

Linear Form of the Radiative Transfer Equation Revisited

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Abstract

A linear form of the radiative transfer equation for the simultaneous retrieval of atmospheric temperature and absorbing gas profiles and surface temperature from radiance spectra was derived in the classic paper by Smith *et al.* (1991). The derivation started with the RTE difference between the true and initial radiance spectra. It is shown that there exists a dual representation of this RTE difference, and the resulting dual linear form of the RTE appears more general than the original linear form.

Introduction

The spectrum of radiance exiting the earth-atmosphere system, as described by the radiative transfer equation (RTE)¹, is a nonlinear functional of atmospheric temperature and absorbing gas profiles as well as surface temperature and emissivities. The physical retrieval of these meteorological variables from the RTE is a mathematically ill-posed problem². With the advance in infrared sensor technology from the multispectral sounders (*e.g.* HIRS³, GOES⁴, MODIS⁵) with tens of bands to the so-called hyperspectral sounders (*e.g.* HIS⁶, NAST-I⁷, AIRS⁸, IASI⁹, CrIS¹⁰, GIFTS¹¹) with thousands of channels, the physical retrieval has evolved from a mathematically underdetermined problem into an overdetermined one as respect to a typical fast RTM with hundreds of atmospheric variables. The advance in infrared sensor technology may also affect NWP data assimilation. For multispectral sounders, assimilation of tens of radiance values instead of hundreds of retrieved meteorological variables per field of view (FOV) in a global or regional 3D/4D-VAR assimilation system has not only shown improved assimilation accuracy but also reduce assimilation time. For hyperspectral sounders, assimilation of hundreds of retrieved meteorological variables instead of thousands of radiance values per FOV may be a foreseeable direction in the future to greatly reduce the assimilation problem size and thus assimilation time if the 3D/4D-VAR system would make the most of full hyperspectral spectra.

For physical retrieval or data assimilation formulated as an optimal variational problem involving radiance observations from a multispectral or hyperspectral sounder, an effective and efficient search direction toward the minimum of the associated cost function relies on the guidance of the so-called Jacobians, which are the Fréchet derivatives of radiances with respect to atmospheric and surface variables in a linear form of the RTE or RTM. Ideally an exact linear form with exact analytical Jacobians is the most desired for accurate and efficient physical retrieval and data assimilation. When such a linear form is not analytically derivable, the next desirable candidate is the tangent linear and adjoint models based on algorithmic differentiation (AD)¹², a technique that uses chain rules to numerically evaluate derivatives of composite functions specified by the computer program of the RTM. This process achieves the same numerical accuracy as the exact analytical Jacobians, but the latter is several times faster in computation. A last resort to compute the Jacobians is the approximation of the Fréchet derivatives by the “brute-force” finite differences for each variable at each pressure level, but this approach is much less accurate and too time-consuming for practical usage in physical retrieval and data assimilation.

Deriving a better linear form of the RTE with more accurate Jacobians for the simultaneous physical retrieval of atmospheric temperature and absorbing gas profiles and surface temperature from radiance spectra has been a continued endeavor since the early 70's¹³⁻¹⁵. In the classic paper by Smith *et al.* (1991)¹⁶, a new approximate linear form of the RTE was presented. This type of monochromatically-approximate linear form has been still used in the physical retrieval by some authors¹⁷⁻¹⁹, and the paper inspired Huang *et al.* (2002)²⁰ to accomplish the derivation of the exact linear form with correct analytical Jacobians for the widely-used McMillin-Fleming-Eyre-Woolf type fast radiative transfer models²¹⁻²⁴ in satellite remote sensing. Examples of this type of fast radiative transfer models are the RTTOV and RT-IASI models (e.g. Eyre²⁵, 1991, Saunders *et al.*²⁶, 1999; Matricardi *et al.*²⁷, 2001). Currently, the RTTOV and RT-IASI models carry the tangent linear and adjoint codes instead of the more computationally-efficient exact analytical Jacobian subroutine for the inverse problems. The quality of analytical Jacobians is crucial for physical retrieval and variational data assimilation in an efficient, reliable and accurate fashion. By numerically comparing the linear form with exact analytical Jacobians with the linear form with monochromatically- approximate analytical Jacobians for the 19 HIRS bands under the 0.1% perturbation of the 1976 U.S. Standard Atmosphere, Huang *et al.*²⁰ showed the latter is lack of accuracy (worse than the “brute-force” finite differences) and even yields the wrong signs for some HIRS bands, implying wrong search directions for finding the optimal inverse solution.

Nevertheless, the classical derivation of the linear form by Smith *et al.* (1991) represents a historic landmark on the simultaneous physical retrieval, signifying the last major endeavor for deriving approximate analytical Jacobians as well as a key inspiration for later successful derivation of exact analytical Jacobians. The derivation of the linear form by Smith *et al.* (1991) is of pedagogical interest. Without resorting to the concepts in calculus of variations, Smith *et al.* started with the finite difference between the RTEs for the true and initial radiance spectra to derive the linear form. In this paper we prove that there exists a *dual* representation of this RTE difference, and show some interesting outcomes from the resulting dual linear form.

The rest of the paper is organized as follows. The section below summarizes the derivation of the linear form by Smith *et al.* and the section following details the derivation of its dual linear form.

Linear Form by Smith *et al.* (1991)

The true spectrum of monochromatic radiance exiting the earth-atmosphere system¹ is

$$R_v = B_v(p_s) \tau_v(p_s) - \int_0^{p_s} B_v(p) d\tau_v(p), \quad (1)$$

where B_v is the Planck radiance with subscript v denoting spectral frequency, $\tau_v(p)$ the total transmittances of the atmosphere above atmospheric pressure level p . The subscript s denotes the earth's surface. The radiance spectrum corresponding to an assumed initial temperature and absorbing gas profiles is

$$R_v^0 = B_v^0(p_s) \tau_v^0(p_s) - \int_0^{p_s} B_v^0(p) d\tau_v^0(p), \quad (2)$$

where a superscript 0 denotes the initial quantity. With the following linear perturbation definitions:

$$\begin{aligned} \delta R_v &\equiv R_v - R_v^0, \\ \delta B_v(p) &\equiv B_v(p) - B_v^0(p), \\ \delta \tau_v(p) &\equiv \tau_v(p) - \tau_v^0(p), \end{aligned} \quad (3)$$

the difference between the true and initial radiance spectra is

$$\delta R_v = B_v(p_s) \delta \tau_v(p_s) + \delta B_v(p_s) \tau_v^0(p_s) - \int_0^{p_s} B_v(p) d[\delta \tau_v(p)] - \int_0^{p_s} \delta B_v(p) d\tau_v^0(p). \quad (4)$$

Performing integration by parts on the first integral term in Eq. (4), the equation becomes

$$\delta R_v = \delta B_v(p_s) \tau_v^0(p_s) - \int_0^{p_s} \delta B_v(p) d\tau_v^0(p) + \int_0^{p_s} \delta \tau_v(p) dB_v(p). \quad (5)$$

Using the linear approximations to the Planck radiance perturbations:

$$\delta B_v(p) = \frac{\partial B_v(T^0(p))}{\partial T(p)} \delta T(p) \equiv \beta_v^0(p) \delta T(p), \quad (6)$$

$$dB_v(p) = \beta_v^0(p) dT(p), \quad (7)$$

and the difference of *monochromatic* transmittances in terms of the difference of the absorbing gas profiles:

$$\delta \tau_v(p) = \tau_v^0(p) \sum_{i=1}^N \delta \ln \tau_{v_i}(p) \approx \tau_v^0(p) \sum_{i=1}^N \delta U_i(p) \frac{d \ln \tau_{v_i}^0(p)}{dU_i^0(p)}, \quad (8)$$

Eq. (5) becomes

$$\begin{aligned} \delta R_v &= \beta_v^0(p_s) \tau_v^0(p_s) \delta T_s - \int_0^{p_s} \beta_v^0(p) \delta T(p) \frac{d\tau_v^0(p)}{dp} dp \\ &\quad + \sum_{i=1}^N \int_0^{p_s} \delta U_i(p) \tau_v^0(p) \frac{d \ln \tau_{v_i}^0(p)}{dU_i^0(p)} \beta_v^0(p) \frac{dT(p)}{dp} dp. \end{aligned} \quad (9)$$

In Eq. (9), N is the number of absorbing gases, and $U_i(p)$ is the path length of the i -th absorbing gas, defined as

$$U_i(p) = \frac{1}{g} \int_0^p q_i(p') dp', \quad (10)$$

where g is the acceleration due to gravity, and q_i is the mixing ratio of the i -th absorbing gas. Note that Eq. (8) ignores the temperature dependence of transmittances. Eq. (9) shows that there is no information about the difference between the true and initial gas concentration profiles, $\delta U_i(p)$, in regions where the lapse rate $dT(p)/dp$ is zero. Using the following identities

$$d\tau_v^0(p) = d \left[\prod_{i=1}^N \tau_{v_i}^0(p) \right] = \tau_v^0(p) \sum_{i=1}^N d \ln \tau_{v_i}^0(p), \quad (11)$$

$$\frac{d \ln \tau_{v_i}^0(p)}{dU_i^0(p)} dT(p) = d \ln \tau_{v_i}^0(p) \frac{dT(p)}{dU_i^0(p)}, \quad (12)$$

Eq. (9) can be rewritten as

$$\begin{aligned} \delta R_v &\approx \beta_v^0(p_s) \tau_v^0(p_s) \delta T_s - \sum_{i=1}^N \int_0^{p_s} \beta_v^0(p) \delta T(p) \tau_v^0(p) d \ln \tau_{v_i}^0(p) \\ &\quad + \sum_{i=1}^N \int_0^{p_s} \delta U_i(p) \tau_v^0(p) \beta_v^0(p) \frac{dT(p)}{dU_i^0(p)} d \ln \tau_{v_i}^0(p). \end{aligned} \quad (13)$$

Define the deviation of the effective temperature profile of the i -th absorbing gas from the true atmospheric temperature profile as

$$\delta T_i(p) \equiv \delta T(p) - \delta U_i(p) \frac{dT(p)}{dU_i^0(p)}. \quad (14)$$

According to Smith *et al.* (1991), the effective temperature for each absorbing gas is that atmospheric temperature profile which would give rise to the radiance observed in spectral regions where the absorbing gas dominates the absorption/emission process, assuming that the initial absorbing gas profile is correct. As seen from Eq. (14), the difference between the effective temperature profile of an absorbing gas and the true atmospheric temperature profile is proportional to the error of the initial absorbing concentration profile.

Using Eq. (14), Eq. (13) becomes

$$\delta R_v \approx W_{T_s} \delta T_s - \sum_{i=1}^N \int_0^{p_s} W_{T_i}(p) \delta T_i(p) dp, \quad (15)$$

where

$$W_{T_s} = \beta_v^0(p_s) \tau_v^0(p_s), \quad (16)$$

and

$$W_{T_i}(p) = \beta_v^0(p) \tau_v^0(p) \frac{d \ln \tau_{v_i}^0(p)}{dp}. \quad (17)$$

Eq. (15) is a linear form of the radiative transfer equation in Eq. (1), with the surface temperature Jacobian W_{T_s} and the effective temperature Jacobians $W_{T_i}(p)$ for each absorbing gas. Eq. (14) can be rewritten as

$$U_i(p) = U_i^0(p) + \frac{dU_i^0(p)}{dT(p)} [T(p) - T_i(p)]. \quad (18)$$

Eq. (18) shows that the retrieval quality of absorbing gas profiles depends only on the quality of the assumed initial absorbing gas profile, regardless of the quality of any assumed initial temperature profile. We will address this issue after we derive the dual linear form in the next section.

Dual Representation of the Linear Form

The idea of a dual linear form was directly inspired from the classic paper of Smith *et al.* (1991). For easy comparison the derivation below is done in a similar fashion as their work wherever it is possible. The true spectrum of monochromatic radiance exiting the earth-atmosphere system is same as Eq. (1):

$$R_v = B_v(p_s) \tau_v(p_s) - \int_0^{p_s} B_v(p) d\tau_v(p). \quad (19)$$

The radiance spectrum corresponding to an assumed initial temperature and absorbing gas profiles is same as Eq. (2)

$$R_v^0 = B_v^0(p_s) \tau_v^0(p_s) - \int_0^{p_s} B_v^0(p) d\tau_v^0(p). \quad (20)$$

Employing the following linear perturbation definitions

$$\begin{aligned} \delta R_v &\equiv R_v - R_v^0, \\ \delta B_v(p) &\equiv B_v(p) - B_v^0(p), \\ \delta \tau_v(p) &\equiv \tau_v(p) - \tau_v^0(p), \end{aligned} \quad (21)$$

the difference between the true and initial spectra is now written as

$$\delta R_v = \delta B_v(p_s) \tau_v(p_s) + B_v^0(p_s) \delta \tau_v(p_s) - \int_0^{p_s} \delta B_v(p) d\tau_v(p) - \int_0^{p_s} B_v^0(p) d[\delta \tau_v(p)]. \quad (22)$$

Note that Eq. (22) is the *dual* representation of Eq. (4). They are different in expression but identical in mathematics. Nevertheless, the following derivation makes their resulting linear forms of the RTE different.

Performing integration by parts on the first integral term in Eq. (22), the linear form becomes

$$\delta R_v = \delta B_v(p_s) \tau_v(p_s) - \int_0^{p_s} \delta B_v(p) d\tau_v(p) + \int_0^{p_s} \delta \tau_v(p) dB_v^0(p). \quad (23)$$

Using the following approximations, which are identical to or similar to those assumed by Smith *et al.* (1991):

$$\delta B_v(p) = \frac{\partial B_v(T^0(p))}{\partial T(p)} \delta T(p) \equiv \beta_v^0(p) \delta T(p), \quad (24)$$

$$\delta \tau_v(p) = \tau_v^0(p) \sum_{i=1}^N \delta \ln \tau_{v_i}(p) \approx \tau_v^0(p) \sum_{i=1}^N \delta U_i(p) \frac{d \ln \tau_{v_i}^0(p)}{d U_i^0(p)}, \quad (25)$$

$$d\tau_v(p) = \tau_v^0(p) \sum_{i=1}^N d \ln \tau_{v_i}(p) \approx \tau_v^0(p) \sum_{i=1}^N d U_i(p) \frac{d \ln \tau_{v_i}^0(p)}{d U_i^0(p)}, \quad (26)$$

$$\tau_v(p_s) \approx \tau_v^0(p_s), \quad (27)$$

and the identity

$$d B_v^0(p) = \beta_v^0(p) d T^0(p), \quad (28)$$

Eq. (23) becomes

$$\begin{aligned} \delta R_v = & \beta_v^0(p_s) \tau_v^0(p_s) \delta T_s - \sum_{i=1}^N \int_0^{p_s} \beta_v^0(p) \delta T(p) \tau_v^0(p) \frac{d U_i(p)}{d p} \frac{d \ln \tau_{v_i}^0(p)}{d U_i^0(p)} d p \\ & + \sum_{i=1}^N \int_0^{p_s} \tau_v^0(p) \delta U_i(p) \frac{d \ln \tau_{v_i}^0(p)}{d U_i^0(p)} \beta_v^0(p) \frac{d T^0(p)}{d p} d p, \end{aligned} \quad (29)$$

where N is the number of absorbing gases, and $U_i(p)$ is the path length of the i -th absorbing gas, defined in Eq. (10). Like its counterpart in Eq. (9), Eq. (29) also shows no information about the difference between the true and initial gas concentration profiles, $\delta U_i(p)$, in regions where the initial lapse rate $d T^0(p)/d p$ is zero. Using the following relations

$$d U_i(p) \frac{d \ln \tau_{v_i}^0(p)}{d U_i^0(p)} = \frac{d U_i(p)}{d U_i^0(p)} d \ln \tau_{v_i}^0(p), \quad (30)$$

$$d T^0(p) \frac{d \ln \tau_{v_i}^0(p)}{d U_i^0(p)} = \frac{d T^0(p)}{d U_i^0(p)} d \ln \tau_{v_i}^0(p), \quad (31)$$

Eq. (29) can be rewritten as

$$\begin{aligned} \delta R_v = & \beta_v^0(p_s) \tau_v^0(p_s) \delta T_s - \sum_{i=1}^N \int_0^{p_s} \beta_v^0(p) \tau_v^0(p) \delta T(p) \frac{d U_i(p)}{d U_i^0(p)} d \ln \tau_{v_i}^0(p) \\ & + \sum_{i=1}^N \int_0^{p_s} \beta_v^0(p) \tau_v^0(p) \delta U_i(p) \frac{d T^0(p)}{d U_i^0(p)} d \ln \tau_{v_i}^0(p). \end{aligned} \quad (32)$$

Now the deviation of the effective temperature profile of the i -th absorbing gas from the true atmospheric temperature profile is defined as

$$\delta T_i(p) \equiv \delta T(p) \frac{d U_i(p)}{d U_i^0(p)} - \delta U_i(p) \frac{d T^0(p)}{d U_i^0(p)}. \quad (33)$$

Note that Eq. (33) is different from Eq. (14) in the previous section. The effective temperature for any absorbing gas in Eq. (33) can be still that atmospheric temperature profile which would give rise to the radiance observed in spectral regions where the absorbing gas dominates the absorption/emission process, assuming that the initial absorbing gas profile is correct.

Plugging Eq. (33) into Eq. (32) leads to

$$\delta R_v \approx W_{T_s} \delta T_s - \sum_{i=1}^N \int_0^{p_s} W_{T_i}(p) \delta T_i(p) dp, \quad (34)$$

where the surface temperature Jacobian W_{T_s} and the effective temperature Jacobians for each absorbing gas $W_{T_i}(p)$ are respectively

$$W_{T_s} = \beta_v^0(p_s) \tau_v^0(p_s), \quad (35)$$

and

$$W_{T_i}(p) = \beta_v^0(p) \tau_v^0(p) \frac{d \ln \tau_{v_i}^0(p)}{dp}. \quad (36)$$

Eq. (34) is the dual linear form of the radiative transfer equation in Eq. (1), with respect to the original linear form in Eq. (15). Their difference lies in the contents of the effective temperature for any absorbing gas shown in Eqs. (14) and (33). Eq. (33) can be rewritten as

$$\left[T^0(p) - T(p) \right] \frac{dU_i(p)}{dT^0(p)} + U_i(p) = U_i^0(p) + \frac{dU_i^0(p)}{dT^0(p)} \left[T^0(p) - T_i(p) \right]. \quad (37)$$

In the *special* case where $T(p) = T^0(p)$, Eq. (37) reduces to

$$U_i(p) = U_i^0(p) + \frac{dU_i^0(p)}{dT(p)} \left[T(p) - T_i(p) \right], \quad (38)$$

It is interesting to note that Eq. (38) is the same formula for absorbing gas profiles as Eq. (18) originally derived by Smith *et al.* (1991). Eq. (38) shows that the quality of the retrieved absorbing gas profiles depends solely on the quality of the assumed initial absorbing gas profile, only when the assumed initial temperature profile happens to be the truth temperature profile.

In the *general* case where $T(p) \neq T^0(p)$, Eq. (37) is a first-order linear differential equation of $U_i(p)$, which can be rewritten as

$$\left[T^0(p) - T(p) \right] \frac{dU_i(p)}{dp} + \frac{dT^0(p)}{dp} U_i(p) = U_i^0(p) \frac{dT^0(p)}{dp} + \frac{dU_i^0(p)}{dp} \left[T^0(p) - T_i(p) \right]. \quad (39)$$

The general solution to Eq. (39) with the boundary condition $U_i(0) = 0$ is

$$U_i(p) = e^{F(p)} \int_0^p e^{-F(p')} G(p') dp'. \quad (40)$$

where

$$F(p) = - \int_0^p \frac{1}{\left[T^0(p') - T(p') \right]} \frac{dT^0(p')}{dp'} dp', \quad (41)$$

and

$$G(p) = \frac{U_i^0(p) \frac{dT^0(p)}{dp} + \frac{dU_i^0(p)}{dp} [T^0(p) - T_i(p)]}{T^0(p) - T(p)}. \quad (42)$$

Unlike Eqs. (38) and (18), the retrieval of $U_i(p)$ in Eq. (43) has a reasonable dependence on the quality of an assumed initial temperature profile $T^0(p)$, via $G(p)$ and $F(p)$ in Eqs. (41) and (42). As expected, the quality of the retrieved absorbing gas profiles depends on both the quality of both the assumed initial temperature and absorbing gas profiles.

Conclusions

The classical derivation of the linear form of the radiative transfer equation by Smith *et al.* is reviewed. A dual representation of the linear form is derived. The dual linear form is able to show that the quality of the retrieved absorbing gas profiles also depends also on the quality of the assumed initial temperature profile. The formulation for retrieving absorbing gas profiles in the original linear form appears to be a special case of its counterpart in the dual linear form when the assumed initial temperature profile happens to be the true temperature profile. Only in this case the dual linear form is reduced to the original linear form with the identical solution.

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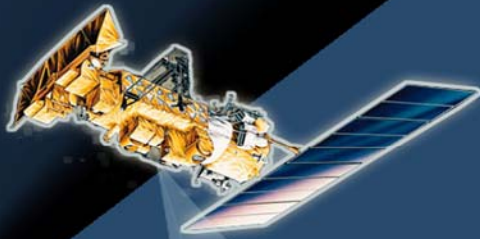
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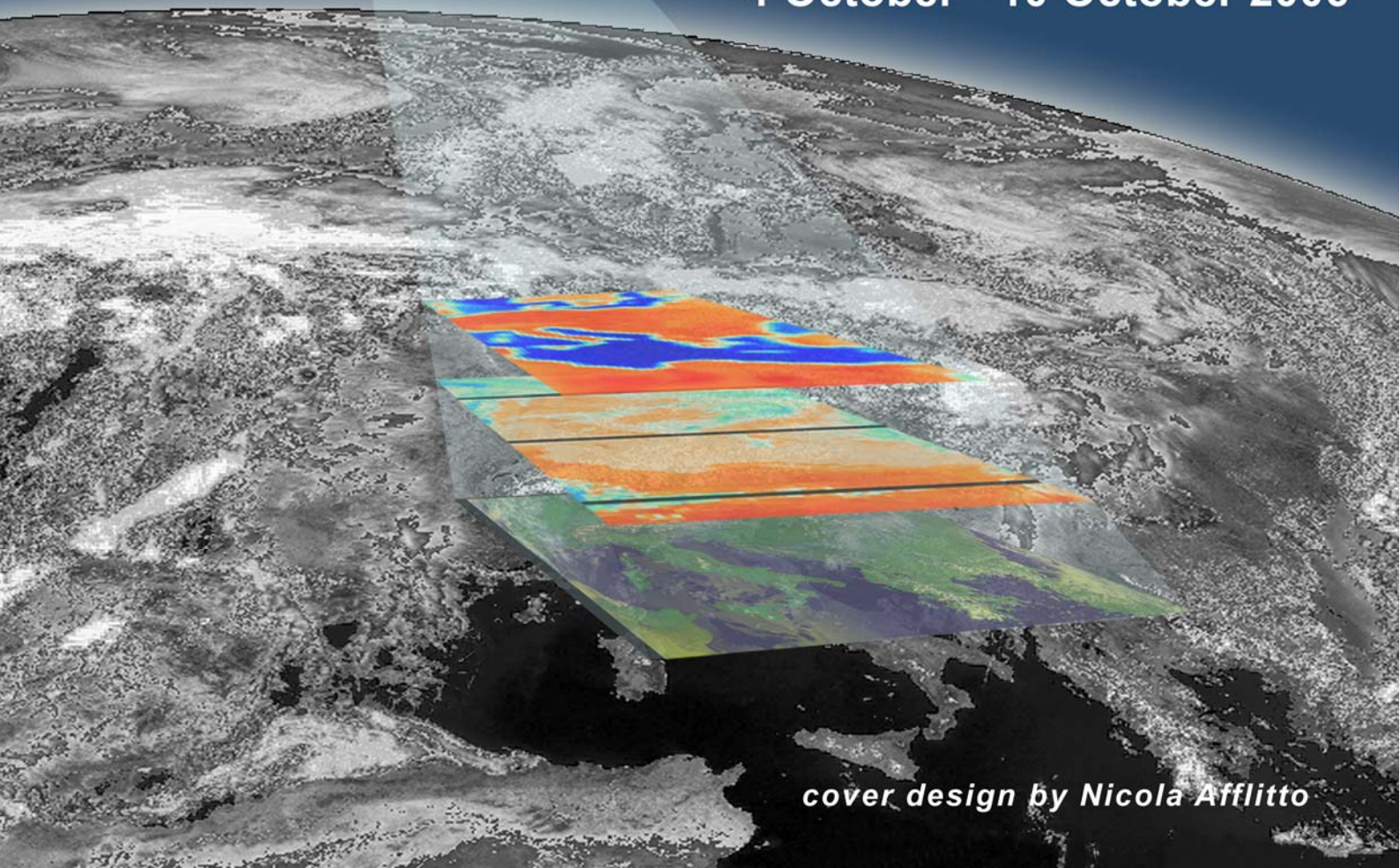
using space-based observations



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