with all orders of scattering, and for this, the OCO algorithm is currently using the pseudo-spherical VLIDORT polarization model (R. Spurr, private communication). In this regard, development of a vector version of Radiant has now begun.

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Figure Captions

1. **Figure 1**. Illustration of *Radiant's* normal mode of operation.

2. **Figure 2**. Illustration of *Radiant's* layer-saving mode of operation.

Figure 1

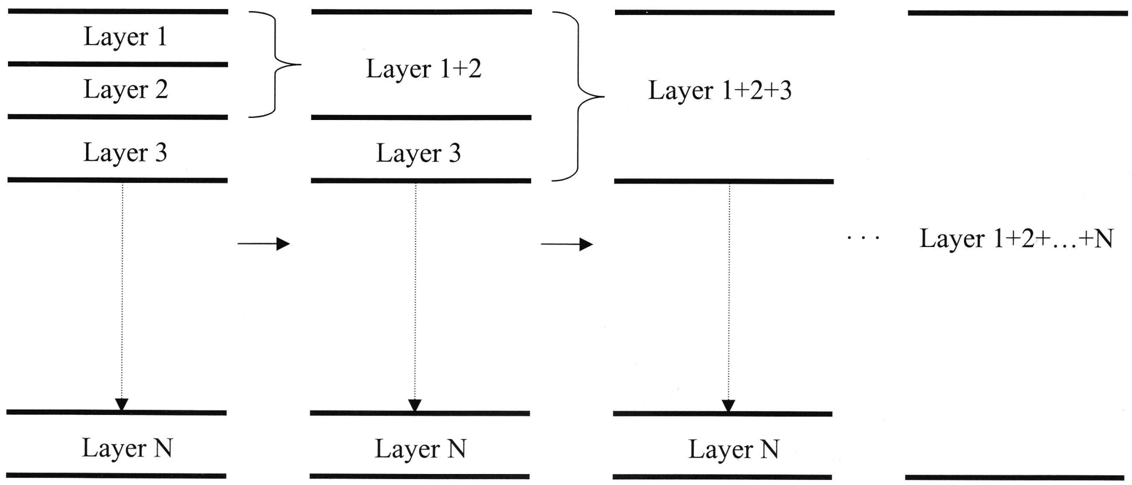

Figure 1: Illustration of *Radiant's* normal mode of operation.

Figure 2

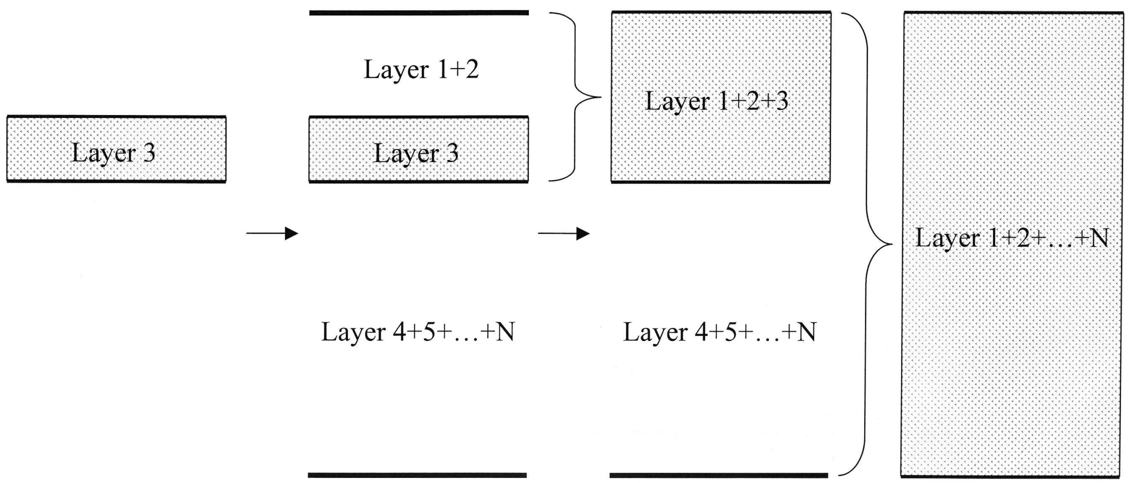

Figure 2: Illustration of *Radiant's* layer-saving mode of operation.