*Atmósfera (1994), 7, pp. 75-86*

*SHORT CONTRIBUTION*

# Reply to the paper by D. G. Cacuci and M. E. Schlesinger

YURI N. SKIBA[1]

*Institute of Numerical Mathematics, Russian Academy of Sciences, Moscow*
[1] *Present address: Centro de Ciencias de la Atmósfera, UNAM*
*Circuito Exterior, CU, 04510, México, D. F., México*

(Manuscript received April 19, 1993; accepted in final form June 18, 1993)

RESUMEN

Se dan explicaciones para demostrar la exactitud del enfoque del método adjunto usado por Marchuk y Skiba (1992). Varias observaciones también son hechas sobre el desarrollo histórico de los métodos adjuntos y su aplicación en los trabajos de Cacuci (1981), Cacuci y Schlesinger (1993), Hall (1986), Hall y Cacuci (1983) y Hall *et al.* (1982).

SUMMARY

The correctness of the adjoint approach used in Marchuk and Skiba (1992) is demonstrated. Remarks are made on the historical development of the adjoint methods and its application in the works by Cacuci (1981), Cacuci and Schlesinger (1993), Hall (1986), Hall and Cacuci (1983) and Hall *et al.* (1982).

## On the validity of the Marchuk and Skiba (1992) adjoint model

I now want to correct two accidental errors made by me in the Marchuk and Skiba (1992) text (henceforth, "MS92"). Unfortunately these errors resulted in incorrect conclusions by Cacuci and Schlesinger (1993) (henceforth, "CS93") on the invalidity of formula (25), and hence, the adjoint model (14)–(20) obtained in MS92.

Two main formulae based on integration by parts and applying Green's formula are used in MS92 to obtain (25):

$$\int_{D_2} T^* \mu \nabla_2 \cdot \nabla_2 T dD = \int_{\Omega} T^* \mu \frac{\partial T}{\partial n} dS$$

$$- \int_{\Omega} T\mu \frac{\partial T^*}{\partial n} dS + \int_{D_2} T\mu \nabla_2 \cdot \nabla_2 \, T^* dD \tag{1}$$

$$\int_{D_1 U D_2} T^* \nabla \cdot (\vec{u}T) dD = \int_{\partial D_1 U \partial D_2} u_n T T^* dS - \int_{D_1 U D_2} T \nabla \cdot (\vec{u}T^*) dD \tag{2}$$

where $D_1$ is the atmosphere domain (spherical layer) with the boundary $\partial D_1$ consisting only of the surface $z = h_1$ and the parts of the surface $z = 0$; $D_2$ is the oceanic domain with the boundary $\partial D_2$ being the union of the lateral boundary $\Omega$ and the parts of the spherical surfaces $z = 0$ and $z = -h_2$; $\nabla_2$ is the 2-dimensional gradient written in the spherical coordinates $(\lambda, \vartheta)$; $\nabla_2 \cdot \nabla_2$ is the scalar product of the gradients; $u_n$ is the component of the velocity vector $\vec{u}$ in the direction of the outward normal $\vec{n}$ to the boundary surface $\partial D_1 \; U \; \partial D_2$ (the union of $\partial D_1$ and $\partial D_2$); and $\frac{\partial}{\partial n}$ is the derivative along the normal $\vec{n}$. In the model, the ocean lateral boundary $\Omega$ is composed only of the parts parallel to either the surface $\lambda =$ Const or the surface $\vartheta =$ Const. Therefore the normal component $u_n$ of $\vec{u}$ on $\Omega$ always coincides with either $\pm u$ or $\pm v$ components of $\vec{u}$ along $\lambda$ or $\vartheta$. Similarly, the derivative $\frac{\partial}{\partial n}$ on $\Omega$ coincides with either $\pm\frac{\partial}{\partial \lambda}$ or $\pm\frac{\partial}{\partial \vartheta}$.

*Mistake 1.* In fact, $\mu = \mu(z, \; t)$. The form $\mu(x, \; t)$ is the misprint made in the MS92 text (see Marchuk and Skiba, 1990, p. 336, where $\mu = \mu(z)$). As was mentioned above, the geometry of the ocean lateral boundary $\Omega$ and independence $\mu(z, \; t)$ of $\lambda$ and $\vartheta$ enable us to use in MS93 the form $\mu\nabla_2 \cdot \nabla_2 T$ instead of the common form $\nabla_2 \cdot (\mu\nabla_2 T)$ (used in Marchuk and Skiba, 1976, 1978, and Skiba, 1980). Thus the boundary conditions (5) and (18) of MS92 lead to the zero values of the first two integrals over $\Omega$ in the right–hand side of (1).

*Mistake 2.* The vertical component $w$ of the wind and current velocities in MS92 satisfy the condition $w = 0$ (or $u_n = 0$) at the parts of the boundary $\partial D_1 U \partial D_2$ that coincide with the surfaces $z = h_1$, $z = 0$ and $z = -h_2$. These conditions (given by Marchuk and Skiba, 1990, p. 336, just after the continuity equation) are accidentally overlooked and absent in the MS92 text. In fact, the normal component $u_n$ is zero everywhere on the boundary $\partial D_1 U \partial D_2$. As a result, the first integral in the right–hand side of (2) is zero.

Section 4.1 of CS93 shows that Cacuci and Schlesinger do not separate two completely different moments: 1) any initial condition for the ajoint problem (14)–(20) given in MS92, must be put at the moment $T = \bar{t}$ (not at the moment $t = 0$) so as to obtain a well posed adjoint problem; 2) the function $T^*(x, \; \bar{t})$ in the initial condition (15) in MS92 was specially taken as zero so as to obtain

$$\int_D \alpha(z)T^*(x, \; \bar{t})T(x, \; \bar{t})dD = 0 \tag{3}$$

that allows us to eliminate this term from the formula (25).

We emphasize that the orography is not taken into account in our linear model. These arguments show the validity of the formula (25) and the adjoint problem (14)–(20) in MS92, and show that within the model limits mentioned above, all the conclusions made by Cacuci and Schlesinger (1993) are incorrect.

## 2. Remarks on the adjoint method development

It should be pointed out that the model considered in MS92 was linear. Therefore it comes as no surprise that the references given in MS92 do not go into the perturbation theory for nonlinear problem. However, since the priority question on applying the adjoint approach in the nonlinear problem sensitivity study was raised in CS93, I would like to remind that the adjoint method in the perturbation theory for quasilinear problems was developed by Marchuk (1973; 1974a, b; 1975a, b), and for discrete nonlinear atmospheric systems by Penenko (1975, 1977, 1979).

Before Cacuci (1981), the interpretation of the adjoint solution as "an influence function" and "the value of information" was given by Marchuk and Orlov (1961) for linear problems, and by Marchuk (1975a, p. 26) for nonlinear problems. Note that the method used by Hall *et al.* (1982), Hall and Cacuci (1983) and Hall (1986) is analogous to that earlier developed by Penenko (1975, 1979), Marchuk *et al.* (1978) and Marchuk and Penenko (1979 a, b).

One rigorous mathematical definition of the adjoint operator for nonlinear problems was given by Vainberg (1979) at least one year before Cacuci *et al.* (1980) and Cacuci (1981). Another definition of the adjoint operator was suggested by Vladimirov and Volovich (1984). The adjoint equations in nonlinear problems were also studied by Marchuk and Agoshkov (1988), Marchuk *et al.* (1991), Shutyaev (1991a, b, c; 1992).

In addition to the works cited in MS92 and CS93, the adjoint method was used in various linear and nonlinear problems by Marchuk (1958), Marchuk and Orlov (1961), Marchuk (1986; 1992), Barkmeijer (1992), Ehrendorfer (1992), Robertson (1991, 1992) and many others. Unfortunately, I can not comment them for reasons of space.

## 3. Remarks on the method by Cacuci, Hall and Schlesinger

*Remark 1*

The linearized matrix form of the main and adjoint small perturbation problems in the interval $(0,\ \bar{t})$ can be written as

$$\frac{\partial \vec{\phi}}{\partial t} + A\vec{\phi} = \vec{F}, \qquad -\frac{\partial \vec{g}}{\partial t} + A^{*}\vec{g} = \vec{G} \tag{4}$$

where $A$ depends on the basic solution of nonlinear problem, and hence, may have arbitrary structure. If $A$ is positive semidefinite ($A \geq 0$) then the adjoint matrix $A^*$ is also positive semidefinite ($A^* \geq 0$), and the main $\vec{\phi}$–problem (4) (solved from $t = 0$ to $t = \bar{t}$) as well as the adjoint $\vec{g}$– problem (solved in the opposite time direction from $t = \bar{t}$ to $t = 0$) are well posed in the Hadamard sense:

$$\frac{\partial}{\partial t}||\vec{\phi}|| \leq 0 \qquad \text{and} \qquad -\frac{\partial}{\partial t}||\vec{g}|| \leq 0 \tag{5}$$

for the unforced ($\vec{F} = 0,\ \vec{G} = 0$) problems (4) where $||\vec{\phi}|| = \sqrt{\vec{\phi}^{*}\vec{\phi}}$ is the norm in the complex Euclidean vector space. In the MS92 model these conditions are fulfilled since the problem is simple and specially formulated. But typically, and also in Hall and Cacuci (1983), Hall (1986) and Hall *et al.* (1982), the matrices $A$ and $A^*$ are of arbitrary structure and have both the stable and unstable modes. Hence there are both stable and unstable manifolds of perturbations $\vec{\phi}$ as, for instance, in the very simple example with the symmetric $(2 \times 2)$–matrices

$$A = A^* = \begin{pmatrix} 2 & 0 \\ 0 & -3 \end{pmatrix}. \tag{6}$$

Then both the problems (4) are ill posed in the Hadamard sense regardless of the direction in which they are solved. The unstable component $\phi_2$ of the perturbation $\vec{\phi} = (\phi_1,\ \phi_2)$ grows exponentially, and the solution $\vec{\phi}(t)$ leaves very fast the domain of infinitesimal perturbations where the adjoint approach is the only applicable. Cacuci, Hall and Schlesinger apparently ignore this important problem. It seems very likely that the eigenvalue problems should be solved first for $A$ and $A^*$ to determine the stable and unstable manifolds. Then the sensitivity analysis can be carried out separately for each such manifold.

*Remark 2*

Consider now a numerical scheme used by Cacuci, Hall and Schlesinger to solve the adjoint problem (4). Given $\vec{G} = 0$, the scheme (Hall and Cacuci, 1983, p. 2545; Hall 1986, p. 2647) can be written as

$$\vec{g}(n+1) = [E - \Delta t A^*]\vec{g}(n) \tag{7}$$

where $E$ is the unit matrix, and $n$ is the number of time steps. Let us consider simple and very favorable for the authors example when $A^*$ is the skew symmetric $(2 \times 2)$–matrix

$$A^* = \begin{pmatrix} iR & 0 \\ 0 & -iR \end{pmatrix} \tag{8}$$

where $R > 0$, and $i$ is the imaginary unit. Then, for any $R$, there is the conservation law $\|\vec{g}(t)\| =$ $=$ Const for the homogeneous different problem (4). But the von Neumann stability analysis leads to

$$|g_k(n+1)| = [1 + (\Delta t R)^2]^{1/2} |g_k(n)| \tag{9}$$

i.e. the scheme (7) is absolutely unstable for any time step $\Delta t$. Moreover, the larger $R$ is, the faster is the growth of the vector components $g_k(n)$ of the solution ($k = 1,\ 2$). Besides, even infinitesimal step $\Delta t$ can not remove the instability. Obviously, the situation is much worse in case of the general matrix $A$.

Thus Cacuci, Hall and Schlesinger try to study the sensitivity of their model to very small perturbations by solving the ill posed adjoint problem with the help of the absolutely unstable scheme (7). In other words, the good theoretical work by Cacuci (1981) is accompaniend by rather bad practical realizations.

## REFERENCES

Barkmeijer, J., 1992. Local error growth in a barotropic model. *Tellus*, **44**A, 314-323.

Cacuci. D. G., 1981. Sensitivity theory for nonlinear systems. Part I. Nonlinear functional analysis approach. *J. Math. Phys.*, **22**, 2794-2802. Part II. Extensions to additional classes of responses. Ibid, 2803-2812.

Cacuci, D. G. and M. E. Schlesinger, 1993. On the application of the adjoint method of sensitivity analysis in the atmospheric sciences. *Atmósfera*, this issue.

Cacuci, D. G., C. F. Wever, E. M. Oblow and J. H. Marable, 1980. Sensitivity theory for general systems of nonlinear equations. *Nucl. Sci. Eng.*, **75**, 88-110.

Ehrendorfer, M, 1992. Four–dimensional data assimilation comparison of variational and sequential algorithms. *Q. J. R. Meteorol. Soc.*, **118**, 673-713.

Hall, M. C. G., 1986. Application of adjoint sensitivity theory to an atmospheric general circulation model. *J. Atmos. Sci.*, **42**, 2644-2651.

Hall, M. C. G. and D. G. Cacuci, 1983. Physical interpretation of the adjoint functions for sensitivity analysis of atmospheric models. *J. Atmos. Sci.*, **40**, 2537-2546.

Hall, M. C. G., D. G. Cacuci and M. E. Schlesinger, 1982. Sensitivity analysis of a radiative–convective model by the adjoint method. *J. Atmos. Sci.*, **39**, 2038-2050.

Marchuk, G. I., 1958. Numerical methods of nuclear reactor design. *Atomizdat*, Moscow.

Marchuk, G. I., 1973. Perturbation theory and the statement of inverse problems. *Lect. Notes Comput. Sci.*, No. **4**, 159-166.

Marchuk, G. I., 1974a. Methods of the long–range weather forecast on a basis of solving the main and adjoint problems. *Meteorologia y Gidrologia*, No. **3**, 17-34.

Marchuk, G. I., 1974b. Numerical solution of the atmosphere and ocean dynamics problems. Leningrad, Gidrometeoizdat.

Marchuk, G. I., 1975a. Formulation of the theory of perturbations for complicated models. *Appl. Math. Optimiz.*, **2**, No. 1, 1-33.

Marchuk, G. I., 1975b. Methods of numerical mathematics. Springer–Verlag, New York.

Marchuk, G. I., 1986. Mathematical models in environmental problems. Elsevier Science Publishers B. V., New York. (Russian edition: Nauka, Moscow, 1982).

Marchuk, G. I., 1992. Adjoint equations and analysis of complex systems. Nauka, pp. 1-335.

Marchuk, G. I. and V. I. Agoshkov, 1988. Conjugate operators and algorithms of perturbations in nonlinear problems. Part I. Principles of construction of conjugate operators. *Sov. J. Numer. Analys. Math. Modelling*, **3**, No. 1, 21-46. Part II. Perturbation algorithms. *Ibid*, No. 2, 115-136.

Marchuk, G. I., V. I. Agoshkov, and V. P. Shutyaev, 1991. Adjoint equations and perturbation algorithms in nonlinear problems of mathematical physics. *Dept. Numer. Mathematics, The USSR Academy of Sciences,* Moscow, pp. 1-341 (1993: Nauka, Moscow).

Marchuk, G. I. and V. V. Orlov, 1961. On theory of the adjoint functions. Gosatomizdat, Moscow (Russian).

Marchuk, G. I. and V. V. Penenko, 1979a. The sensitivity study of the discrete atmosphere and ocean dynamics model *Izvestiya Akad. Nauk SSSR, Atmos. Ocean. Phys.*, **15**, No. 11, 279-284.

Marchuk, G. I. and V. V. Penenko, 1979b. Application of optimization methods to the problem of mathematical simulation of atmospheric processes and environment. In: Modelling and optimization of complex systems: Proc. of the IFIP-TC7 Work Conf., Novosibirsk: 240-252.

Marchuk, G. I., V. V. Penenko and A. Protasov, 1978. Variational principle in miniparametric model for atmospheric dynamics. In: Variational–Difference Methods in Mathematical Physics, Novosibirsk, 213-224.

Marchuk, G. I and Yu. N. Skiba, 1976. Numerical calculation of the conjugate problem for a model of thermal interaction of the atmosphere with the oceans and continents. *Izvestiya Akad. Nauk SSSR, Atmos. Ocean Phys.*, No. **12**, 279-284.

Marchuk, G. I. and Yu. N. Skiba, 1978. On a model for forecasting mean temperature anomalies. Preprint No. 120, Computer Centre, Akad. Nauk SSSR, Siberian branch, Novosibirsk, 40 p.

Marchuk, G. I and Yu. N. Skiba, 1990. Role of ajoint functions in studying the sensitivity of a model of the thermal interaction of the atmosphere and ocean to variations in input data. *Izvestiya, Akad. Nauk SSR, Atmos. ocean Phys.*, **26**, No. 5, 335-342.

Marchuk, G. I. and Yu. N. Skiba, 1992. Role of adjoint equations in estimating monthly mean air surface temperature anomalies. *Atmósfera*, **5**, 119-133.

Penenko, V. V., 1975. Computational aspects of modeling the atmospheric process dynamics and estimation of effects of various factors on the dynamics of the atmosphere. In collection: Certain problems of numerical and applied mathematics. Nauka Press, Novosibirsk, 61-77 (in Russian).

Penenko, V. V., 1977. Energy-balanced discrete models of atmospheric process dynamics. *Sov. Meteorol. Hydrology*, No. **10**, 1-16.

Penenko, V. V., 1979. Estimation of the parameters of discrete models of the dynamics of atmosphere and ocean. *Sov. Meteorol. Hydrology*, No. **7**, 57-68.

Robertson, A. W., 1991. Diagnosis of regional monthly anomalies using the adjoint method. Part I. Temperature. *J. Atmos. Sci.,* **49**, 885-905. Part II. Potential vorticity. *Ibid,* 906-918.

Robertson, A. W., 1992. The investigation of regional climate anomalies with a linear barotropic model and an adjoint technique. *Q. J. R. Meteorol. Soc.*, **118**, 1187-1209.

Shutyaev, V. P., 1991a. Justification of perturbation algorithm for a weakly nonlinear elliptic second-order boundary problem. *Sov. J. Numer. Anal. Math. Modelling,* **6**, 263-276.

Shutyaev, V. P., 1991b. On perturbation method for a weakly nonlinear first order hyperbolic problem. *Math. Notes*, **50**, No. 5. 156-158.

Shutyaev, V. P., 1991c. On computing of functionals in a nonlinear problem using the adjoint equation. *J. Numer. Math. Math. Physics*, **31**, No. 9, 1278-1288.

Shutyaev, V. P., 1992. On properties of the adjoint equation in a nonlienar hyperbolic problem. *Differential Equations*, **28**, No. 4. 706-715.

Skiba, Yu. N., 1980. On formulation of the basic and adjoint heat propagation problems in the atmosphere-ocean-soil system. In: *Mathematical Modelling of Atmosphere and Ocean Dynamics,* Part I, Computer Center, Akad. Nauk SSSR, Siberian Branch, Novosibirsk, 156-169 (Russian).

Vainberg, M. M., 1979. Functional analysis. Prosveschenie, Moscow. (Russian)

Vladimirov, V. S. and I. V. Volovich, 1984. Conservation laws for nonlinear equations. *Doklady Akad. Nauk SSSR,* **279**, No. 4, 843-847.