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On the application of the adjoint method of sensitivity analysis to problems in the atmospheric sciences

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RESUMEN

Motivados por un reciente trabajo publicado en esta revista por Marchuk y Skiba (1992), presentamos una breve revisión del desarrollo del método adjunto de análisis de sensibilidad, destacando sus limitaciones y aplicabilidad tanto a sistemas lineales como a los no lineales. Así mismo el trabajo de Marchuk y Skiba (1992), es analizado desde el punto de vista matemático e histórico.

ABSTRACT

Motivated by a recent article published in this journal by Marchuk and Skiba (1992), we present a brief review of the development of the adjoint method of sensitivity analysis, highlighting its limitations and applicability to both linear and nonlinear systems. In the process, the work of Marchuk and Skiba (1992) is set in perspective, both historically and mathematically.

1. Introduction

In a recent paper published in this journal, henceforth referred to as "MS92", Marchuk and Skiba (1992) have discussed a sensitivity analysis, using adjoint functions, of a simple atmosphere–ocean–soil thermal interaction model. This model is used by the authors to calculate three-dimensional, time-dependent, global temperature deviations $T(\lambda, \theta, z, t)$ from some unspecified (albeit assumed known) reference temperature distribution, subject to prescribed nondivergent atmospheric winds and nondivergent oceanic currents. Two simple linear functionals of $T(\lambda, \theta, z, t)$ are defined to be the model responses of interest. An "adjoint problem" is then formulated, ostensibly for the purpose of performing a sensitivity analysis of these responses to variations in the model's initial data and forcing functions. However, a sensitivity analysis is not presented; instead, the authors present several contour plots of the solutions to their "adjoint problem" and some vague conclusions about their significance. In addition, they make several unsubstantiated claims, with misleading implications regarding both their specific model and, more generally, regarding the adjoint method of sensitivity analysis.

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This work has two objectives: first, to highlight the advantages and limitations of the adjoint method of sensitivity analysis; and second, to alleviate the misleading claims of MS92 regarding both the origins of the adjoint method of sensitivity analysis and its specific application to the MS92 model. For this purpose, we present in Section 2 a brief overview of the historical development of the adjoint method of sensitivity analysis. This overview places Marchuk's contribution to this field in the proper perspective, thereby providing a counterbalance to the exaggerated claims of pioneering implied in MS92. In Section 3, we discuss the salient features of the adjoint method of sensitivity analysis of nonlinear systems, highlighting its range of applicability and limitations. Section 4 addresses the proper application of this method to the MS92 model, including the full treatment of boundary conditions. Several inaccuracies in the MS92 work are pointed out in the process. Finally, we summarize our conclusions briefly in Section 5.

2. Historical development of the adjoint method

The use of adjoint functions for analyzing the effects of small perturbations on system responses for linear systems arose in the then–emerging field of nuclear reactor physics, and is attributed (Glasstone and Edlund, 1952, p. 372; see also Weinberg and Wigner, 1958) to Wigner (1945; see also Brooks, 1948), while the introduction of variational principles for analyzing such perturbation effects is generally acknowledged (see, e.g., Stacey, 1974) to have evolved from the works of Schwinger (Levine and Schwinger, 1949). Wigner also appears to have been the first to interpret the adjoint function (in that case, the adjoint neutron flux) as the *importance function*. As acknowledged by Weinberg and Wigner (1958, p. 556), additional contributions came from the works of Fuchs (1949) and Usachev (1955). These early methods were subsequently developed further, yet still within the field of nuclear reactor physics, by Selengut (1959, 1963) Usachev (1964), Lewins (1965), Pomraning (1965), Gandini (1967) and others – too numerous to list here. These works established a fully developed, deterministic methodology for performing a systematic and exhaustive *sensitivity analysis of linear systems*. Marchuk(1974, 1975) appears to have been the first to use this methodology – already fully developed for linear systems – to assess the effects of small perturbations in *linear atmospheric models*. It is crucial to note here, however, that *the methodology used by Marchuk cannot be applied to nonlinear models.*

The first formulation of a methodology using adjoint functions for performing a systematic sensitivity analysis for *nonlinear systems* – continuous and/or discrete – was provided by Cacuci *et al.* (1980). This methodology was subsequently set on a rigorous mathematical basis (Cacuci, 1981a) and fundamentally extended (Cacuci, 1981b) to nonlinear operator–type responses and responses defined by critical points. In particular, Cacuci (1981a,b) stressed that the corresponding adjoint functions for nonlinear systems depend on the unperturbed forward (i.e., nonlinear) solution. Cacuci (1981a,b) has also shown that the adjoint functions corresponding to nonlinear systems can be interpreted as *importance functions* – in that they measure the importance of a region and/or event in phase–space in contributing to the system's response under consideration; this interpretation is similar to that originally assigned by Wigner (1945) to the adjoint functions in the linear problems underlying nuclear reactor physics.

The first application of the nonlinear sensitivity analysis methodology developed by Cacuci (1981a) to a *nonlinear model of interest to atmospheric sciences* – namely the radiative–convective model of the atmosphere developed by Schlesinger – was by Hall, Cacuci and Schlesinger (1982). They presented not only an exhaustive sensitivity analysis using adjoint functions for that model, but also illustrated the use of sensitivities for uncertainty analysis. The physical intepretation of the adjoint functions for this radiative–convective model was discussed by Hall and Cacuci (1983) who showed that the respective adjoint functions quantify the importance of previous (antecedent) states to the current response. In a similar vein, Errico and Vukicevic (1992) have recently applied Cacuci's sensitivity theory (1981a) to the PSU–NCAR mesoscale model and showed that the respective adjoint fields quantify the antecedent conditions that most affect a specified forecast.

The work of Cacuci (1981a) was subsequently extended to nonlinear systems with feedback (Cacuci and Hall, 1984). The first application of Cacuci's sensitivity theory (1981a) to a large-scale, realistic climate model was by Hall (1986) to the Oregon State University atmospheric general circulation model. This study not only simultaneously determined the sensitivities of global-mean surface-air temperature to variations in CO_2, solar insolation, sea surface temperature, surface albedo and stratospheric ozone, but also presented the temporal evolution and spatial distribution of these five sensitivities and ranked the contributions to them by each of the GCM's seven prognostic quantities. A milestone application of Cacuci's adjoint sensitivity theory (1981b) for nonlinear systems with operator-type responses is the recent adjoint sensitivity study by Zou *et al.* (1993) of blockings in a two-layer climate model. In this work, the blocking index is represented as a time- and space-dependent operator of the model's dynamic fields and parameters. The sensitivities of blockings to all model parameters were obtained both in grid-space and spectral-space using Cacuci's adjoint method (1981b). As Zou *et al.* (1993) demostrate, it would have been impossible to obtain the same amount of sensitivity information in any other way (e.g., via recalculations or statistical methods), because of the prohibitive amount of computations that would have been required.

Adjoints of atmospheric and oceanic models have also been used for purposes other than sensitivity analysis. We mention here briefly the three other areas where such adjoints have been used: (1) variational data assimilation (LeDimet and Talagrand, 1986; Talagrand and Courtier, 1987; Thépaut and Courtier, 1992; Navon *et al.*, 1992); (2) optimal parameter estimation (Smedstad and O'Brien, 1991; Zou *et al.*, 1992); and (3) evaluation of optimal growth rates of initial perturbations (Farrell, 1990; Barkmeijer, 1992).

3. Applicability of the adjoint method

It is important to note that the sensitivities yielded by either the sensitivity analysis methods for linear systems (i.e., perturbation theory *a la* Wigner or variational method *a la* Schwinger–Selengut) or the sensitivity analysis method of Cacuci (1981a,b) for nonlinear systems are *local sensitivities*, valid only in sufficiently small neighborhoods of the nominal values of the respective parameters. In the simplest case, these sensitivities are equivalent to the first-order partial derivatives of the system's response with respect to the system parameters.

The ideas underlying the method presented by Cacuci (1990) opened the way for a bona fide global sensitivity analysis of linear and/or nonlinear systems. This method involves a simultaneous marching with the forward system and the adjoint system through a global phase-space to determine (with probability one) all of the system's critical points, namely, the solution's bifurcation and turning points, and the maxima, minima, and saddle points for the response – as the system's parameters are allowed to vary globally over their entire physical ranges. In addition, this method provides simultaneously the local sensitivities around any point in phase-space, including the critical points – thus providing, in particular, information about the linear stability of the respective points. Although applications involving relatively small-scale nonlinear systems have been presented for illustrative purposes, applications to large-scale nonlinear systems, such as those underlying meteorological and climate problems, require a careful analysis of the computational structures specific to each application in order to minimize computational costs associated with the global search of critical points. Of course, searching for efficient computational algorithms is an obvious characteristic that permeates all global analyses of large-scale systems.

A straightforward application of perturbation theory and/or Cacuci's method for nonlinear systems to calculate second-order sensitivities – thereby presumably extending the range of applicability of these methods – is not profitable. This is because, as discussed by Cacuci (1990), the adjoint systems required to calculate second- (and higher-) order sensitivities depend on the value of the perturbation, and this dependence cannot be avoided. This situation is in stark contrast to the adjoint system needed to calculate the first-order sensitivities, which is independent of the perturbation value, although, as shown by Cacuci (1981a,b), the adjoint system for nonlinear problems depends on the nominal values of the respective response, parameters and forward dependent variables (i.e., state functions). Note that the corresponding adjoint system for linear problems is also independent of the forward variables. Since the adjoint systems for second- and higher-order sensitivities necessarily depend on the parameter perturbation values, it follows that as many adjoint systems as there are parameter values would need to be solved in practice to obtain the second- and higher-order sensitivities. This would negate the tremendous practical advantages brought by the adjoint method for calculating the first-order sensitivities, where, as already mentioned, the adjoint system is independent of the parameter perturbations, so only one adjoint system needs to be solved per response.

It has been shown by Cacuci (1990) that even if all the second- and higher- order sensitivities could be obtained, the information gained over that provided by the first-order sensitivities would be minimal; this is because the higher-order sensitivities still provide information about only the *local, not the global, behavior* of the response and system around the nominal parameter values. In other words, calculating the first-order sensitivities by the adjoint method (Cacuci, 1981a,b) provides a high ratio of payoff-to-effort (analytical and computational); this ratio decreases dramatically starting with the calculation of second-order sensitivities.

4. Application of the adjoint method of sensitivity analysis to the MS92 model

The aim of this section is to present the proper application of the adjoint method of sensitivity analysis to the MS92 model – several inaccuracies present in MS92 becoming apparent in the process. The MS92 model is described by its authors as a "simplified three-dimensional global heat interaction model of the atmosphere and ocean" that "has been linearized by using the climatic monthly mean wind in the atmosphere and the climatic seasonal currents in the World Ocean". The actual mathematical formulation of the MS92 model is quoted bellow:

$$\alpha \frac{\partial T}{\partial t} + div(\vec{u}T) - \frac{\partial}{\partial z}\left(\nu \frac{\partial T}{\partial z}\right) - \mu \Delta_2 T = 0, \quad t \epsilon (0,\ \bar{t}), \quad x \epsilon D_1 \cup D_2, \tag{1}$$

$$T(x,\ t) = T^o(x), \text{ at } t = 0, \tag{2}$$

$$\nu \frac{\partial T}{\partial z} = 0, \text{ at } z = h_1,\ z = -h_2,\ z = -h_3, \tag{3}$$

$$\nu \frac{\partial T}{\partial z} = -F(\lambda,\ \theta,\ t), \text{ at } z = 0 \text{ on } S_1, \tag{4}$$

$$T(\lambda,\ \theta,\ -0,\ t) - T(\lambda,\ \theta, +0,\ t) = 0, \text{ on } S_2 \cup S_3, \tag{5}$$

$$\nu\frac{\partial T}{\partial z}(\lambda,\ \theta,\ -0,\ t) - \nu\frac{\partial T}{\partial z}(\lambda,\ \theta,\ +0,\ t) = F,\ \text{on}\ S_2 \cup S_3, \tag{6}$$

$$\mu\frac{\partial T}{\partial \vec{n}} = 0,\ \text{on the lateral surface}\ \Omega\ \text{of}\ D_2, \tag{7}$$

$$\vec{u}\cdot\vec{n} = 0,\ \vec{u}\epsilon\Omega, \tag{8}$$

$$div\ \vec{u} = 0,\ \vec{u}\epsilon D_1 \cup D_2, \tag{9}$$

where $x = (\lambda,\ \theta,\ z)$, with λ = longitude, θ = colatitude, z = altitude above the Earth's surface (mean sea level); $D_1 = \{(\lambda,\ \theta,\ z) : (\lambda,\ \theta)\epsilon S,\ 0 < z < h_1\}; D_2 = \{(\lambda,\ \theta,\ z) : (\lambda,\ \theta)\epsilon S_2,\ -h_2 < z < 0\}; D_3 = \{(\lambda,\ \theta,\ z) : (\lambda,\ \theta)\epsilon S_3,\ -h_3 < z < 0\}; D = D_1 \cup D_2 \cup D_3; S_1$ = snow–and ice–covered surface; S_2 = ocean surface; S_3 = continental surface, free of snow and ice; $S = S_1 \cup S_2 \cup S_3; T(x,\ t)$ = temperature deviation from a basic–state value, $\tilde{T}(x,\ t); T^o(x)$ = initial value of $T(x,\ t)$; div = divergence operator; Δ_2 = spherical part of the Laplace operator; $F(\lambda,\ \theta, t)$ = surface heat flux deviation (n.b., due to all processes other than turbulent transport); $\vec{n}$ = unit outward normal vector on $\Omega; \alpha(z)$ is the specific heat times a standard density, $\rho(z); \vec{u}(x,\ t)$ is $\alpha(z)$ times the prescribed velocity vector, $\vec{U}(x,\ t)$; and $\mu(x,\ t)$ and $\nu(x,\ t)$ are the horizontal and vertical turbulent diffusivity coefficients. It is assumed that $\alpha(z)$, $\vec{u}(x,\ t)$, $\mu(x,\ t)$ and $\nu(x,\ t)$ are known functions in the time–space domain, $D \times (0,\ \bar{t})$, where $(0,\ \bar{t})$ is the time interval under consideration, for example, one month.

Two *linear* model responses are considered in MS92, defined as the following linear functionals of T,

$$\Im_{p^*}(T) = \int_o^{\bar{t}} \int_D p^*(x,\ t)T(x,\ t)dx\ dt, \tag{10}$$

and

$$\Im_{F^*}(T) = \int_o^{\bar{t}} \int_S F^*(\lambda,\ \theta,\ t)T(\lambda,\ \theta,\ 0,\ t)dS\ dt, \tag{11}$$

where $p^*(x,\ t)$ and $F^*(\lambda, \theta, t)$ are known functions.

They then claim that the following results holds,

$$\Im(T) = \Im_{p^*}(T) + \Im_{F^*}(T) = \int_o^{\bar{t}} \int_S T^*(\lambda,\ \theta,\ 0,\ t)F(\lambda,\ \theta,\ t)dS\ dt$$

$$+ \int_D \alpha(x)T^*(x,\ 0)T^o(x)dx, \tag{12}$$

where $T^*(x,\ t)$ is the solution of the following system,

$$-\alpha\frac{\partial T^*}{\partial t} - div(\vec{u}T^*) - \frac{\partial}{\partial z}\left(\nu\frac{\partial T^*}{\partial z}\right) - \mu\Delta_2 T^* = p^*, \tag{13}$$

$$T^*(x,\ \bar{t}) = 0,\ \text{at}\ t = \bar{t}, \tag{14}$$

$$\nu\frac{\partial T^*}{\partial z} = 0,\ \text{at}\ z = h_1,\ z = -h_2,\ \text{and}\ z = -h_3, \tag{15}$$

$$\nu\frac{\partial T^*}{\partial z} = -F^*(\lambda,\ \theta,\ t),\ \text{at}\ z = 0\ \text{on}\ S_1, \tag{16}$$

$$T^*(\lambda,\ \theta,\ -0,\ t) - T^*(\lambda,\ \theta,\ +0,\ t) = 0,\ \text{on}\ S_2 \cup S_3, \tag{17}$$

$$\nu\frac{\partial T^*}{\partial z}(\lambda,\ \theta,\ -0,\ t) - \nu\frac{\partial T^*}{\partial z}(\lambda,\ \theta,\ +0,\ t) = F^*,\ \text{on}\ S_2 \cup S_3, \tag{18}$$

$$\mu\frac{\partial T^*}{\partial \vec{n}} = 0,\ \text{on}\ \Omega, \tag{19}$$

where $\vec{u}(x,\ t)$ satisfies Eqs. (8) and (9). In MS92, the problem described by Eqs. (13) through (19), together with Eqs. (8) and (9), is referred to as "the adjoint problem".

It will be shown in the following that the problem described by Eqs. (13) through (19), augmented by Eqs. (8) and (9), is *not the rigorously correct adjoint problem* to the MS92 model described by Eqs. (1) through (9). Thus, multiplying Eq. (1) by $T^*(x,\ t)$ and integrating the result over $x \epsilon D$ and $t \epsilon (0,\ \bar{t})$ yields,

$$\int_o^{\bar{t}}\int_D \left[T^*(x,\ t)\alpha(z)\frac{\partial T}{\partial t}\right] dx\ dt + \int_o^{\bar{t}}\int_D \{T^*(x,\ t) div[\vec{u}(x,\ t)T(x,\ t)]\} dx\ dt$$

$$-\int_o^{\bar{t}}\int_D \left\{T^*(x,\ t)\frac{\partial}{\partial z}\left[\nu(x,\ t)\frac{\partial T(x,\ t)}{\partial z}\right]\right\} dx\ dt - \int_o^{\bar{t}}\int_D \{T^*(x,\ t)\mu(x,\ t)\Delta_2 T(x,\ t)\} dx\ dt = 0. \tag{20}$$

Integrating the first term on the left-hand side of Eq. (20) by parts over t yields

$$\int_o^{\bar{t}}\int_D \left[T^*(z,\ t)\alpha(z)\frac{\partial T}{\partial t}\right] dt\ dx = \int_D \alpha(z)\left\{T^*(x,\ \bar{t})T(x,\ \bar{t}) - T^*(x,\ 0)T(x,\ 0)\right\} dx$$

$$-\int_o^{\bar{t}}\int_D \left[T(x,\ t)\frac{\partial}{\partial t}(\alpha T^*)\right] dx\ dt, \tag{21}$$

and integrating the remaining terms on the left–hand side of Eq. (20) by parts over the respective spatial variables gives

$$\int_o^{\bar t}\int_D \{T^*(x,\ t)div[\vec u(x,\ t)T(x,\ t)]\}dx\ dt = -\int_o^{\bar t}\int_D \{T(x,\ t)div[\vec u(x,\ t)T^*(x,\ t)]\}dx\ dt$$

$$+\int_o^{\bar t}\int_D T(x,\ t)T^*(x,\ t)div\ \vec u(x,\ t)dx\ dt + \int_o^{\bar t} dt\left[\int_\theta\int_\lambda \{TT^*u_z\}_z a^2\sin\theta d\theta d\lambda + \right.$$

$$\left. + \int_z\int_\lambda \{TT^*\sin\theta u_\theta\}_\theta adzd\lambda + \int_z\int_\theta \{TT^*u_\lambda\}_\lambda adzd\theta\right], \tag{22}$$

$$\int_o^{\bar t}\int_D T^*(x,\ t)\frac{\partial}{\partial z}\left[\nu(x,\ t)\frac{\partial T(x,\ t)}{\partial z}\right]dx\ dt = \int_o^{\bar t}\int_D T(x,\ t)\frac{\partial}{\partial z}\left(\nu(x,\ t)\frac{\partial T^*}{\partial z}\right)dx\ dt +$$

$$+\int_o^{\bar t} dt\int_\lambda\int_\theta a^2\sin\theta d\lambda\ d\theta\left\{T^*(x,\ t)\nu(x,\ t)\frac{\partial T(x,\ t)}{\partial z} - T(x,\ t)\nu(x,\ t)\frac{\partial T^*}{\partial z}\right\}_z, \tag{23}$$

$$\int_o^{\bar t}\int_D T^*(x,\ t)\mu(x,\ t)\Delta_2 T(x,\ t)dx\ dt = \int_o^{\bar t}\int_D T(x,\ t)\Delta_2(\mu T^*)dx\ dt +$$

$$+\int_o^{\bar t} dt\left[\int_z\int_\lambda\left\{T^*\mu\sin\theta\frac{\partial T}{\partial\theta} - T\sin\theta\frac{\partial(\mu T^*)}{\partial\theta}\right\}_\theta dz\ d\lambda + \right.$$

$$\left. + \int_z\int_\theta\left\{T^*\mu\frac{\partial T}{\partial\lambda} - T\frac{\partial(\mu T^*)}{\partial\lambda}\right\}_\lambda\frac{dz\ d\theta}{\sin\theta}\right], \tag{24}$$

where a is the radius of the Earth, u_λ, u_θ and u_z are the longitudinal, colatitudinal and vertical components of $\vec u(x,\ t)$, and the symbolic notation

$$\{A\}_y \equiv A(y_2) - A(y_1)$$

has been used to denote the result obtained by performing and evaluating a definite integral with respect to any independent variable y.

Substituting Eqs. (21)–(24) into Eq. (20) gives

$$\int_o^{\bar{t}}\int_D T^*(x,\ t)\left[\alpha(z)\frac{\partial T}{\partial t}+div(\vec{u}T)-\frac{\partial}{\partial z}\left(\nu(x,\ t)\frac{\partial T}{\partial z}\right)-\mu(x,\ t)\Delta_2 T\right]dx\ dt=$$

$$=\int_o^{\bar{t}}\int_D T(x,\ t)\left[-\frac{\partial}{\partial t}(\alpha T^*)-div(\vec{u}T^*)-\frac{\partial}{\partial z}\left(\nu\frac{\partial T^*}{\partial z}\right)-\Delta_2(\mu T^*)\right]dx\ dt$$

$$+\int_D \alpha(z)\{T^*(x,\ \bar{t})T(x,\ \bar{t})-T^*(x,\ 0)T(x,\ 0)\}dx+\int_o^{\bar{t}}\int_D TT^* div(\vec{u})dx\ dt$$

$$+\int_o^{\bar{t}} dt\left[\int_\theta\int_\lambda a^2\sin\theta d\theta d\lambda\left\{TT^*u_z-T^*\nu\frac{\partial T}{\partial z}+T\nu\frac{\partial T^*}{\partial z}\right\}_z\right.$$

$$+\int_z\int_\lambda dz\ d\lambda\left\{TT^*u_\theta a\sin\theta-T^*\mu\sin\theta\frac{\partial T}{\partial\theta}+T\sin\theta\frac{\partial(\mu T^*)}{\partial\theta}\right\}_\theta$$

$$\left.+\int_z\int_\theta dz\ d\theta\left\{TT^*u_\lambda a-T^*\mu\frac{\partial T}{\sin\theta\partial\lambda}+T\frac{\partial(\mu T^*)}{\sin\theta\partial\lambda}\right\}\right]_\lambda$$

$$=0. \tag{25}$$

From Eq. (25) the *formal adjoint operator* $\mathcal{L}^*$ for Eq. (1) is

$$\mathcal{L}^*(T^*)=-\frac{\partial}{\partial t}(\alpha T^*)-div(\vec{u}T^*)-\frac{\partial}{\partial z}\left(\nu\frac{\partial T^*}{\partial z}\right)-\Delta_2(\mu T^*). \tag{26}$$

To obtain the functional $\Im_{p^*}(T)$ in Eq. (25) of MS92, one must use Eq. (25) above and set $\mathcal{L}^*(T^*)=p^*$, that is,

$$-\frac{\partial}{\partial t}(\alpha T^*)-div(\vec{u}T^*)-\frac{\partial}{\partial z}\left(\nu\frac{\partial T^*}{\partial z}\right)-\Delta_2(\mu T^*)=p^*. \tag{27}$$

Then one must use Eq. (1); the initial condition for T, eq. (2); the boundary conditions for T, Eqs. (3)–(6); the boundary condition for $\vec{u}$, Eq. (8); and the condition for nondivergent motion, Eq. (9). The functional $\Im_{p^*}(T)$ is then given by

$$\Im_{p^*}(T)=-B-I+\int_D\alpha(z)T^*(x,\ 0)T^o(x)dx$$

$$+\int_o^{\bar{t}}\int_S[T^*(\lambda,\ \theta,\ 0,\ t)F(\lambda,\ \theta,\ t)-T(\lambda,\ \theta,\ 0,\ t)F^*(\lambda,\ \theta,\ t)]dS\ dt \tag{28}$$

where

$$B = \int_0^{\bar{t}} \int_{z\leq 0}^{z} \left[\int_{\lambda} \left\{ T \sin\theta \frac{\partial(\mu T^*)}{\partial\theta} \right\}_{\theta} d\lambda + \int_{\theta} \left\{ T \frac{\partial(\mu T^*)}{\sin\theta \partial\lambda} \right\}_{\lambda} d\theta \right] dz\, dt - \int_o^{\bar{t}} \int_S \{TT^* u_z\}_z dS\, dt \quad (29)$$

is the residual of the boundary terms in Eq. (25), and

$$I = \int_o^{\bar{t}} \alpha(z) T^*(x,\ \bar{t}) T(x,\ \bar{t}) dx \quad (30)$$

is the term involving the "initial condition" for T^* at time $t = \bar{t}$.

In order to proceed further, it is necessary to choose properly the initial and boundary conditions for T^*. Below we discuss how this should be done in principle, and then discuss the conditions imposed by MS92 to obtain the functional $\Im_{p^*}(T)$ in their Eq. (25) from the correct functional $\Im_{p^*}(T)$ in Eq. (28).

4.1. Initial condition for T^*

Contrary to the assertion of MS92 (p. 124), the requirement that $T^*(x,\ t) = 0$ at $t = \bar{t}$, given by Eq. (14), is *not* imposed out of the desire to obtain a well-posed adjoint problem; rather, *this requirement is the result of wishing to eliminate the appearance of the forward function $T(x,\ t)$ in the adjoint problem for $T^*(x,\ t)$.* In other words, if we did not impose $T^*(x,\ t) = 0$ at $t = \bar{t}$, we could not eliminate the appearance of (the unknown value of) $T(x,\ t)$ in the adjoint problem, a fact that would immediately annihilate the very reason for using the adjoint method! The fact that setting $T^*(x,\ t) = 0$ at $t = \bar{t}$ leads to a well-posed adjoint problem is, of course, important, but of secondary importance. For example, one could set $T^*(x,\ t) = f(x)$ at $t = \bar{t}$ and still obtain a well-posed adjoint problem. However, as shown by Eq. (28), the term $\int_D \alpha(z) f(x) T(x,\ \bar{t}) dx$ would then not drop out; furthermore, the evaluation of this term would require calculation of the value for the forward function, $T(x,\ \bar{t})$, which, again, would annihilate the very reason for using the adjoint method. As shown by Cacuci (1981a,b), the requirement that the initial and boundary conditions for the adjoint be selected such that all unknown values and parameters of the forward problem are eliminated becomes even more important for nonlinear problems.

4.2. Boundary conditions for T^*

It is useful here to state the general principle that underlies the derivation of the correct form of the adjoint boundary conditions. This general principle requires that the adjoint boundary conditions be independent of any and all variations in: (a) the state variables [in the MS92 model – variations in the dependent variable $T(x,\ t)$], and (b) the model's parameters [in the MS92 model –variations in $\mu(x,\ t)$, $\nu(x,\ t)$, $\alpha(z)$], and any boundary parameters. *Note that for the MS92 model, the application of this principle will cause the correct adjoint boundary conditions to be also independent of the forward state function, $T(x,\ t)$; this is because the MS92 model given by Eqs. (1)-(9) is actually linear in $T(x,\ t)$! Note that this independence of the forward state function(s) is in distinct contrast to the general case of nonlinear models, where – as shown generally by Cacuci (1981a,b) – the adjoint system is tied to (i.e., depends on) the normal values of both the model's dependent forward variables and parameters.*

In view of the preceding discussion, it becomes clear that the correct adjoint boundary conditions to be associated with the correct formal adjoint of Eq. (1) given by Eq. (26), are to be obtained by: (i) using the complete set of forward boundary conditions on the right-hand side of Eq. (25), and (ii) ensuring that the remaining terms reduce precisely to the expression

$$\int_o^{\bar{t}} \int_S [F^*(\lambda,\ \theta,\ t)T(\lambda,\ \theta,\ 0,\ t) - F(\lambda,\ \theta,\ t)T^*(\lambda,\ \theta,\ 0,\ t)]dS\ dt.$$

This requires that the boundary term in Eq. (28) must be zero, that is $B = 0$. This, in turn requires that

$$u_z = 0,\ \text{at } z = h_1 \text{ and } z = -h_2 \tag{31a}$$

$$u_z = 0,\ \text{at } z = 0 \text{ on } S_1 \cup S_3, \tag{31b}$$

$$TT^* u_z(\lambda,\ \theta,\ -0,\ t) - TT^* u_z(\lambda,\ \theta,\ +0,\ t) = 0,\ \text{on } S_2, \tag{31c}$$

and

$$\frac{\partial(\mu T^*)}{\partial \vec{n}} = 0,\ \text{on } \Omega \tag{32a}$$

or, equivalently,

$$\mu \frac{\partial T^*}{\partial \vec{n}} = -T^* \frac{\partial \mu}{\partial \vec{n}},\ \text{on } \Omega. \tag{32b}$$

MS92 do not state the boundary conditions given by Eq. (31). Furthermore, condition (31b) means that the Earth's surface orography is ignored. In a more-comprehensively formulated adjoint problem, even one including all the nonlinearities of a GCM, it is not necessary to impose this "flat earth" assumption (see Hall, 1986).

MS92 also does not use the boundary condition given by Eq. (32b). Instead they use Eq. (19),

$$\mu \frac{\partial T^*}{\partial \vec{n}} = 0,\ \text{on } \Omega, \tag{19}$$

which is valid only if μ is independent of both λ and θ, an idealization which contradicts the MS92 statement that μ is a function of t *and* x, that is, $\mu(x,\ t)$.

4.3. Other remarks

MS92 define the adjoint operator by the left-hand-side of Eq. (13), that is,

$$\mathcal{L}^*(T^*) = -\alpha \frac{\partial T^*}{\partial t} - div(\vec{u}T^*) - \frac{\partial}{\partial z}\left(\nu \frac{\partial T^*}{\partial z}\right) - \mu \Delta_2 T^*. \tag{33}$$

This is an approximation of the correct $\mathcal{L}^*(T^*)$ given by Eq. (26), which approximation is valid only if α is independent of t, an idealization which MS92 do explicitly assume, and μ is independent of both λ and θ, again which contradicts the MS92 statement that $\mu = \mu(x, t)$.

It is important also to note that the MS92 model, Eqs. (1)–(9), is *independent* of what MS92 refer to as the "basic state [temperature] value $\tilde{T}(\lambda, \theta, z, t)$" [cf. MS92, p. 121]. The only way a "linearized" model can become completely independent of the "basic state value" – in the sense used by MS92 – is if the *original forward model were linear to begin with, or if this "basic state value" were a constant.* In contrast, if the original forward model is *nonlinear* in the "basic state value" $\tilde{T}(\lambda, \theta, z, t)$, then the *linearized* model, corresponding in this case to Eqs. (1)–(9), must necessarily depend on $\tilde{T}(\lambda, \theta, z, t)$ explicitly. These considerations highlight the discrepancy between the mathematical structure of the MS92 model and the implied claim of original nonlinearities set forth in MS92 [cf. the quotes at the beginning of our Section 4]. Thus, the results, claims and interpretations of the adjoint functions presented in MS92 must be viewed with considerable caution.

5. Summary and conclusions

In this paper we have derived the correct form of the adjoint system (operator and boundary/initial conditions) that results from the proper application of the adjoint method of sensitivity analysis for the simple, linear model of atmosphere–ocean–soil interaction presented by MS92. We have also outlined the historical development of the adjoint method of sensitivity analysis. For *linear systems,* the adjoint method of sensitivity analysis had its origins in the works of Wigner (1945) and Schwinger (Levine and Schwinger, 1949), and has been developed in the field of nuclear reactor physics by many, many authors. Marchuk (1974, 1975) appears to have been the first to apply these already well-developed adjoint method for *linear systems* to simple *linear* problems in weather and climate modeling. For *nonlinear systems*, with and without feedback, and with general operator–type responses, the adjoint method of sensitivity analysis has been developed by Cacuci (Cacuci *et al.*, 1980; Cacuci, 1981a,b, 1988, 1990; Cacuci and Hall, 1984).

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