Physical Interpretation of the Adjoint Functions for Sensitivity Analysis of Atmospheric Models[1]

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ABSTRACT

The adjoint functions for an atmospheric model are the solution to a system of equations derived from a differential form of the model's equations. The adjoint functions can be used to calculate efficiently the sensitivity of one of the model's results to variations in any of the model's parameters. This paper shows that the adjoint functions themselves can be interpreted as the sensitivity of a result to instantaneous perturbations of the model's dependent variables. This interpretation is illustrated for a radiative convective model, although the interpretation holds equally well for general circulation models. The adjoint functions are used to reveal the three time scales associated with 1) convective adjustment, 2) heat transfer between the atmosphere and space and 3) heat transfer between the ground and atmosphere. Calculating the eigenvalues and eigenvectors of the matrix of derivatives occurring in the set of adjoint equations reveals similar physical information without actually solving for the adjoint functions.

The sensitivities given by the adjoint functions are verified by comparison with sensitivities obtained directly from recalculations. Despite sharp changes in the adjoint functions arising from convective adjustment switching on and off during a diurnal cycle, a first-order numerical scheme to solve the adjoint equations gives agreement with direct recalculations to three significant figures. For a model with N time steps, this comparison has also shown that the adjoint method is at least $N/2$ times more efficient than recalculation. Such an efficient method of calculating the sensitivity of a simulated synoptic state to all previous synoptic states is valuable not only to identify the time scales of various physical processes, but also to assimilate data for initialization.

1. Introduction

Our understanding of atmospheric processes relies in part on the use of mathematical models to test the consequences of a collection of physical assumptions. As mathematical models increase in sophistication, though, the reasons for the results they give become less clear, making the results more difficult to interpret. A quantitative procedure to help interpret the results of a mathematical model is to perform a sensitivity analysis, i.e., to investigate how the results of the model change when parameters in the model are varied. Hall, Cacuci and Schlesinger (1982) have illustrated the use of an efficient method—the adjoint method—to perform such a sensitivity analysis for a radiative convective model.

This adjoint method involves solving a set of adjoint equations derived from a differential form of the model's equations. Each component of the solution to the adjoint equations is an adjoint function that uniquely corresponds to one of the model's dependent variables. The purpose of this paper is to show that each adjoint function can be interpreted as the sensitivity to instantaneous perturbations in the corresponding dependent variable. Furthermore these adjoint functions can be used to reveal the time scales associated with the most important physical processes in the model.

Throughout this paper, illustrative results are provided using the radiative convective model described in Section 2. Starting with the adjoint equations, Section 3 derives the physical interpretation of the adjoint functions. Section 4 illustrates this interpretation for the radiative convective model and discusses the physical processes that the adjoint functions reveal. In Section 5, equivalent physical information is deduced, without solving the adjoint equations, by examining the eigenvalues and eigenvectors associated with these equations. Section 6 verifies the adequacy of the numerical method used to solve the adjoint equations. This section also highlights the efficiency of obtaining sensitivities using adjoint functions instead of actually perturbing dependent variables and recalculating the results. The summary and conclusions are presented in Section 7.

2. The radiative convective model

The radiative convective model used in this work is the same as that described by Hall, Cacuci, and

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Schlesinger (1982). Note, though, that different options are now in effect so that clouds and convective adjustment switch on and off during a diurnal cycle.

The specific humidities in both atmospheric layers are now fixed so that the relative humidity becomes a function of temperature. The lower level relative humidity determines the fractional cloud cover. Diurnal insolation, corresponding to a perpetual equinox at 30° latitude, causes both convective adjustment of lapse rate and cloud cover to switch on and off periodically. The ground has a thermal capacity equivalent to a 0.1 m depth of water.

The model proceeds by integrating from time a to time b the equations

$$\left.\begin{array}{l} du_i/dt = f_i(\mathbf{u}, \boldsymbol{\alpha}) \\ u_i(a) = \alpha_i \end{array}\right\}, \quad i = 1, \ldots, I, \qquad (1)$$

where $I = 3$. The dependent variables u_1 and u_2 represent, respectively, the temperatures at the upper and lower atmospheric levels, and u_3 represents the temperature of the ground. The components of the vector $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_P)$ are the parameters in the model. The diurnal insolation causes some of these parameters to be explicit functions of time (e.g., angle of solar zenith).

The time integration starts at time a from arbitrary initial values of the dependent variables u_i. These initial values are the first I components of $\boldsymbol{\alpha}$. The integration proceeds until the final time b. For the results presented in this paper, the total time span of the model (i.e., $b - a$) is 200 days. Table 1 shows the values of some of the model variables during the last integration day. Convective adjustment occurs from 1500 to 0200, and clouds exist from 0800 to 1300 (all times are local standard). The temperature of the air at the earth's surface (the surface air temperature) is obtained by linearly extrapolating the temperatures of the two atmospheric layers (i.e., $-0.5u_1 + 1.5u_2$). The seasonal and regional conditions simulated by this model could be interpreted to correspond to late March at the same latitude as Florida.

3. Physical interpretation of the adjoint functions: Theory

Eq. (1) describes both radiative convective and general circulation models. For general circulation models, the vector of dependent variables $\mathbf{u}$ represents a spatially discrete form of the synoptic state, and $\mathbf{f}$ includes terms that represent spatial derivatives of $\mathbf{u}$. Although the number I of dependent variables is of practical importance, it does not affect the interpretation of the adjoint functions.

To highlight the physical interpretation of the ad-

TABLE 1. Values of variables during the last integration day of the radiative convective model.

Day:hour	Upper level atmospheric temperature (K)	Lower level atmospheric temperature (K)	Surface air temperature (K)	Ground temperature (K)	Convective adjustment	Fractional cloud cover
199:0000	226.69	275.17	299.41	301.82	yes	0
199:0100	226.66	275.14	299.38	300.16	yes	0
199:0200	226.64	275.10	299.34	298.65	no	0
199:0300	226.61	275.05	299.28	297.26	no	0
199:0400	226.58	275.00	299.21	295.98	no	0
199:0500	226.56	274.94	299.12	294.80	no	0
199:0600	226.53	274.86	299.03	293.71	no	0
199:0700	226.52	274.80	298.94	294.18	no	0
199:0800	226.51	274.74	298.86	296.23	no	0.00023
199:0900	226.51	274.74	298.86	299.59	no	0.00122
199:1000	226.51	274.70	298.80	303.84	no	0.00184
199:1100	226.52	274.72	298.83	308.47	no	0.00199
199:1200	226.52	274.77	298.90	312.96	no	0.00161
199:1300	226.53	274.85	299.01	316.80	no	0.00068
199:1400	226.53	274.95	299.16	319.54	no	0
199:1500	226.57	275.03	299.26	320.87	yes	0
199:1600	226.63	275.10	299.33	320.62	yes	0
199:1700	226.67	275.15	299.39	318.74	yes	0
199:1800	226.70	275.19	299.43	315.59	yes	0
199:1900	226.72	275.21	299.46	312.72	yes	0
199:2000	226.73	275.22	299.47	310.12	yes	0
199:2100	226.73	275.22	299.46	307.75	yes	0
199:2200	226.72	275.21	299.46	305.60	yes	0
199:2300	226.71	275.20	299.44	303.62	yes	0
200:0000	226.69	275.17	299.41	301.82	yes	0

joint functions, it is sufficient to consider results of the model that are of the form

$$R(\mathbf{u}, \alpha) = \int_a^b \mathbf{d} \cdot \mathbf{u}(t) r(t) dt. \quad (2)$$

In this equation, $\mathbf{d}$ is a constant vector, and $r(t)$ is a function of time. In general, the vector $\mathbf{d}$ represents the spatial and physical properties that characterize the result, and the function $r(t)$ defines either an averaging time period or an instantaneous time for the result. For example, with the radiative convective model, if $\mathbf{d}$ is the vector $(-0.5, 1.5, 0)$, then $\mathbf{d} \cdot \mathbf{u}$ is the surface air temperature. If, in addition, $r(t)$ is the Heaviside function $[(1/\tau)H(t-b+\tau)]$, then the result defined by (2) is the average surface air temperature from time $b-\tau$ to time b. On the other hand, if $r(t)$ is the Dirac delta function $\delta(t-c)$, then the result defined by (2) is the instantaneous surface air temperature at time c. Henceforth this result will be denoted by R_c.

Using the nominal values α^0 for the vector of parameters α in (1) gives the solution $\mathbf{u}^0$ for the dependent variables, and gives the corresponding result $R(\mathbf{u}^0, \alpha^0)$. Variations in the nominal values of the parameters can arise either from uncertainties in the parameters' values, or from tests of model sensitivity. If the variation in the nominal values of the parameters is $\mathbf{g}$, then the adjoint method gives, to first order in $\mathbf{g}$, the following expression for the variation in $R(\mathbf{u}^0, \alpha^0)$:

$$VR = \int_a^b \sum_{i=1}^{I} v_i \sum_{p=1}^{P} g_p\{(\partial/\partial\alpha_p)f_i\}(\mathbf{u}^0, \alpha^0)dt + \sum_{j=1}^{I} v_j(a)g_j. \quad (3)$$

[Here, and in the following, $\{\lambda\}(\mu)$ means "λ evaluated at μ." As explained in the reference, VR is the G-differential of R.] In this equation, $v_i(i = 1, \ldots, I)$ are the adjoint functions that satisfy the adjoint equations

$$\left.\begin{aligned} -dv_i/dt - \sum_{j=1}^{I} v_j\{(\partial/\partial u_i)f_j\}(\mathbf{u}^0, \alpha^0) = d_i r(t) \\ v_i(b) = 0 \end{aligned}\right\}, \quad (4)$$

where t is in the interval (a, b).

The adjoint functions $\mathbf{v}$ are independent of the parameter variations $\mathbf{g}$, so once (4) is solved, Eq. (3) immediately gives the value of VR for any combination of parameter variations. The adjoint functions, though, are dependent on the source term $d_i r(t)$ derived from the result functional (2). Thus for each result there is a different set of adjoint functions. For example, $\mathbf{v}^c$ denotes the adjoint functions associated with the result R_c.

Note from (3) that, if a variation occurs only in the initial value of the jth dependent variable [i.e., $\mathbf{g} = (0, \ldots, 0, g_j, 0, \ldots, 0)$, $j \leq I$], then Eq. (3) becomes $VR = v_j(a)g_j$. This implies that the value of the adjoint function v_j at the initial time is the sensitivity of the result to the initial value of the corresponding dependent variable u_j. The following shows the more general result that the value of the adjoint function v_j at an arbitrary time s is the sensitivity of the result to an impulsive perturbation at time s of the corresponding dependent variable u_j.

If the system is perturbed impulsively so that the solution $\mathbf{u}$ of (1) jumps by an amount γ at time s, then this perturbed solution satisfies the equations

$$\left.\begin{aligned} du_i/dt = f_i(\mathbf{u}, \alpha) + \delta(t-s)\gamma_i \\ u_i/(a) = \alpha_i \end{aligned}\right\}, \quad i = 1, \ldots, I. \quad (5)$$

For Eqs. (1) and (5) to describe the same nominal model, the elements of γ must be parameters with vanishing nominal values (i.e., $\gamma^0 = \mathbf{0}$). Then Eqs. (1) and (5) have the same nominal solution $\mathbf{u}^0$ and lead to the same adjoint solution $\mathbf{v}$, although a variation of $\mathbf{y}$ about $\gamma^0 = \mathbf{0}$ represents an impulsive perturbation to the nominal solution $\mathbf{u}^0$ at time s. Fig. 1 illustrates schematically the effect of such a perturbation; at times after s the perturbed solution differs from $\mathbf{u}^0$.

Deriving the adjoint equations for (5) uses the same procedure as deriving the adjoint equations for (1), except that $\mathbf{f} + \delta(t-s)\gamma$ replaces $\mathbf{f}$, (α, γ) replaces α, and $(\mathbf{g}, \mathbf{y})$ replaces $\mathbf{g}$. Introducing these replacements in (4) shows explicitly that the same adjoint equations arise respectively from (1) and (5). Introducing the same replacements in (3), though, introduces additional terms since (3) becomes

$$VR = \int_a^b \sum_{i=1}^{I} v_i\{[\sum_{p=1}^{P} g_p(\partial/\partial\alpha_p) + \sum_{j=1}^{I} y_j(\partial/\partial\gamma_j)] \times [f_i + \delta(t-s)\gamma_i]\}(\mathbf{u}^0, \alpha^0, \gamma^0)dt + \sum_{j=1}^{I} v_j(a)g_j.$$

Note that $(\partial/\partial\alpha_p)\gamma_i = 0$, $(\partial/\partial\gamma_j)f_i = 0$ and $(\partial/\partial\gamma_j)\gamma_i = \delta_{ij}$ (where δ_{ij} is the Kronecker delta), so the above expression reduces to

$$VR = \int_a^b \sum_{i=1}^{I} v_i \sum_{p=1}^{P} g_p(\partial/\partial\alpha_p)f_i dt + \sum_{j=1}^{I} v_j(s)y_j + \sum_{j=1}^{I} v_j(a)g_j.$$

Choosing $(\mathbf{g}, \mathbf{y}) = (0, 0, \ldots, 0, y_j, 0, \ldots, 0)$ (i.e., all parameters variations are zero except for the perturbation y_j at time $t = s$) gives

$$VR = v_j(s)y_j. \quad (6)$$

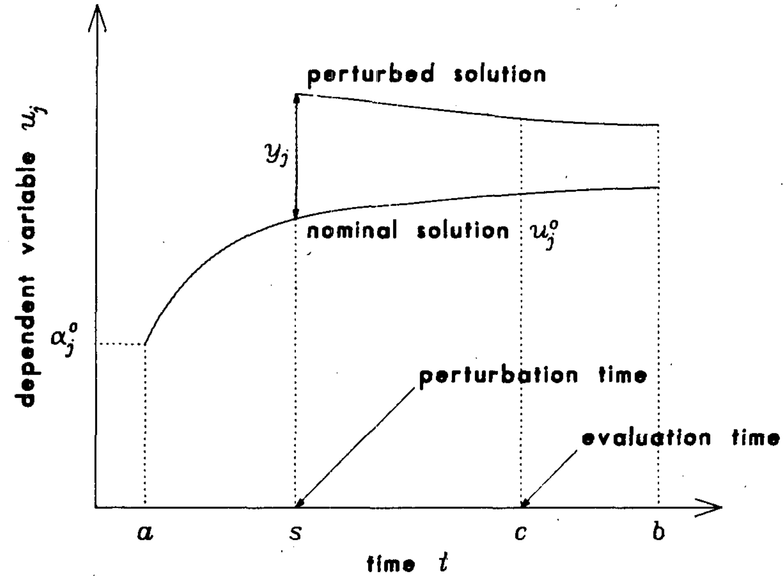

FIG. 1. Illustration of the effect of an impulsive perturbation y_j at time s on the nominal solution.

This equation shows that the adjoint function v_j at time s is the sensitivity of the result R to an impulsive perturbation y_j of the solution u_j^0 at time s.

4. Physical interpretation of the adjoint functions: Results

Using the radiative convective model, this section discusses the physical interpretation of the adjoint functions $v_1^c(s)$, $v_2^c(s)$ and $v_3^c(s)$; these are associated with the result R_c, i.e., the surface air temperature at time c. As discussed in Section 3, the explicit form of R_c is $\mathbf{d} \cdot \mathbf{u}(c)$, where $\mathbf{d}$ is the vector $(-0.5, 1.5, 0)$.

The three graphs in Fig. 2 show respectively the time-dependent behavior of $v_1^c(s)$, $v_2^c(s)$ and $v_3^c(s)$. The vertical axes measure the values of the adjoint functions. Since the value of the adjoint function $v_i^c(s)$ is the sensitivity of R_c to a perturbation in the dependent variable u_i at time s, these axes are labeled "sensitivity." The longer horizontal axes measure the value of s; each of these axes labels indicate the perturbation time of the dependent variable that corresponds to the adjoint function. The remaining axes measure the value of c, so these axes are labeled "evaluation time of surface air temperature."

The value of c ranges from day 199 to day 200 in hourly intervals. Thus the surface air temperature is evaluated at 25 different times, so that Fig. 2 presents 25 different sets of adjoint functions. Although the perturbation can occur at times $0 \leqslant s \leqslant 200$ days, the range of s in Fig. 2 is only for 196 days $\leqslant s \leqslant 200$ days. This is to highlight the detailed transient behavior of the adjoint functions.

When the perturbation time is greater than the evaluation time (i.e., $s > c$), then the sensitivity must be zero. The flat triangular areas at the bottom of each graph in Fig. 2 illustrate this. When the perturbation time equals the evaluation time (i.e., $s = c$), then a perturbation y_j of the dependent variable $u_j(s)$ is also the perturbation of $u_j(c)$. Since the surface air temperature R_c is equal to $\mathbf{d} \cdot \mathbf{u}^0(c)$, the variation in this result caused by y_j is $d_j y_j$. Therefore when $s = c$ the sensitivity is d_j; Fig. 2 illustrates this. Perturbation and evaluation times are equal adjacent to the hypotenuse of each of the flat triangular areas mentioned previously: as expected, adjacent to each hypotenuse there is a ridge of constant sensitivity equal to the respective component $(-0.5, 1.5$, or $0)$ of $\mathbf{d}$.

When the perturbation time is less than the evaluation time, the sensitivity depends on the radiative and convective processes that occur between these two times. For example, in this model, the convective adjustment process reacts to a perturbation of either the upper or lower level air temperature more quickly than do radiation processes. Therefore, the sensitivity of the surface air temperature to such a perturbation depends strongly on whether or not convective adjustment has occurred between perturbation time and evaluation time. Fig. 2 illustrates this phenomenon: sharp changes in the sensitivity occur both at the evaluation time 199:1500 (i.e., the 15th hour of day 199) when convective adjustment switches on, and at the perturbation time 199:0200 when convective adjustment switches off. The sharpness of these changes is a reflection of the fact that full convective adjustment occurs every time step in this model.

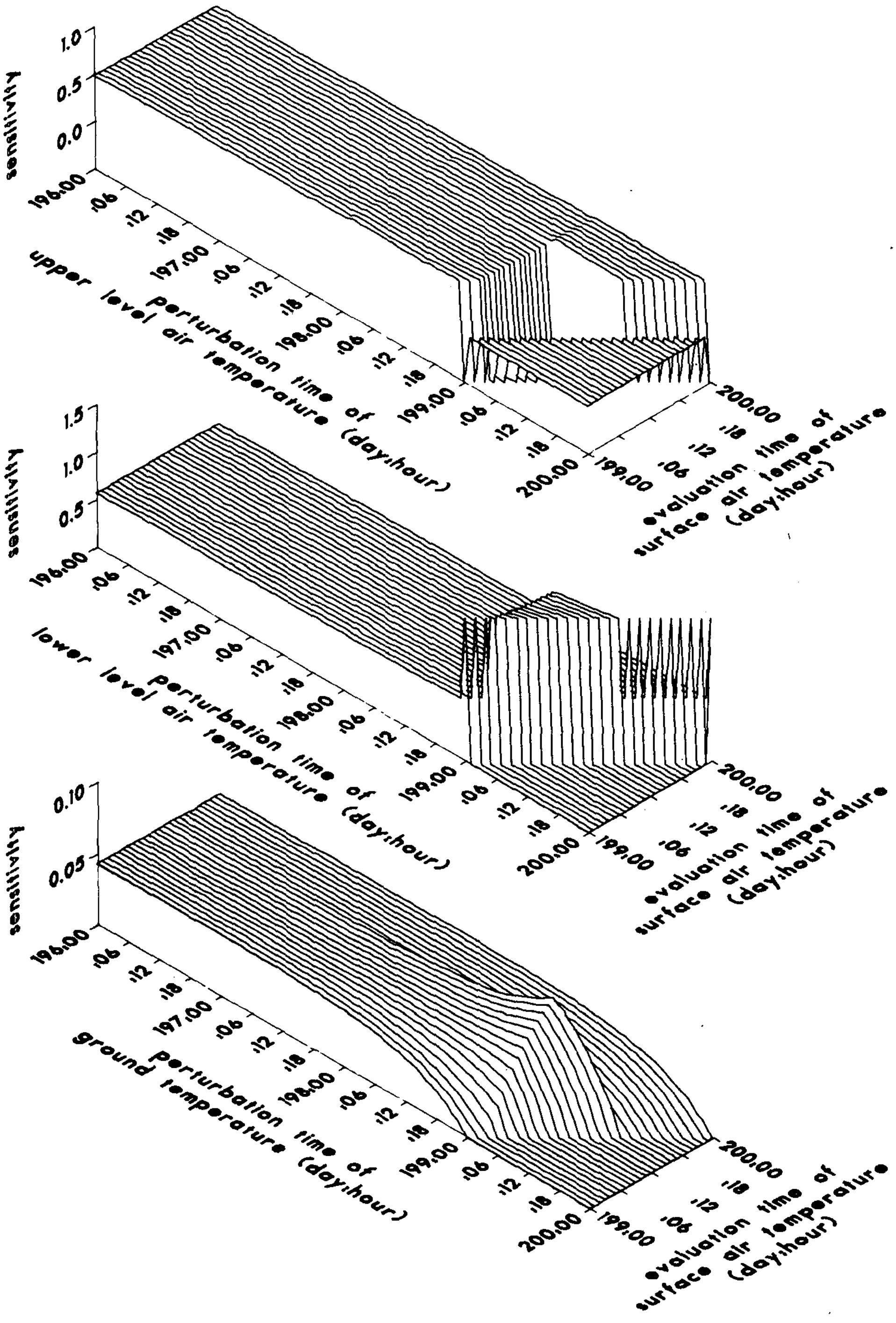

FIG. 2. Numerical adjoint solution for the radiative convective model from day 196 to day 200.

For perturbation times before 199:0000, the sensitivities in the uppermost two graphs of Fig. 2 each have a constant value of ~0.5. This value is explained by considering the effects of both convective adjustment and the relative values of the heat capacities of the atmospheric layers and the ground. Each atmospheric layer has a pressure thickness $\Delta p = 4 \times 10^4$ Pa, so the heat capacity of c_a of each is approximately $c_p\Delta p/g = 4.1 \times 10^6$ J K^{-1} m^{-2} (where c_p is the specific heat of dry air at constant pressure and g is the acceleration of gravity). On the other hand, the ground in this model is equivalent to a 0.1 m depth of water, so its heat capacity c_g is 4.2×10^5 J K^{-1} m^{-2}. Note that c_g is an order of magnitude smaller than c_a. Since convective adjustment tends to maintain a constant temperature difference between both atmospheric layers (i.e., $\delta u_1 = \delta u_2$), neglecting the heat capacity of the ground means that a temperature perturbation y of either atmospheric layer will be equally divided between both (i.e., $\delta u_1 = \delta u_2 = 0.5y$). Therefore the corresponding change in surface air temperature (i.e., $-0.5\delta u_1 + 1.5\delta u_2$) is $0.5y$. It follows that the sensitivity of surface air temperature to perturbations in the temperature of either atmospheric layer is 0.5.

As the lowest graph in Fig. 2 shows, the sensitivity to perturbations of the ground temperature varies more smoothly as a function of perturbation time than the sensitivities to perturbations of the air temperature. This smooth behavior reflects the effect of the heat transfer mechanism from the ground to the atmosphere. The rate Q of this heat transfer is $C_s[u_3 - (-0.5u_1 + 1.5u_2)] + \sigma u_3^4$, where C_s is the prescribed heat transfer coefficient 4.9 W m^{-2} K^{-1}, and σ is the Stefan-Boltzmann constant. Perturbing the ground temperature from its nominal value u_3^0 by an amount y at time s gives rise to a time-dependent perturbation $\delta u_3(t)$. When the heat capacity c_a is much larger than c_g, the time evolution of δu_3 is mainly governed by the change δQ in Q, with u_1 and u_2 treated as constant. In this case δu_3 evolves according to

$$\left.\begin{aligned} c_g\delta\dot{u}_3 &= -\delta Q = -[C_s + 4\sigma(u_3^0)^3]\delta u_3 + \mathrm{O}[(\delta u_3)^2] \\ \delta u_3(s) &= y \end{aligned}\right\},$$

where the dot denotes differentiation with respect to t. Solving these equations shows that perturbing the ground temperature by y at time s gradually heats the lower level air at a rate δQ, where

$$\delta Q = c_g y \exp\{(s - t)/[c_g/C_s + 4\sigma(u_3^0)^3]\}. \quad (7)$$

Thus an instantaneous perturbation in the ground temperature has the same effect as a series of perturbations in lower level air temperature over a time period of approximately $c_g/[C_s + 4\sigma(u_3^0)^3]$. The results in Table 1 show that the ground temperature u_3^0 is approximately 305 K, so this time period is ~11 h. Fig. 2 illustrates this conclusion: the lowest graph (ground temperature) is similar to the middle graph (lower level air temperature) smoothed over a perturbation time of approximately half a day.

Comparing each of the uppermost two graphs in Fig. 2 to the lowest graph shows that the sensitivity to perturbations of the ground temperature is approximately an order of magnitude smaller than the sensitivity to perturbations of the air temperature. This is a consequence of the relative magnitudes of the heat capacities of the ground and atmospheric layers. Since c_g is much less than c_a, most of the heat $c_g y$ associated with a perturbation y of the ground temperature will transfer to the atmosphere, and, as previously discussed, this transfer will take place within approximately 11 h. As before, convective adjustment will distribute this heat as a uniform temperature change in the atmosphere while conserving energy (i.e., $c_a\delta u_1 = c_a\delta u_2 = 0.5c_g y$), so the resulting change in surface air temperature (i.e., $-0.5\delta u_1 + 1.5\delta u_2$) is $0.5(c_g/c_a)y$. Therefore the sensitivity of surface air temperature to perturbations in the ground temperature is $0.5(c_g/c_a) \approx 0.05$.

The three graphs in Fig. 3 show the behavior of the adjoint function over the entire time range $0 \leqslant s \leqslant 200$ days. These graphs show that all the sensitivities gradually diminish with decreasing perturbation time. The characteristic time governing this behavior can be understood by considering the time evolution of a temperature perturbation δu of a blackbody with temperature u^0 subject to incident radiation. The temperature perturbation $\delta u(t)$ resulting from the initial perturbation y at time s satisfies the equation

$$\left.\begin{aligned} c_b\delta\dot{u} &= -4\sigma(u^0)^3\delta u + \mathrm{O}[(\delta u)^2] \\ \delta u(s) &= y \end{aligned}\right\},$$

where c_b is the heat capacity of the black body. Thus at time c, δu is given by

$$\delta u(c) = y \exp\{-(c - s)/[c_b/4\sigma(u^0)^3]\}.$$

Applying this expression to the model atmosphere with heat capacity $c_b = 2c_a = 8.2 \times 10^6$ J K^{-1} m^{-2} and nominal temperature $u^0 = (u_1^0 + u_2^0)/2 \approx 251$ K indicates that the sensitivities should diminish with an exponential time constant of ~26 days. This corresponds to the behavior seen in Fig. 3.

5. Interpretation of eigenvalues and eigenvectors associated with the adjoint equations

The adjoint equations (4) in matrix form are

$$\left.\begin{aligned} \dot{\mathbf{v}} + \mathbf{A}(t)\mathbf{v} &= -\mathbf{d}\delta(t - c) \\ \mathbf{v}(b) &= 0 \end{aligned}\right\},$$

where the dot denotes differentiation with respect to t, and where

$$A_{ij}(t) = \{(\partial/\partial u_i)f_j\}(\mathbf{u}^0, \alpha^0), \quad i, j = 1, \ldots, I.$$

The matrix $\mathbf{X}(t)$ is now defined to consist of the normalized column eigenvectors of $\mathbf{A}(t)$, i.e., $\mathbf{X} = (\mathbf{x}^1, \ldots, \mathbf{x}^I)$ where $\mathbf{A}\mathbf{x}^k = \lambda_k\mathbf{x}^k$ and $\mathbf{x}^k \cdot \mathbf{x}^k = 1$, $k = 1, \ldots, I$. Provided the eigenvectors of $\mathbf{A}$ are linearly independent, the use of the linear transformation $\mathbf{v}(t) = \mathbf{X}(t)\mathbf{w}(t)$ in the above equations leads to

$$\left.\begin{aligned} \dot{\mathbf{w}} + \mathbf{X}^{-1}\dot{\mathbf{X}}\mathbf{w} + \mathbf{D}\mathbf{w} &= -\mathbf{X}^{-1}\mathbf{d}\delta(t - c) \\ \mathbf{w}(b) &= 0 \end{aligned}\right\}, \quad (8)$$

where the diagonal matrix $\mathbf{D}$ of eigenvalues is given in terms of the Kronecker delta by

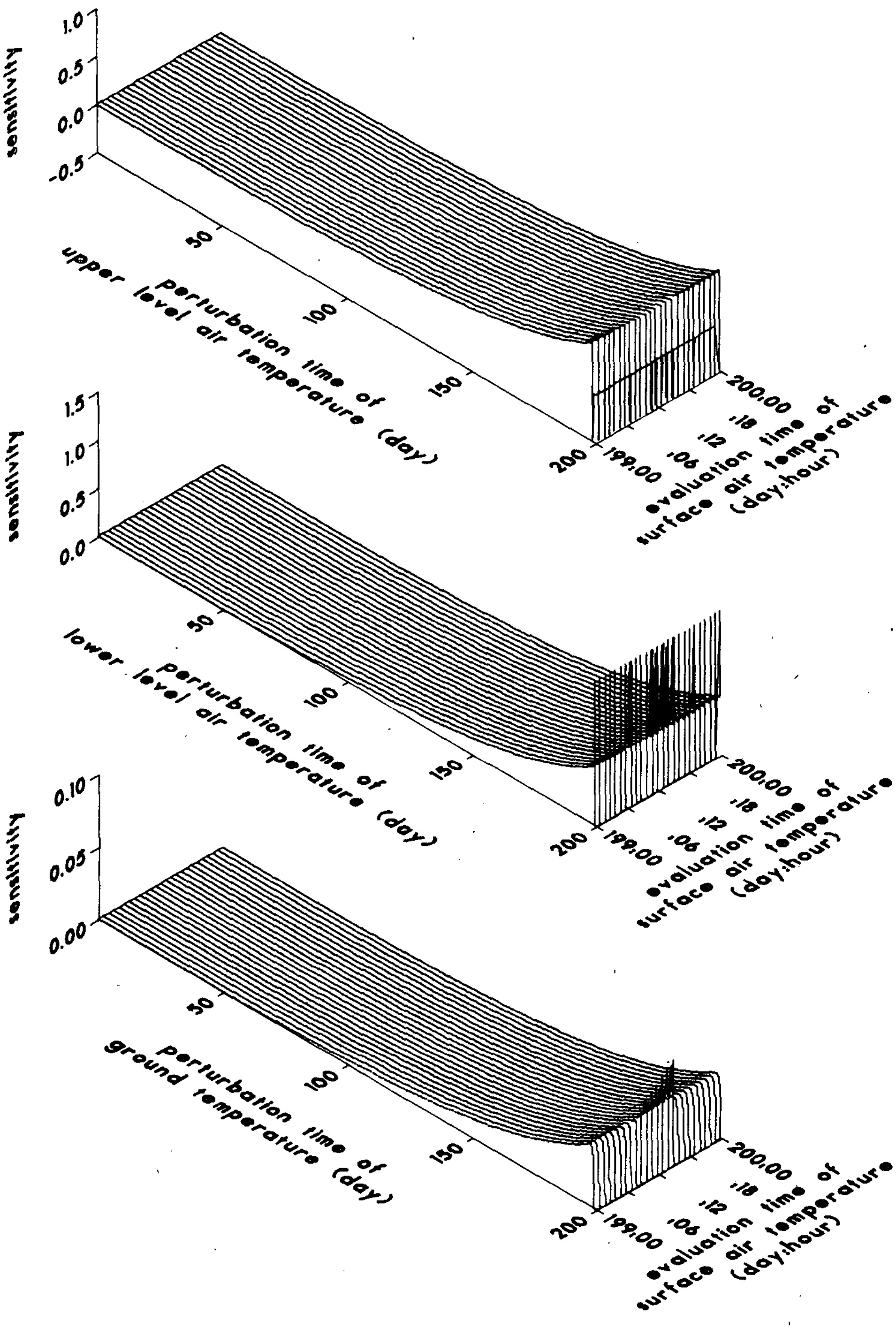

FIG. 3. Numerical adjoint solution for the radiative convective model from day 0 to day 200.

$$D_{ij}(t) = \delta_{ij}\lambda_j(t).$$

The physical significance of the eigenvectors of $\mathbf{A}$ can be analyzed by choosing the vector $\mathbf{d}$ to be the kth eigenvector of $\mathbf{A}$ evaluated at $t = c$, i.e., $\mathbf{d} = \mathbf{x}^k(c)$. Substituting this value in (8) gives the equations

$$\left.\begin{aligned} \dot{w}_i + \lambda_i w_i &= -\delta_{ik}\delta(t - c) \\ &\quad - \sum_{j=1}^{I} (\mathbf{X}^{-1}\dot{\mathbf{X}})_{ij} w_j \\ w_i(b) &= 0 \end{aligned}\right\}, \quad i = 1, \ldots, I. \tag{9}$$

Treating the right side of (9) as an inhomogeneous source term, and solving this equation using the integrating factor method gives

$$w_i(t) = -\int_b^t \exp\left[\int_t^{t'} \lambda_i(t'')dt''\right] \sum_{j=1}^{I} w_j(t')\{(\mathbf{X}^{-1}\dot{\mathbf{X}})_{ij}\}(t')dt' + \delta_{ik} \exp\left[\int_t^c \lambda_i(t'')dt''\right], \quad t < c. \quad (10)$$

This equation can be solved iteratively.

The initial iterate w_i^0 is chosen to be

$$w_i^0(t) = H(c - t)\delta_{ik} \exp\left[\int_t^c \lambda_i(t'')dt''\right], \quad (11)$$

where H is the Heaviside function. The fractional difference between the next iterate $\mathbf{w}^1$ and the initial iterate $\mathbf{w}^0$ can be obtained by substituting (11) in the right side of (10) and evaluating the resulting expression using the mean value theorem. This gives

$$[w_k^1(t) - w_k^0(t)]/w_k^0(t) = (c - t)\{(\mathbf{X}^{-1}\dot{\mathbf{X}})_{kk}\}(\tau_1), \quad (12)$$

$$\begin{aligned}[w_i^1(t) - w_i^0(t)]/w_k^0(t) &= [\lambda_i(\tau_2) - \lambda_k(\tau_3)]^{-1}\{(\mathbf{X}^{-1}\dot{\mathbf{X}})_{ik}\}(\tau_4) \\ &\times (\exp\{[\lambda_i(\tau_2) - \lambda_k(\tau_5)](c - t)\} \\ &- \exp\{[\lambda_k(\tau_3) - \lambda_k(\tau_5)](c - t)\}), \quad i \neq k, \quad (13)\end{aligned}$$

where τ_n, $n = 1, 2, \ldots, 5$, are times somewhere in the range $t \leqslant \tau_n \leqslant c$. Provided the magnitude of the right side of both (12) and (13) is much less than unity, the first iterate $\mathbf{w}^0$ given by (11) is an adequate solution to (10). Further use of the linear transformation $\mathbf{v}(t) = \mathbf{X}(t)\mathbf{w}(t)$ on (11) then implies that the adjoint solution $\mathbf{v}(t)$ associated with the result,

$$R_k = \mathbf{x}^k(c) \cdot \mathbf{u}(c), \quad (14)$$

is

$$\mathbf{v}^k(t) = \mathbf{x}^k(t)H(c - t) \exp[\bar{\lambda}_k(c - t)], \quad (15)$$

where

$$\bar{\lambda}_k = \int_t^c \lambda_k(t'')dt''/(c - t). \quad (16)$$

Eqs. (14), (15) and (16) show that each eigenvector $\mathbf{x}^k$ of $\mathbf{A}(c)$ defines a result (14) whose sensitivity (15) to previous states is governed solely by the eigenvalue λ_k. Furthermore, the mean value (16) of this eigenvalue determines the exponential rate at which this sensitivity changes.

The practical usefulness of the preceding mathematical discussion is now illustrated by using the radiative convective model with the value of c taken as midnight on the 200th day after the start of time integration of the model, i.e., $c = a + 200{:}0000$. At this value of c, convective adjustment is occurring and the unphysical transients in the model have decayed. In view of (14), the matrix $\mathbf{X}(t)$ of eigenvectors of $\mathbf{A}(t)$ needs to be evaluated at time c. The matrix $\mathbf{A}(c)$ is

$$\mathbf{A}(c) = \begin{pmatrix} -0.587 & 0.501 & -0.0291 \\ 0.480 & -0.418 & 0.0923 \\ 0.00308 & 0.00374 & -0.0855 \end{pmatrix} \text{h}^{-1},$$

giving the matrix of normalized column eigenvectors,

$$\mathbf{X}(c) = \begin{pmatrix} 0.772 & 0.648 & -0.405 \\ -0.636 & 0.759 & -0.353 \\ 4.84 \times 10^{-13} & 0.0576 & 0.844 \end{pmatrix}. \quad (17)$$

Recall that (15) is valid provided the magnitude of the right side of both (12) and (13) is much less than unity. Investigation of these magnitudes requires evaluation of the matrices $\mathbf{D}(\tau)$ and $\{\mathbf{X}^{-1}\dot{\mathbf{X}}\}(\tau)$ at times τ anywhere in the range $t \leqslant \tau \leqslant c$. At $\tau = c$, these matrices are

$$\mathbf{D}(\tau) = \begin{pmatrix} -1.000 & 0 & 0 \\ 0 & -1.53 \times 10^{-3} & 0 \\ 0 & 0 & -8.86 \times 10^{-2} \end{pmatrix} \text{h}^{-1}, \quad (18)$$

$$\{\mathbf{X}^{-1}\dot{\mathbf{X}}\}(\tau) = \begin{pmatrix} 2.28 \times 10^{-14} & -3.88 \times 10^{-6} & 9.03 \times 10^{-5} \\ -1.72 \times 10^{-12} & 8.29 \times 10^{-5} & -5.70 \times 10^{-3} \\ -8.38 \times 10^{-14} & 1.71 \times 10^{-4} & -2.72 \times 10^{-3} \end{pmatrix} \text{h}^{-1}. \quad (19)$$

Evaluation of the matrices $\mathbf{D}$ and $\mathbf{X}^{-1}\mathbf{X}$ at several additional values of t shows that in the range $c_{-10} \leqslant \tau \leqslant c$, where $c_{-10} = c - 10$ h $= a + 199{:}1400$, the eigenvalues appearing in $\mathbf{D}(\tau)$ vary by only a few percent and the elements of $\{\mathbf{X}^{-1}\dot{\mathbf{X}}\}(\tau)$ remain at the same order of magnitude. But since the right side of both (12) and (13) involves τ_n in the range $t \leqslant \tau_n \leqslant c$, use of (18) and (19) imposes on t the lower bound $t \geqslant c_{-10}$. (Note that, as Table 1 shows, this is the range where convective adjustment is occurring.)

For $k = 1$, the quantities appearing on the right sides of (12) and (13) are, as obtained using (18) and (19):

$$|\{(\mathbf{X}^{-1}\dot{\mathbf{X}})_{11}\}(\tau_1)| \sim 10^{-14} \text{ h}^{-1},$$

$$|\lambda_i(\tau_2) - \lambda_1(\tau_3)| \sim 1 \text{ h}^{-1}, \quad i = 2, 3,$$

$$|\{(\mathbf{X}^{-1}\dot{\mathbf{X}})_{i1}\}(\tau_4)| < 10^{-12} \text{ h}^{-1}, \quad i = 2, 3,$$

$$\exp\{[\lambda_i(\tau_2) - \lambda_1(\tau_5)](c - t)\} \sim \exp\{(1\ \mathrm{h}^{-1})(c - t)\}, \quad i = 2, 3,$$

$$\exp\{[\lambda_1(\tau_3) - \lambda_1(\tau_5)](c - t)\} \sim 1,$$

for $c_{-10} \leqslant \tau_n \leqslant c$, $n = 1, 2, \ldots, 5$. Therefore, for $c_{-10} \leqslant t \leqslant c$, the right side of (12) has a magnitude less than 10^{-13}, and the right side of (13) has a magnitude less than 10^{-8}. Thus Eq. (15) is valid for $k = 1$, and for $t = s$ the sensitivity of the result $R_1 = \mathbf{x}^1(c)\cdot\mathbf{u}(c)$ where $\mathbf{x}^1(c) = (0.772, -0.636, 4.84 \times 10^{-13})$ decays as $\exp[(c - s)\bar{\lambda}_1]$ with $1/\bar{\lambda}_1 = -1.000$ h.

The physical significance of $R_1 = \mathbf{x}^1\cdot\mathbf{u}$ can be deduced by examination of the above components of $\mathbf{x}^1$. The last component of $\mathbf{x}^1$ is effectively zero, indicating that R_1 is independent of the ground temperature. The first and second components of $\mathbf{x}^1$ are approximately equal and opposite, indicating that R_1 is related to the difference between the two atmospheric temperatures, i.e., R_1 is related to the lapse rate. In this model, the critical lapse rate for convective adjustment occurs when $u_1 = 0.824u_2$. Note that R_1 can be written $R_1 = 0.772(u_1 - 0.824u_2)$; therefore R_1 measures the departure of the lapse rate from its critical value for convective adjustment. Thus, it can be concluded that convective adjustment of lapse rate takes place on a time scale of $|1/\bar{\lambda}_1| = 1.000$ h. Since the time step in this model is one hour, this conclusion agrees with the observation made in Section 4 that convective adjustment occurs every time step in this model.

A similar line of reasoning to that above can be used to deduce the physical significance of $\mathbf{x}^k$ and λ_k when $k = 2$ and $k = 3$. Evaluation of (12) and (13) shows that (15) is valid for both $k = 2$ and $k = 3$. The components of $\mathbf{x}^2 = (0.648, 0.759, 0.0576)$ are approximately in the ratio $c_a:c_a:c_g$ (recall that $c_a \approx 4.1 \times 10^6$ J k^{-1} m^{-2} is the heat capacity of each atmospheric layer, and $c_g \approx 4.2 \times 10^5$ J K^{-1} m^{-2} is the heat capacity of the ground). Therefore $R_2 = \mathbf{x}^2\cdot\mathbf{u}$ is a measure of the total heat energy of both the ground and the atmosphere. Since (15) is valid, it can be concluded that changes in the total heat energy of the ground and atmosphere take place on a time scale of $|1/\bar{\lambda}_2| = 27$ days. Since in this model most of the heat resides in the atmosphere, this conclusion agrees with the conclusion in Section 4 that perturbations to atmospheric temperature decay on a time scale of 28 days.

The components of $\mathbf{x}^3 = (-0.405, -0.353, 0.844)$ are in the ratio -0.48:-0.42:1.00. Thus $R_3 = \mathbf{x}^3\cdot\mathbf{u}$ indicates the difference between the ground temperature and an average atmospheric temperature. Again since (15) is valid, it can be concluded that changes in this difference take place on a time scale of $|1/\bar{\lambda}_3| = 11$ h. This conclusion agrees with the conclusion in Section 4 that a perturbation of the ground temperature diminishes because of heat transfer to the atmosphere on a time scale of 11 h.

6. Numerical efficiency and accuracy

The dependent variables $\mathbf{u}$ have been obtained numerically using a first-order finite difference approximation for Eq. (1). This gives

$$\mathbf{u}^{m+1} = \mathbf{u}^m + \Delta t\mathbf{f}(\mathbf{u}^m, \alpha^0),$$

where $\mathbf{u}^m$ is the approximate value of $\mathbf{u}$ at time $t^m = a + m\Delta t$, and the time step Δt is 1 h. The numerical adjoint solution has been obtained similarly, leading to the equation

$$\mathbf{v}^{m-1} = \mathbf{v}^m - \Delta t\mathbf{A}(t^m)\mathbf{v}^m - \int_{t^{m-1}}^{t^m} \mathbf{d}r(t)dt,$$

where the matrix $\mathbf{A}$ of derivatives is obtained using

$$A_{ij}(t^m) = \{\partial f_j/\partial u_i\}(\mathbf{u}^0, \alpha^0) \approx (1/\epsilon)\{f_j(u_1^0, \ldots, u_i + \epsilon, \ldots, u_I^0, \alpha^0) - f_j(\mathbf{u}^0, \alpha^0)\}(t^m),$$

with $\epsilon = 0.01f_i(\mathbf{u}^0, \alpha^0)\Delta t$.

The adequacy of this numerical method to solve the adjoint equations has been verified using Eq. (6). Each graph in Fig. 1 actually plots the function v_j^m superimposed on sensitivities obtained by recalculations. These recalculations involve actually perturbing the numerical solution u_j^m by y_j, recalculating each result R_c, and dividing the difference between the recalculated and original results by y_j. For $y_j = 0.01f_j(\mathbf{u}^0, \alpha^0)\Delta t$, the sensitivities obtained by recalculations agree with the numerical values of the adjoint function to three significant figures. Because of this close agreement, the two plots in each of the three graphs in Fig. 1 appear to be identical.

The calculations involved in obtaining Fig. 1 highlight the numerical advantages of the adjoint method over recalculation. In the radiative convective model, most of the computation consists of evaluating the function $f(\mathbf{u}, \alpha)$ at each time step. Since there is a 1 h time step, the numerical solution requires 96 evaluations of $\mathbf{f}$ during days 196–200. The perturbation to u_j^m occurs at the mth time step, and recalculation of the solution occurs for all time steps after the mth. For three different values of j and 96 different values of m, these recalculations require $3 \times 96 \times (96 + 1)/2 = 13\,968$ evaluations of $\mathbf{f}$. To obtain the adjoint function $\mathbf{v}$ requires values of $\partial\mathbf{f}/\partial u_j$ at each time step. Calculating these derivatives for three different values of j using a finite difference expression requires $3 \times 96 = 288$ evaluations of $\mathbf{f}$. In general, using the adjoint method to calculate sensitivity to perturbations in dependent variables is more efficient than recalculation by a factor of half the number of time steps.

7. Summary and conclusions

The adjoint method of sensitivity analysis for an atmospheric model involves solving a set of adjoint equations derived from a differential form of the model's equations. Then, the sensitivity of a result of the model to any of the model's parameters can be obtained efficiently using the adjoint solution. But, as this paper has shown, the adjoint solution itself has a physical interpretation: each adjoint function v_i at time s is the sensitivity of the result to an instantaneous perturbation of the dependent variable u_i at time s. This interpretation holds for any model described by first-order equations of time evolution, including general circulation models.

Analysis of numerical solutions to the adjoint equations for a radiative convective model has revealed three characteristic time scales associated with different physical processes: convective adjustment reacts instantaneously, heat transfer between the atmosphere and space occurs with a characteristic time of 27 days, and heat transfer between the ground and the atmosphere occurs with a characteristic time of 11 h. Calculating the eigenvalues and eigenvectors of the matrix of derivatives occuring in the set of adjoint equations has revealed similar physical information without actually solving for the adjoint functions; the eigenvalues have been identified with the characteristic times, and the respective eigenvectors have been identified with the associated physical processes.

Sensitivities to instantaneous perturbations of the dependent variables have been obtained directly (i.e., by impulsively varying the value of a dependent variable and recalculating the result). Sensitivities obtained in this way agree within three significant figures to sensitivities obtained using the adjoint method. This agreement shows that the first-order numerical method of solving the adjoint equations accurately determines the adjoint solution including the sharp changes caused by convective adjustment. For a model with N time steps, this comparison has also shown that the adjoint method is at least $N/2$ times more efficient at calculating sensitivity to the N previous atmospheric states than recalculation.

This work illustrates that the adjoint method is a powerful and efficient way of analyzing the effects of physical processes in an atmospheric model. Although the results presented were for a radiative convective model, the physical interpretation of the adjoint function will hold for general circulation models. The adjoint approach promises to be particularly useful where the time scales of various physical processes need to be known, or where four-dimensional data initialization is of interest.

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