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Numerical algorithm for the adjoint sensitivity study of the Adem Ocean Thermodynamic Model

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RESUMEN

Se aplica el método adjunto para derivar fórmulas integrales simples para el estudio de sensibilidad del Modelo Termodinámico de Adem para océanos a variaciones pequeñas tanto en el forzamiento de calor como en las condiciones iniciales y de frontera. En cada fórmula, la solución del modelo adjunto es una fuente útil de información acerca de la contribución de tales variaciones a las anomalías promedio de la temperatura de la superficie del mar en una región seleccionada. Gracias al conjunto de condiciones especiales en las fronteras "líquidas" de entrada y salida, los modelos principal y adjunto son bien-puestos en el sentido de Hadamard (1923) no solamente para cuencas oceánicas cerradas, sino también para abiertas.

Se construyen esquemas en diferencias finitas implícitos, absolutamente estables y balanceados con aproximación de segundo orden tanto en espacio como en tiempo para los modelos termodinámicos principal y adjunto para océanos. Los esquemas están basados en el método de separación y son resueltos fácilmente por factorización. Ambos operadores en diferencias (separados y no separados) de esos esquemas satisfacen la identidad de Lagrange discreta en cada paso de tiempo. En el caso no-disipativo y no-forzado cuando no hay flujo a través de las fronteras "líquidas", cada uno de los esquemas tiene dos leyes de conservación.

ABSTRACT

The adjoint method is applied to derive simple integral formulas for the sensitivity study of the Adem Ocean Thermodynamic Model to small variations both in the heat forcing and in the initial and boundary conditions. In each formula, the adjoint model solution is a useful source of information about the contribution of such variations to average sea surface temperature anomaly in a certain region. Thanks to special conditions set at inflow and outflow liquid boundaries, the main and adjoint thermodynamic models are well-posed in the sense of Hadamard (1923) not only for closed, but also for open oceanic basins.

Balanced and absolutely stable implicit finite-difference schemes of the 2nd order approximation both in space and in time are constructed for the main and adjoint ocean thermodynamic models. The schemes are based on the splitting method and easily solved by the factorization. Both unsplit and split difference operators of these schemes satisfy the discrete Lagrange identity at every time step. In the nondissipative and unforced case when there is no flux across the liquid boundaries, the schemes have two conservation laws each.

1. Introduction

During the past two decades many applications of the adjoint equations have been developed in the dynamic meteorology and oceanology. Marchuk (1974, 1975) suggested to use the adjoint equation solutions for estimating the time-space average anomalies of hydro-meteorological fields and for studying the linear response of the models to variations in the initial conditions and forcing. For the three-dimensional global linear model of thermal interaction of the troposphere with the oceans and continents, the adjoint solutions were constructed by Marchuk and Skiba (1976) and Skiba (1978). Results obtained with a more refined version of this model were published later (Marchuk and Skiba 1990, 1992). For the average troposphere temperature equation the adjoint solutions were calculated by Sadokov and Shteinbok (1977), Musaelyan *et al.* (1983), Voronov *et al.* (1984) and others.

Rigorous mathematical definitions of the adjoint operator in nonlinear problems were given by Vainberg (1979) and Cacuci (1981a,b). The method of the adjoint sensitivity study was developed, improved and generalized for nonlinear discrete systems by Penenko (1979) and Marchuk and Penenko (1979), and for nonlinear differential systems by Cacuci (1981a,b), Marchuk *et al.* (1993) and Marchuk (1995).

This methodology was applied for the nonlinear sensitivity analysis of the radiative-convective model (Hall *et al.*, 1982), of the OSU general circulation model (Hall 1986), and of the PSU-NCAR mesoscale model (Errico and Vukicevic, 1992). It was used by Robertson (1991, 1992, 1993) in the diagnosis of regional anomalies, and by Zou *et al.* (1993) - in the blocking sensitivity study. The adjoint equation solutions were also used to construct the explicit scheme whose stability properties approximate those of the implicit Crank-Nicholson scheme (Marchuk *et al.*, 1985a), and to calculate the first two moments of random fields in the Kalman filtering (Marchuk *et al.*, 1985b).

Adjoint atmospheric and oceanic equations have also been applied for the variational data assimilation (Penenko, 1981; Lewis and Derber, 1985; LeDimet and Talagrand, 1986; Courtier and Talagrand 1987, 1990; Talagrand and Courtier, 1987; Thépaut and Courtier, 1991; Erendorfer, 1992; Navon *et al.*, 1992; Rabier *et al.*, 1992). Besides, Farrell (1990) and Barkmeijer (1992, 1993) applied adjoint solutions for estimating the optimal growth rates of the model initial perturbations.

In this work, a balanced absolutely stable numerical algorithm is constructed for the adjoint sensitivity study of the Adem ocean thermodynamic climate model (Adem, 1991). Physical basis of the model was laid in Adem (1962, 1964a,b, 1970a,b, 1975) and Morales-Acoltzi and Adem (1994), while numerical results were discussed in Adem (1963, 1975, 1979, 1982), Adem and Donn (1981), Donn *et al.* (1985), and Adem *et al.* (1991, 1994a,b).

Mathematical formulation of the model for closed and open oceanic basins as well as balanced absolutely stable finite-difference schemes based on the splitting method are given by Skiba and Adem (1995).

Two types of the model oceanic basin, both closed and open are considered in the present work, too. Remind that the closed basin boundary everywhere coincides with a coast line, while some part of the open basin boundary is liquid. The model dynamic operator is positive for both the basins. For the open basin case it was achieved by setting different boundary conditions at the "inflow" and "outflow" liquid boundaries of the basin. The original 2-D dynamic operator of the model is split into the sum of two 1-D operators each of which is also positive. The positive definiteness of these operators offers two main advantages:

1) the splitting method (Marchuk, 1982; Skiba and Adem, 1995) can be used for the construction of economical balanced and absolutely stable finite-difference schemes;

2) The oceanic model is well posed in the sense of Hadamard (1923) for closed and open basins: either model solution is unique and stable to initial perturbations.

The last property means that exponential growth of initial perturbations is impossible, and the adjoint method can properly be applied to the sensitivity study of the model to small forcing variations. On the contrary, whenever the real parts of the model operator eigenvalues are opposite in sign, some initial perturbations grow exponentially and rapidly leave the domain of small perturbations where the adjoint method is the only applicable. It presents additional problems, and therefore the adjoint sensitivity study of any ill posed problem merits special investigation.

The model is briefly described in Section 2. A concept of the adjoint operator as well as some examples are given in Section 3. The adjoint thermodynamic models for closed and open oceanic basins are set in Section 4. Application of the adjoint model solutions in the model sensitivity study is explained in Section 5, whereas the role of the boundary conditions is discussed in Section 6. The 2nd order finite - difference approximations (in space and time) of the thermodynamic model and its adjoint are given in Sections 7 and 8. Although there is generally a difference between the discretized adjoint operator $(A^*)^h$ and the adjoint $(A^h)^*$ of the discretized operator A^h , the boundary conditions are approximated in Section 8 in such a way that $(A^*)^h = (A^h)^*$ for any type of oceanic basin, both closed and open. This equality is also valid for each of the split 1-D main and adjoint operators used in the splitting algorithm (Section 9). Thus the discrete Lagrange identity is satisfied not only for unsplit, but also for split operators at each fractional time step. Balanced and absolutely stable finite-difference schemes for the main and adjoint ocean thermodynamic models are constructed in Section 10. In the case when both dissipation and forcing are absent, either scheme has two conservation laws. Conclusions are drawn in Section 11.

2. Description of the model in closed and open basins

The Adem Thermodynamic Climate Model written for climatic temperature anomaly $T(\mathbf{r},\ t)$ in the ocean upper layer is described by the two-dimensional heat balance equation

$$\frac{\partial T}{\partial t} + \mathbf{U} \cdot \nabla T - \mu \nabla^2 T + \gamma T = f \tag{1}$$

in an oceanic basin Ω and time interval $(0, \bar{t}\ )$. The solution $T(\mathbf{r}, t)$ is the sea surface temperature (SST) anomaly defined as the difference between an actual SST, $T_s(\mathbf{r}, t)$, and the climatic SST, $T_{sc}(\mathbf{r}, t)$; $\mathbf{U}(\mathbf{r}, t)$ is the known vector of the ocean currents; ∇ is the horizontal gradient; ∇^2 is the spherical part of the Laplacian; $\mathbf{r} = (\lambda, \vartheta)$ is the ocean basin point identified by its longitude λ and colatitude ϑ in the geographic coordinate system; and μ is a positive turbulent diffusion coefficient.

The Adem Climate Model forcing $F(T_s)$ taking into account such processes as evaporation, radiation and vertical turbulent transport, depends on the sea surface temperature $T_s(\mathbf{r}, t)$ (Adem, 1967, 1971). It is assumed here that the SST anomaly $T(\mathbf{r}, t)$ is small enough, so that $F(T_s)$ can be expanded into the power series of $T(\mathbf{r}, t)$ in a vicinity of the climatic SST, $T_{sc}(\mathbf{r}, \mathbf{t})$. Then the term γT in the equation (1) with a positive function $\gamma(\mathbf{r}, \mathbf{t})$ represents a linear part of this series (Adem, 1971), while the Eq.(1) forcing

$$f(\mathbf{r}, t) = F(T_s) - F(T_{sc}) + \gamma T \tag{2}$$

includes its higher order terms. Note that though the term γT makes the sea surface temperature T_s to return to the climatic value T_{sc}, the heat forcing $f(\mathbf{r}, t)$ can generate the SST anomalies.

Equation (1) can be written as

$$\frac{\partial T}{\partial t} + AT = f \tag{3}$$

where

$$AT = \mathbf{U} \cdot \nabla T - \mu \nabla^2 T + \gamma T \tag{4}$$

We take

$$T(\mathbf{r},0) = T^o(\mathbf{r}) \qquad \text{in } \Omega \tag{5}$$

as the initial condition, and

$$\mu\frac{\partial T}{\partial n} = 0 \qquad \text{at S} \tag{6}$$

as the condition at the boundary S of a closed 2-D oceanic basin Ω. Here n is the unit outward normal vector to S, $\frac{\partial T}{\partial n}$ is the normal derivative, and S is formed only from segments of the lines λ=Const or ϑ=Const. Besides,

$$U_n = \mathbf{U}\cdot\mathbf{n} = 0 \qquad \text{at S} \tag{7}$$

where U_n is the normal component of U at S. Thus there is no anomalous heat flux across the boundary S in the case of the closed basin Ω. It is also believed that the oceanic flow is incompressible:

$$div\ \mathbf{U} = 0 \tag{8}$$

If $\gamma = 0$ then the operator (4) is positive semidefinite (Skiba and Adem, 1995), and hence, A is positive definite for $\gamma > 0$:

$$\int_\Omega T\ AT\ d\mathbf{r} > 0, \tag{9}$$

Thus either solution of (2)-(8) is unique and stable to initial perturbations.

In the case of open oceanic basin Ω, the conditions (6) and (7) are again valid at the part of S being a coast line. However, unlike the closed basin, a nonzero anomalous heat flux across a liquid part of the boundary S is now a possibility. Therefore we put (Skiba, 1993; Skiba and Adem, 1995):

$$\mu\frac{\partial T}{\partial n} - U_nT = 0 \qquad \text{at } S^- \tag{10}$$

$$\mu\frac{\partial T}{\partial n} = 0 \qquad \text{at } S^+ \tag{11}$$

Here S^- is the inflow part of the boundary S where $U_n \leq 0$, and by (10), the total (advective plus diffusive) anomalous heat flux is zero at S^- . The outflow part of the boundary S where $U_n \geq 0$ is denoted by S^+ (Fig. 1), and (11) means that the turbulent anomalous heat flux at S^+ is neglected as compared to the advective anomalous heat outflux by the current U.

Where S coincides with the coast line the conditions (10) and (11) automatically satisfy (6) due to (7). Thus when (7) is imposed at the solid part of S, conditions (10) and (11) can be used at the entire boundary S without separating S into solid and liquid segments.

Eqs. (10) and (11) are well known boundary conditions of the 3d and 2nd kind, respectively (Ladyzhenskaya, 1973). In the limiting no-diffusive case ($\mu = 0$), (10) is reduced to the reasonable condition $T = 0$ at the inflow part of the boundary, while the condition (11) vanishes as it should, since for pure advection, no condition is required at the outflow boundary, where the solution is defined by the method of characteristics (Skiba and Adem, 1995).

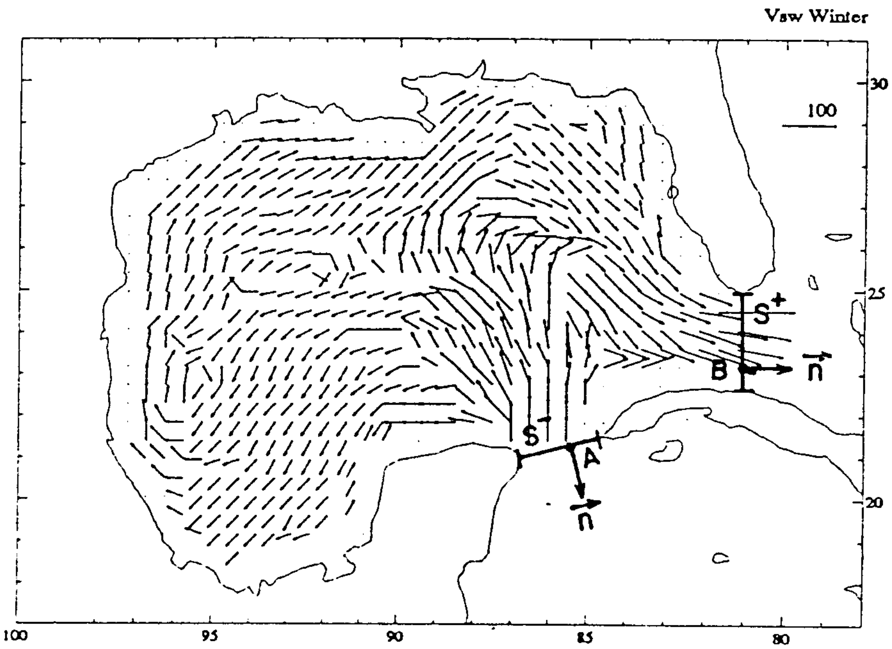

Fig. 1. The open oceanic domain **D**. The boundary points A and B belong to the boundary parts $\mathbf{S}^-$ and $\mathbf{S}^+$ respectively; $\mathbf{U}_n$ is a projection of the current velocity vector $\mathbf{U}$ on the outward unit normal to the boundary **S**.

By analogy with Skiba and Adem (1995), it can easily be shown that the problem (1), (5), (8)-(11) is well posed in the sense of Hadamard (1923). Indeed, the uniqueness and stability of each model solution follows from the fact that the operator A of the open oceanic basin model is positive, too.

3. Concept of the adjoint operator

Let us consider a Hilbert space **H** of such real functions $\varphi(\mathbf{r})$ defined in a domain Ω that the norm

$$\| \varphi \| = \{ \int_\Omega |\varphi(\mathbf{r})|^2 d\mathbf{r} \}^{1/2} \tag{12}$$

is finite. Then the inner product of any two functions $\varphi(\mathbf{r})$ and $\psi(\mathbf{r})$ of **H** can be defined as

$$< \varphi, \psi > = \int_\Omega \varphi(\mathbf{r}) \psi(\mathbf{r}) d\mathbf{r} \tag{13}$$

Obviously, $\| \varphi \| = < \varphi, \varphi >^{1/2}$. Let A be a linear operator with a domain D(A), i.e., the result $A\varphi(\mathbf{r})$ is determined in **H** for any function $\varphi(\mathbf{r})$ of D(A). Then the adjoint operator A^* can be defined by the Lagrange identity (Kato, 1966)

$$< A\varphi, g > = < \varphi, A^* g > \tag{14}$$

which holds for any $\varphi(\mathbf{r})$ of D(A) and any function $g(\mathbf{r})$ of a domain $D(A^*)$ of the adjoint operator A^* . We now consider 4 simple examples of the adjoint operator in various Hilbert spaces $\mathbf{H}$. Operators in the examples 1, 3 and 4 are parts of the thermodynamic model operator (4) and therefore elucidate formulation of the continuous adjoint model. The example 2 is helpful in setting up a finite-difference adjoint model (see Sections 7-10).

Example 1. A self-adjoint operator

Let $\mathbf{H}$ be a space of square integrable functions $\varphi(\mathbf{r})$ defined in Ω with inner product (13), and $A\varphi(\mathbf{r}) = \gamma\varphi(\mathbf{r})$ where $\gamma = \text{Const}$. Obviously, the domain D(A) coincides with $\mathbf{H}$, and A is bounded: $\| A \| = \gamma$ (Kato, 1966). Then, due to (14),

$$< A\varphi, g > = \int_{\Omega} [\gamma\varphi(\mathbf{r})] g(\mathbf{r}) d\mathbf{r} = \int_{\Omega} \varphi(\mathbf{r}) [\gamma g(\mathbf{r})] d\mathbf{r} = < \varphi, A^* g > \tag{15}$$

Thus A is self-adjoint: $A^* g(\mathbf{r}) = \gamma g(\mathbf{r})$, and $D(A^*) = D(A)$.

Example 2. The adjoint to a matrix

Let $\mathbf{H}$ be a real Euclidean $n - D$ vector space, and A be a $n \times n$ matrix. Define by $< \vec{\varphi}, \vec{g} > = \vec{g}^T \vec{\varphi}$ the inner product of vectors $\vec{\varphi}$ and $\vec{g}$ in $\mathbf{H}$ where $\vec{g}^T$ is the transpose. Then

$$< A\vec{\varphi}, \vec{g} > = \vec{g}^T A\vec{\varphi} = (\vec{g}^T A)\vec{\varphi} = (A^T \vec{g})^T \vec{\varphi} = < \vec{\varphi}, A^T \vec{g} > \tag{16}$$

and, due to (14), $A^* = A^T$. Thus the adjoint of A is merely the transpose of A. In particular, $A^* = A$ if A is symmetric, and $A^* = -A$ if A is skew-symmetric.

Example 3. A skew-symmetric advection operator

Let $\mathbf{H}$ be a space of square integrable periodic real functions $\varphi(x)$ in interval $[a, b]$ with the inner product

$$< \varphi, \psi > = \int_a^b \varphi(x)\psi(x) dx \tag{17}$$

and the norm

$$\| \varphi \| = < \varphi, \psi >^{1/2} \tag{18}$$

Consider the simplest advection operator

$$A\varphi(x) = \frac{\partial}{\partial x}\varphi(x) \tag{19}$$

in the domain $D(A)$ of all continuously differentiable periodic functions: $\varphi(b) = \varphi(a)$. Since

$D(A)$ is a part of $\mathbf{H}, A$ is unbounded, and by (17),

$$< A\varphi, g >= \int_a^b \frac{\partial \varphi}{\partial x}(x)g(x)dx = \varphi(b)g(b) - \varphi(a)g(a)$$

$$+ \int_a^b \varphi(x)[-\frac{\partial g}{\partial x}(x)]dx \tag{20}$$

We now are in a good position to explain the role of boundary conditions in the definition of the adjoint operator. Indeed, if $D(A^*) = D(A)$, i.e., $D(A^*)$ is also the set of continuously differentiable periodic functions in $[a, b]$ then

$$< A\varphi, g >= \int_a^b \varphi(x)[-\frac{\partial g(x)}{\partial x}]dx \tag{21}$$

and by (14), A is skew symmetric ($A^* = -A$):

$$A^* g = -\frac{\partial g}{\partial x} \tag{22}$$

The formula (22) is also valid if $D(A^*)$ is a set of all continuously differentiable functions $g(x)$ in $[a, b]$ such that $g(b) = 0$ and $g(a) = 0$. However the domain $D(A^*)$ of the adjoint A^* is now more narrow. Thus although two adjoint operators have the same structure (22), they are not identical because of different domains $D(A^*)$.

Lastly, suppose that $D(A)$ is a set of such continuously differentiable functions $\varphi(x)$ that $\varphi(a) = c$, $\varphi(b) = d$, $c \neq d$. Then $A^* = -A$ only if $D(A^*)$ consists of continuously differentiable functions $g(x)$ such that $g(a) = d$ and $g(b) = c$. In this case, φ and g have different boundary conditions, and $D(A^*)$ and $D(A)$ differ from each other. Thus the adjoint A^* is defined not only by its formal structure (22), but also by its domain $D(A^*)$ and boundary conditions. This fact is taken into account in the construction of the adjoint model operator in open oceanic basin (see boundary conditions (10), (11) and (32), (33)).

Example 4. A symmetric diffusion operator

Let $\mathbf{H}$ be the same space as in example 3, and let A has the diffusion operator form (see (4)):

$$A\varphi(x) = \frac{\partial^2}{\partial x^2}\varphi(x) \tag{23}$$

besides, $D(A)$ contains such two times continuously differentiable in $[a, b]$ functions that

$$\varphi(a) = 0 \qquad \text{and} \qquad \frac{\partial \varphi}{\partial x}(b) = 0 \tag{24}$$

Then

$$< A\varphi, g >= -g(a)\frac{\partial \varphi}{\partial x}(a) - \varphi(b)\frac{\partial g}{\partial x}(b) + \int_a^b \varphi[\frac{\partial^2 g}{\partial x^2}]dx \tag{25}$$

for any two times continuously differentiable function $g(x)$.

Hence

$$A^*g = \frac{\partial^2 g}{\partial x^2} \tag{26}$$

if

$$g(a) = 0 \qquad \text{and} \qquad \frac{\partial g}{\partial x}(b) = 0 \tag{27}$$

Thus $D(A^*) = D(A)$, and A is unbounded and symmetric.

4. The adjoint thermodynamic model

We now formulate the adjoint thermodynamic model in oceanic basins, both closed and open.

a) A closed basin Ω. Then operator A is defined by the formulas (4) and (6). Using (7) and the Lagrange identity (14) it is easy to show that

$$A^*g = -\nabla \cdot (\mathbf{U}g) - \mu\nabla^2 g + \gamma g \tag{28}$$

is the adjoint operator under the boundary condition

$$\mu\frac{\partial g}{\partial n} = 0 \qquad \text{at} \qquad \mathrm{S} \tag{29}$$

Due to (8), A^* can be written as

$$A^*g = -\mathbf{U} \cdot \nabla g - \mu\nabla^2 g + \gamma g \tag{30}$$

Since $D(A^*) = D(A)$, we can put $\varphi = g$ in (14), and obtain

$$< g, A^*g >=< Ag, g > > 0 \tag{31}$$

Thus the adjoint A^* is also positive definite.

b) An open basin Ω. Application of the identity (14) to the model operator (4), (10) and (11), results in the fact that the adjoint operator A^* regains the form (28) or (30) if any function $g(\mathbf{r})$ of $D(A^*)$ satisfies the following boundary conditions (see Skiba, 1993):

$$\mu\frac{\partial g}{\partial n} = 0 \qquad \text{at} \qquad \mathrm{S}^- \tag{32}$$

$$\mu\frac{\partial g}{\partial n} + U_n g = 0 \qquad \text{at} \qquad \mathrm{S}^+ \tag{33}$$

Since $D(A^*)$ does not coincide with $D(A)$, the identity (31) can not be used in this case to prove the positive definiteness of the adjoint operator A^*. However, calculating directly the scalar product (13) of g and A^*g, we obtain

$$< g, A^*g >= \mu \int_{\Omega} | \nabla g |^2 \, d\mathbf{r} + \gamma \int_{\Omega} g^2 d\mathbf{r}$$

$$+\frac{1}{2}\{\int_{S^+} U_n \, g^2 dS - \int_{S^-} U_n \, g^2 dS\} \tag{34}$$

The boundary conditions (32) and (33) have been used here. Since $U_n \geq 0$ at S^+, and $U_n \leq 0$ at S^-, the adjoint A^* is positive.

As the adjoint thermodynamic model in the domain Ω and time interval $(0, \bar{t}\ )$ we consider the equation

$$-\frac{\partial g}{\partial t} + A^*g = R \tag{35}$$

The adjoint forcing R will be defined later. As the boundary conditions for the adjoint model we take (29) if Ω is a closed oceanic basin, and (32), (33) if the basin Ω is open. Since $A^* > 0$, we have

$$\frac{\partial}{\partial t} \| g \| > 0 \tag{36}$$

if the adjoint forcing R is zero. Hence the adjoint thermodynamic model is well-posed in the sense of Hadamard only if solved backward in time: from $t = \bar{t}$ to $t = 0$. Therefore the initial condition for Eq. (35) is put at the moment $t = \bar{t}$:

$$g(\mathbf{r}, \bar{t}\ ) = Z(\mathbf{r}) \qquad \text{at} \qquad t = \bar{t} \tag{37}$$

Let us denote $t' = \bar{t} - t$. Then

$$\frac{\partial g}{\partial t'} = -\frac{\partial g}{\partial t} \tag{38}$$

and (35) can be written as

$$\frac{\partial g}{\partial t'} + A^*g = R \tag{39}$$

It is easily seen that the formal structures (30) and (4) of the adjoint and the main operators are differed only by the sign of the current vector $\mathbf{U}$. Since these vectors are directly opposed in the main and adjoint problems, the inflow and outflow boundaries S^- and S^+ of the main model (4), (10), (11) become, respectively, the outflow and inflow boundaries for the adjoint model (39). It explains the replacement of the boundary conditions (10), (11) by (32), (33), respectively.

Note that the adjoint model is a convenient mathematical tool used to solve some physical problems. Besides, the choice of the forcing $R(\mathbf{r}, t)$ and initial condition $Z(\mathbf{r})$ for the adjoint model is determined by the purpose of a concrete investigation. One of such problems, the model sensitivity study, will be considered in the next section. Physical and mathematical interpretation of the adjoint solution will be given too.

5. Adjoint sensitivity study of the open basin model

Let us consider the open basin model (3), (4), (10), (11) with initial condition (5). Suppose that we have to study the response of the model to variations in the initial anomalies $T^o(\mathbf{r})$ and forcing anomalies $f(\mathbf{r},t)$ within a time interval $(0,\bar{t}\ )$. We now consider and compare two different approaches to the problem.

1) The direct method

Assume that there is a set of various initial temperature anomalies $T_k^o(\mathbf{r})$ and forcing anomalies $f_k(\mathbf{r},t)(k=1,2,\ldots,N)$. The direct method of the model sensitivity study consists in solving the model (3), (10), (11) within $(0,\bar{t}\ )$ for each k, and finding all N solutions $T_k(\mathbf{r},t)$. This way gives comprehensive information about each solution T_k in the domain Ω and time interval $(0,\bar{t}\ )$. However, if the interval $(0,\bar{t}\ )$ and the number N of the numerical experiments are too large, this method is rather costly because of considerable computing time consumption. It is especially costly for complicated multi - dimensional models. In such cases the adjoint method described below can be used as alternative and more economical.

2) The adjoint method

We now apply the standard combination of the main and adjoint equations (Marchuk, 1974) to the Adem Thermodynamic Model. The inner product (13) of Eq. (3) with the solution $\mathbf{g}$ of Eq. (35) yields

$$< \frac{\partial T}{\partial t}, g > + < AT, g > = < f, g >, \tag{40}$$

while the inner product of (35) with the solution T of Eq. (3) gives

$$- < T, \frac{\partial g}{\partial t} > + < T, A^* g > = < T, R > \tag{41}$$

Subtracting (41) from (40) and using the Lagrange identity (14) we obtain

$$\frac{\partial}{\partial t} < T, g > = < f, g > - < T, R > \tag{42}$$

Finally, the integration of (42) over time from $t=0$ to $t=\bar{t}$, and taking into account (37) lead to

$$< T(\mathbf{r},\bar{t}\ ), Z(\mathbf{r}) > - < T^o(\mathbf{r}), g(\mathbf{r},0) > = \int_o^{\bar{t}} [< f, g > - < T, R >] dt \tag{43}$$

Let us define the value

$$J_R(T) \equiv \int_o^{\bar{t}} < T, R > dt = \int_o^{\bar{t}} \int_\Omega R(\mathbf{r},t) T(\mathbf{r},t) d\mathbf{r} dt \tag{44}$$

as a sensitivity characteristic of the linear response of the model (3). Obviously (44), can be used in the direct method of the model sensitivity study. Note that $J_R(T)$ is completely defined by the function $R(\mathbf{r},t)$ which, in such event, is taken as the adjoint model forcing. By setting $Z(\mathbf{r}) = 0$ in (37) we eliminate the first term in (43), and therefore (43) and (44) give

$$J_R(T) = \int_\Omega g(\mathbf{r},0) T^o(\mathbf{r}) d\mathbf{r} + \int_o^{\bar{t}} \int_\Omega g(\mathbf{r},t) f(\mathbf{r},t) d\mathbf{r} dt \tag{45}$$

which is fundamental in the adjoint sensitivity study. Any of the dual formulas (44) and (45) can be used for studying the model response. However, the main advantage of (45) lies in the fact that it directly relates the model sensitivity characteristic $J_R(T)$ with initial condition $T^o(\mathbf{r})$ and forcing $f(\mathbf{r},t)$ of the model, besides, the adjoint solution $g(\mathbf{r},t)$ appears here as a weight function (multiplier) for $T^o(\mathbf{r})$ and $f(\mathbf{r},t)$. Unlike (44) that involves the thermodynamic model solution, the formula (45) uses a solution of the adjoint thermodynamic model. Since (45) can be written in the form

$$J_R(T) =< g(\mathbf{r},0), T^o(\mathbf{r}) > + \int_o^{\bar{t}} < g(\mathbf{r},t), f(\mathbf{r},t) > dt \tag{46}$$

(see (13)), the model response $J_R(T)$ is insensitive to any initial temperature anomaly $T^o(\mathbf{r})$ whose spatial structure is orthogonal to $g(\mathbf{r},0)$ in the sense of the inner product (13). It is the case, for example, if the regions of nonzero values $g(\mathbf{r},0)$ and $T^o(\mathbf{r})$ in Ω have empty intersection. In a similar manner, the sensitivity of $J_R(T)$ to the forcing anomaly $f(\mathbf{r},t)$ in any subinterval (t_1,t_2) of $(0,T)$ depends on the projection of $f(\mathbf{r},t)$ onto $g(\mathbf{r},t)$ within this subinterval. In particular, the response (46) can be significant if the positions of local maxima of $g(\mathbf{r},0)$ and $g(\mathbf{r},t)$ coincide with the positions of local maxima of $T^o(\mathbf{r})$ and $f(\mathbf{r},t)$, respectively. Since a fixed characteristic (44) cannot be sensitive to any $T^o(\mathbf{r})$ and $f(\mathbf{r},t)$, a few such characteristics (for various $R(\mathbf{r},t)$) are generally chosen in the model adjoint sensitivity study.

Thus the adjoint solution $g(\mathbf{r},t)$ can be interpreted as an influence function which may tell preliminary information about the spatial and temporal structure of the model response to the forcing and initial temperature anomalies (Wigner, 1945; Marchuk and Orlov, 1961). Besides, where the influence function $g(\mathbf{r},t)$ has local maxima, the anomalies $T^o(\mathbf{r})$ and $f(\mathbf{r},t)$ are especially important, since they may contribute significantly to the characteristic (45).

Assume that we want to analyze the linear response of the model in M subdomains $\Omega_i \subset \Omega$ $(i = 1, 2, \ldots, M)$ within a time interval $(\bar{t} - \Delta t, \bar{t})$ of length Δt. To this end, we introduce M functions

$$R_i(\mathbf{r},t) = p_i(\mathbf{r}) q(t) \tag{47}$$

with such nonnegative functions $p_i(\mathbf{r})$ and $q(t)$ that

$$\int_{\Omega_i} p_i(\mathbf{r}) d\mathbf{r} = 1 \tag{48}$$

for each i $(i = 1, 2, \ldots, M)$, and

$$\int_{\bar{t}-\Delta t}^{\bar{t}} q(t)dt = 1 \tag{49}$$

In particular, $p_i(\mathbf{r})$ and $q(t)$ can be taken as in Marchuk and Skiba (1976):

$$p_i(\mathbf{r}) = \begin{cases} \frac{1}{\text{mes } \Omega_i}, & \text{if } \mathbf{r} \epsilon \, \Omega_i, \\ 0, & \text{otherwise} \end{cases} \tag{50}$$

and

$$q(t) = \begin{cases} \frac{1}{\Delta t}, & \text{if } t \epsilon \, (\bar{t} - \Delta t, \bar{t}) \\ 0, & \text{otherwise} \end{cases} \tag{51}$$

where mes Ω_i is the area of Ω_i, and ϵ denotes the membership to a set. The values $\bar{t}$ and Δt as well as the form and location of Ω_i are determined by the purpose of the study. Under the assumptions (47) - (51), either sensitivity characteristic

$$J_i(T) \equiv J_{R_i}(T) = \frac{1}{\Delta t \text{ mes } \Omega_i} \int_{\bar{t}-\Delta t}^{\bar{t}} \int_{\Omega_i} T(\mathbf{r}, t) d\mathbf{r} dt \tag{52}$$

$(i = 1, 2, \ldots, M)$ is the SST anomaly averaged over domain Ω_i and time interval $(\bar{t} - \Delta t, \bar{t})$, and can be calculated as soon as the solution $T(\mathbf{r}, t)$ of the model (3) is found. At the same time, (52) can also be computed using the dual formula (45) of the adjoint sensitivity study:

$$J_i(T) = < g_i(\mathbf{r}, 0), T^o(\mathbf{r}) > + \int_o^{\bar{t}} < g_i(\mathbf{r}, t), f(\mathbf{r}, t) > dt \tag{53}$$

To this end, for each i $(i = 1, 2, \ldots, M)$, the adjoint solution $g_i(\mathbf{r}, t)$ should be found with the zero initial condition (37) and forcing (47), and then the formula (53) is used repeatedly to calculate the characteristic $J_i(T)$ for various pairs of small initial temperature anomaly $T_k^o(\mathbf{r})$ and small forcing anomaly $f_k(\mathbf{r}, t)$ $(k = 1, 2, \ldots, N)$.

The main advantage of the direct method of the model sensitivity study is the possibility to use, along with the linear characteristics (52), any nonlinear characteristics. However if the number N of the pairs $\{T_k^o(\mathbf{r}), f_k(\mathbf{r}, t)\}$ is sufficiently large then the direct method becomes rather costly (time-consuming), since the thermodynamic model has to be solved N times (for each k). In this connection, whenever the number M of the sensitivity characteristics (52) is considerably less than N, the adjoint model sensitivity study is more economical, since it requires to solve only M adjoint problems before using the simple formulas (53).

Since the operator A^* of the adjoint problem (35), (37) is positive definite for both types of the oceanic basins (see (31) and (34)), the adjoint solution is estimated in the norm (12) by

$$|| \, g(\mathbf{r}, t) \, || \leq \int_t^{\bar{t}} || \, R(\mathbf{r}, t) \, || \, dt \tag{54}$$

If the adjoint forcing is defined by (47), (50)-(51) then

$$|| g(\mathbf{r},t) || \le \frac{1}{\sqrt{\text{mes } \Omega_i}} \tag{55}$$

and, due to (53),

$$| J_i(T) | \le \frac{1}{\sqrt{\text{mes } \Omega_i}} \left(|| T^o(\mathbf{r}) || + \int_o^{\bar{t}} || f(\mathbf{r},t) || \, dt \right) \tag{56}$$

Thus the model response (53) depends on the size of Ω_i: the less is mes Ω_i, the stronger can be the model response.

Once again, we stress that the adjoint thermodynamic model is not well posed in the sense of Hadamard if A^* is not positive semidefinite. In this case, the eigenfunctions corresponding to the eigenvalues with negative real part form the unstable manifold. Indeed, a nonzero projection of the adjoint forcing (47) on such a manifold will cause the exponential growth of the adjoint solution $g_i(\mathbf{r},t')$ with $t' \equiv \bar{t} - t$. Therefore, due to (53), the adjoint sensitivity study of the model to small anomalies $T^o(\mathbf{r})$ and $f(\mathbf{r},t)$ can become problematical. This case calls for further investigation which should include such steps as

a) separate sensitivity study of the model with respect to the anomalies $T^o(\mathbf{r})$ and $f(\mathbf{r},t)$ of the stable and unstable invariant manifolds;

b) search of appropriate sensitivity characteristics and a suitable time interval $(0,\bar{t})$;

c) special formulation of the adjoint problems separately for stable and unstable manifold.

6. Role of the boundary conditions

We now analyze the role of the boundary conditions in the linear response of the Adem Thermodynamic Model, and generalize the sensitivity formula (45) to the case when there is also anomalous heat flux at the inflow boundary S^- of the open oceanic basin Ω. To this end, assume that the boundary condition (10) has the form

$$\mu \frac{\partial T}{\partial n} + U_n T = Q \qquad \text{at } S^- \tag{57}$$

while the condition (11) is unchangeable. Here $Q(\mathbf{r},t)$ is a known anomalous heat flux across S^-. Then the sensitivity formula (45) is generalized to

$$J_R(T) = \int_\Omega g(\mathbf{r},0) T^o(\mathbf{r}) d\mathbf{r} + \int_o^{\bar{t}} \int_\Omega g(\mathbf{r},t) f(\mathbf{r},t) \, d\mathbf{r} dt$$

$$+ \int_o^{\bar{t}} \int_{S^-} g(\mathbf{r},t) \; Q(\mathbf{r},t) dS dt \tag{58}$$

which takes into account not only the initial temperature anomaly $T^o(\mathbf{r})$ and heat forcing anomaly $f(\mathbf{r},t)$, but also the anomalous heat flux $Q(\mathbf{r},t)$ across the boundary S^-.

7. Finite-difference approximation of the model operator

The operators A and A^* of the main and adjoint thermodynamic models can be written as

$$A = A_1 + A_2 \quad , \quad A^* = A_1^* + A_2^* \tag{59}$$

where

$$A_1 T = \frac{1}{2a\sin\vartheta}[\frac{\partial}{\partial\lambda}(uT) + u\frac{\partial T}{\partial\lambda}] - \frac{\mu}{a^2\sin^2\vartheta}\frac{\partial^2 T}{\partial\lambda^2} + \frac{\gamma}{2}T \tag{60}$$

$$A_2 T = \frac{1}{2a\sin\vartheta}[\frac{\partial}{\partial\vartheta}(vT\sin\vartheta) + v\sin\vartheta\frac{\partial T}{\partial\vartheta}]$$

$$-\frac{\mu}{a^2\sin\vartheta}\frac{\partial}{\partial\vartheta}(\sin\vartheta\frac{\partial T}{\partial\vartheta}) + \frac{\gamma}{2}T \tag{61}$$

$$A_1^* g = -\frac{1}{2a\sin\vartheta}[\frac{\partial}{\partial\lambda}(ug) + u\frac{\partial g}{\partial\lambda}] - \frac{\mu}{a^2\sin^2\vartheta}\frac{\partial^2 g}{\partial\lambda^2} + \frac{\gamma}{2}g \tag{62}$$

and

$$A_2^* g = -\frac{1}{2a\sin\vartheta}[\frac{\partial}{\partial\vartheta}(vg\sin\vartheta) + v\sin\vartheta\frac{\partial g}{\partial\vartheta}]$$

$$-\frac{\mu}{a^2\sin\vartheta}\frac{\partial}{\partial\vartheta}(\sin\vartheta\frac{\partial g}{\partial\vartheta}) + \frac{\gamma}{2}g \tag{63}$$

The operators (60) - (63) are positive definite if at least one of the following three conditions is satisfied (Skiba, 1993; Skiba and Adem, 1995): $\mu > 0$, $\gamma > 0$ or $U_n \not\equiv 0$ at the boundary of open basin. If $\mu = 0, \gamma = 0$ and $U_n \equiv 0$ then either operator (60)-(63) is skew symmetric.

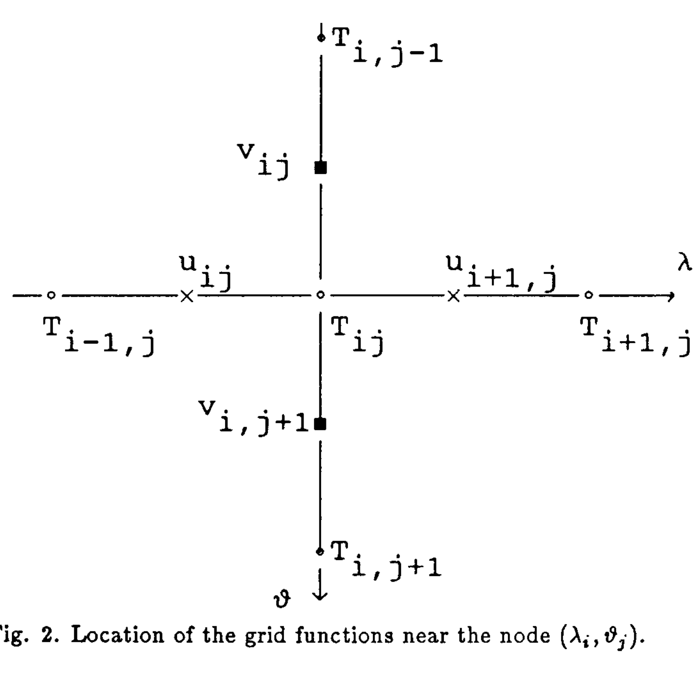

Fig. 2. Location of the grid functions near the node (λ_i, ϑ_j).

We will use the same shifted regular grids as in Skiba and Adem (1995) with constant mesh sizes $\Delta\lambda$ and $\Delta\vartheta$ along the axes λ and ϑ respectively (Fig. 2). Finite-difference approximations A_1^h and A_2^h of the $1-D$ operators A_1 and A_2 are obtained in the same way as in Skiba and Adem (1995). Therefore only the final formulas will be given here:

$$\{A_1^h T\}_{ij} = \frac{1}{2a\Delta\lambda \sin\vartheta_j}(u_{i+1,j}T_{i+1,j} - U_{ij}T_{i-1,j})$$

$$-\frac{\mu}{a^2\Delta\lambda^2\sin^2\vartheta_j}(T_{i+1,j} - 2T_{ij} - T_{i-1,j}) + \frac{\gamma}{2}T_{ij} \tag{64}$$

and

$$\{A_2^h T\}_{ij} = \frac{v_{i,j+1}\sin\vartheta_+ T_{i,j+1} - v_{ij}\sin\vartheta_- T_{i,j-1}}{2a\Delta\vartheta\sin\vartheta_j}$$

$$-\frac{\mu\{\sin\vartheta_+(T_{i,j+1} - T_{ij}) - \sin\vartheta_-(T_{ij} - T_{i,j-1})\}}{a^2\Delta\vartheta^2\sin\vartheta_j} + \frac{\gamma}{2}T_{ij} \tag{65}$$

where u_{ij}, v_{ij} and T_{ij} are the velocity $\mathbf{U}$ components and the temperature anomaly in the grid points, respectively; a is the Earth radius; $\vartheta_j = j\Delta\vartheta$, $\vartheta_+ \equiv (j+1/2)\Delta\vartheta$, and $\vartheta_- \equiv (j-1/2)\Delta\vartheta$.

The adjoint operators A_i^* are approximated by the matrices $(A_i^*)^h$ defined as

$$\{(A_1^*)^h g\}_{ij} = -\frac{1}{2a\Delta\lambda\sin\vartheta_j}\{u_{i+1,j}g_{i+1,j} - u_{ij}g_{i-1,j}\}$$

$$-\frac{\mu}{a^2\Delta\lambda^2\sin^2\vartheta_j}\{g_{i+1,j} - 2g_{ij} + g_{i-1,j}\} + \frac{\gamma}{2}g_{ij} \tag{66}$$

and

$$\{(A_2^*)^h g\}_{ij} = -\frac{v_{i,j+1}\sin\vartheta_+ g_{i,j+1} - v_{ij}\sin\vartheta_- g_{i,j-1}}{2a\Delta\vartheta\sin\vartheta_j}$$

$$-\frac{\mu\{\sin\vartheta_+(g_{i,j+1} - g_{ij}) - \sin\vartheta_-(g_{ij} - g_{i,j-1})\}}{a^2\Delta\vartheta^2\sin\vartheta_j} + \frac{\gamma}{2}g_{ij} \tag{67}$$

Obviously there is generally a difference between the discretized adjoint operator $(A_i^*)^h$ and the adjoint $(A_i^h)^*$ of the discretized operator A_i^h . However the boundary conditions approximation given in Section 8 leads to

Proposition 1. The equality

$$(A_i^*)^h = (A_i^h)^* \tag{68}$$

is valid for any oceanic basin, both closed and open.

The equality (68) means that the operators of the main and adjoint discrete problems satisfy the discrete Lagrange identity (14) (see (72) below).

8. Approximation of boundary conditions

We now approximate the boundary conditions (10), (11) and (32), (33). Assume that the oceanic boundary S consists only of such segments that are parallel either to the lines λ = Const or to the lines ϑ = Const (Fig. 3). Therefore in each boundary node, the normal component U_n of the velocity vector $\mathbf{U}$ coincides either with $\pm u_{ij}$ or with $\pm v_{ij}$, while the normal vector $\mathbf{n}$ to S is always directed along one of the coordinates λ or ϑ. As a result we do not face any difficulties with setting boundary conditions for the 1-D split operators (60)-(63).

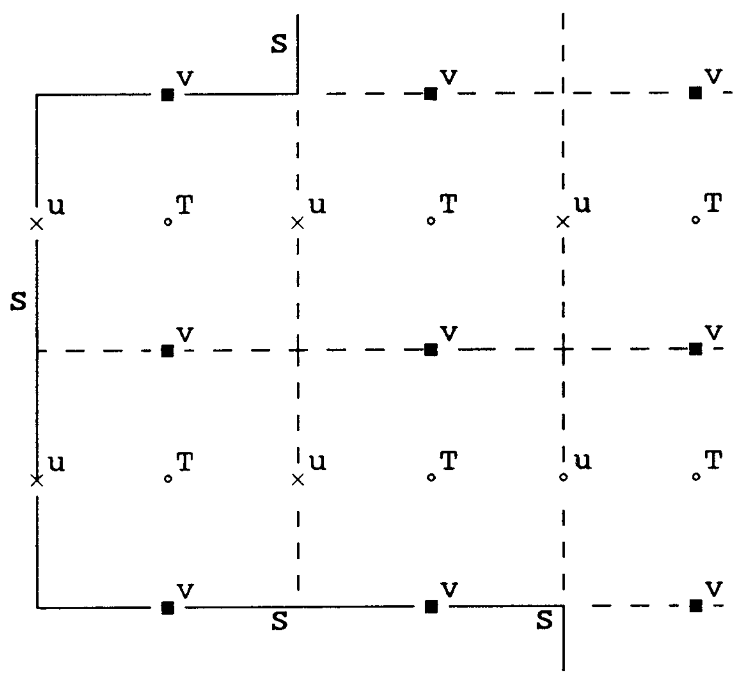

Fig.3. Location of the functions in the grid domain.

Since finite-difference approximation of the boundary conditions for the main split problems is described in Skiba and Adem (1995), we demonstrate approximation of the boundary condition only at a single boundary node for the main and adjoint split operators (64) and (66).

Let a line ϑ_j = Const runs across the oceanic domain, and let $L \equiv (\lambda_L - \Delta\lambda/2, \vartheta_j)$ be the left boundary point on this line. We assume that L belongs to S^- (Fig.4). Then $u_{L,j} > 0$, and the

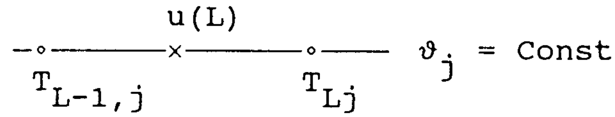

Fig.4. Location of the grid nodes immediately adjacent to the boundary point L on the line $\vartheta_j = Const$.

normal component $U_n(L)$ at L is negative and coincides with $-u_{L,j}$. We denote as T_{Lj} the SST anomaly in the first internal node (λ_L, ϑ_j) adjacent to L. At the point L, the normal vector $\mathbf{n}$ to S is directed from (λ_L, ϑ_j) to the external point $(\lambda_{L-1}, \vartheta_j)$ of the grid ocean domain, and $\frac{\partial T}{\partial n}(L)$ is approximated by $(T_{L-1,j} - T_{L,j})/(a\Delta\lambda \sin\vartheta_j)$. Then the boundary condition (10) is approximated as

$$\frac{\mu}{a\Delta\lambda \sin\vartheta_j}(T_{L-1,j} - T_{Lj}) + \frac{1}{2}u_{Lj}(T_{L-1,j} + T_{Lj}) = 0 \tag{69}$$

while the adjoint problem boundary condition (32) at L is approximated as

$$\mu\frac{g_{L-1,j} - g_{Lj}}{\Delta\lambda} = 0 \qquad \text{or} \qquad g_{L-1,j} = g_{Lj} \tag{70}$$

The boundary conditions at any node of S^+ as well as the boundary conditions for the split operators (65) and (67) are obtained in perfect analogy to this one (see also Skiba and Adem, 1995).

Let us introduce the inner product in the finite - dimensional vector space of the grid functions as

$$< \vec{T}, \vec{g} >_h = a^2\Delta\lambda\Delta\vartheta \sum_{i,j} T_{ij} g_{ij} \sin\vartheta_j \tag{71}$$

where the summation is taken over all interval nodes of the grid oceanic domain Ω. Then it is easy to check using the boundary conditions of the type of (69) and (70) that the finite-difference operators (64) and (66) as well as (65) and (67) satisfy the discrete Lagrange identity:

$$< A_i^h\vec{T}, \vec{g} >_h = < \vec{T}, (A_i^*)^h \vec{g} >_h \tag{72}$$

$(i = 1, 2)$, and hence, Proposition 1 (see (68)) is valid. Moreover, either discrete operator A_i^h and $(A_i^h)^*$ is positive definite in the presence of dissipation ($\mu > 0$ or $\gamma > 0$), or/and when $U_n \not\equiv 0$ at the boundary S (see (34)):

$$< A_i^h\vec{T}, \vec{T} >_h > 0, \qquad < \vec{g}, (A_i^h)^* \vec{g} >_h > 0 \tag{73}$$

If both $\mu = 0, \gamma = 0$ and $U_n \equiv 0$ at S then the operators (64)-(67) are skew-symmetric:

$$< A_i^h\vec{T}, \vec{T} >_h = 0, \qquad < \vec{g}, (A_i^h)^* \vec{g} >_h = 0 \tag{74}$$

Thus discrete operators (64)-(67) conserve the main properties of the corresponding differential operators (60) - (63).

9. Splitting-up method

The equations (3) and (35) discretized in space can be written as

$$\frac{\partial \vec{T}}{\partial t} + (A_1^h + A_2^h)\vec{T} = \vec{f} \tag{75}$$

and

$$-\frac{\partial \vec{g}}{\partial t} + \{(A_1^h)^* + (A_2^h)^*\}\vec{g} = \vec{R} \tag{76}$$

where A_i^h and $(A_i^h)^*$ are defined by (64) - (67), and the column vectors $\vec{T}(t), \vec{f}(t), \vec{g}(t)$ and $\vec{R}(t)$ have as their components the values $T_{ij}(t), f_{ij}(t), g_{ij}(t)$ and $R_{ij}(t)$ of the corresponding functions in the grid nodes (Fig. 3).

In the next section we will discuss approximation of the model boundary conditions and show that all the 1-D matrices A_i^h and $(A_i^h)^*$ are positive definite ($i = 1, 2$). This property is of great importance at the construction of economical implicit absolutely stable difference schemes based on the splitting method.

Since the operators A_1 and A_2 are time-dependent and do not commute: $A_1 A_2 \neq A_2 A_1$, the symmetric version of the splitting method (Marchuk, 1982) is used here to obtain a scheme of the second order approximation in time within each small time interval $(t - \tau, t + \tau)$ (choice of τ is discussed in Skiba and Adem (1995)). The symmetric algorithm for the main model (75) consists of the three successive steps:

1) The equation

$$\frac{\partial \vec{T}_1}{\partial t} + A_1^h \vec{T}_1 = 0 \tag{77}$$

is solved in the interval $(t - \tau, t)$ with the initial condition $\vec{T}_1(t - \tau) = \vec{T}(t - \tau)$ where $\vec{T}(t - \tau)$ is the solution of Eq. (75) obtained in the previous interval $(t - 3\tau, t - \tau)$.

2) The equation

$$\frac{\partial \vec{T}_2}{\partial t} + A_2^h \vec{T}_2 = \vec{f} \tag{78}$$

is solved in the interval $(t - \tau, t + \tau)$ with initial condition $\vec{T}_2(t - \tau) = \vec{T}_1(t)$.

3) The equation

$$\frac{\partial \vec{T}_3}{\partial t} + A_1^h \vec{T}_3 = 0 \tag{79}$$

is solved in $(t, t+\tau)$ with initial condition $\vec{T}_3(t) = \vec{T}_2(t+\tau)$. Then $\vec{T}_3(t+\tau)$ approximates solution $\vec{T}(t + \tau)$ of the unsplit equation (75), and is taken as the initial condition to solve (75) in the next interval $(t + \tau, t + 3\tau)$.

The splitting algorithm used to solve the adjoint model (76) in $(t-\tau, t+\tau)$ has a similar form:

1) The equation

$$-\frac{\partial \vec{g}_3}{\partial t} + (A_1^h)^* \vec{g}_3 = 0 \tag{80}$$

is backward solved within $(t, t+\tau)$ with the initial condition $\vec{g}_3(t+\tau) = \vec{g}(t+\tau)$ where $\vec{g}(t+\tau)$ is the solution of the adjoint equation (76) at the moment $t+\tau$ obtained in the previous interval $(t+\tau, t+3\tau)$.

2) The equation

$$-\frac{\partial \vec{g}_2}{\partial t} + (A_2^h)^* \vec{g}_2 = \vec{R} \tag{81}$$

is backward solved in $(t-\tau, t+\tau)$ with the initial condition $\vec{g}_2(t+\tau) = \vec{g}_3(t)$.

3) The equation

$$-\frac{\partial \vec{g}_1}{\partial t} + (A_1^h)^* \vec{g}_1 = 0 \tag{82}$$

is backward solved within $(t-\tau, t)$ with the initial condition $\vec{g}_1(t) = \vec{g}_2(t-\tau)$. Then $\vec{g}_1(t-\tau)$ approximates the adjoint solution $\vec{g}(t-\tau)$ of the unsplit problem (76).

10. The main and adjoint numerical schemes

Let us divide the whole time interval $(0, \bar{t})$ into a set of equal subintervals (t_n, t_{n+1}) where $t_{n+1} = t_n + \tau$, $t_o = 0$, $t_{N+1} = \bar{t}$, $n = 0, 1, 2, \ldots, N$, and τ is small. Applying the symmetric splitting algorithm (77) - (79) and approximating the 1-D split problems in time by the Crank-Nicholson scheme, we obtain the following implicit numerical scheme for the Adem Ocean Thermodynamic Model:

$$\vec{T}[n-\frac{1}{2}] - \vec{T}[n-1] = -\frac{\tau}{2} A_1^h (\vec{T}[n-\frac{1}{2}] + \vec{T}[n-1])$$

$$\vec{T}[n+\frac{1}{2}] - \vec{T}[n-\frac{1}{2}] = -\tau A_2^h (\vec{T}[n+\frac{1}{2}] + \vec{T}[n-\frac{1}{2}]) + 2\tau \vec{f}[n]$$

$$\vec{T}[n+1] - \vec{T}[n+\frac{1}{2}] = -\frac{\tau}{2} A_1^h (\vec{T}[n+1] + \vec{T}[n+\frac{1}{2}]) \tag{83}$$

where $\vec{T}[n-1]$, $\vec{T}[n+1]$ and $\vec{f}[n]$ are the column vectors $\vec{T}(t_{n-1})$, $\vec{T}(t_{n+1})$ and $\frac{1}{2}[\vec{f}(t_{n+1}) + \vec{f}(t_{n-1})]$ respectively, whereas $\vec{T}[n-\frac{1}{2}]$ and $\vec{T}[n+\frac{1}{2}]$ having the same dimension as $\vec{T}[n-1]$ are the auxiliary vectors of the splitting-up algorithm.

In the same time interval (t_{n-1}, t_{n+1}), the algorithm (80) - (82) leads to the adjoint thermodynamic model scheme

$$\vec{g}[n+\frac{1}{2}] - \vec{g}[n+1] = -\frac{\tau}{2}(A_1^h)^*(\vec{g}[n+\frac{1}{2}] + \vec{g}\,[n+1])$$

$$\vec{g}[n-\frac{1}{2}] - \vec{g}[n+\frac{1}{2}] = -\tau(A_2^h)^*(\vec{g}[n-\frac{1}{2}] + \vec{g}[n+\frac{1}{2}]) + 2\tau\vec{R}[n]$$

$$\vec{g}\,[n-1] - \vec{g}[n-\frac{1}{2}] = -\frac{\tau}{2}(A_1^h)^*(\vec{g}[n-1] + \vec{g}[n-\frac{1}{2}]) \tag{84}$$

Assume now that $\vec{f}\,[n]$ and $\vec{R}[n]$ are identically zero. If we take the inner product (71) of the first equation (83) with the vector $\frac{1}{2}(\vec{T}[n-\frac{1}{2}] + \vec{T}[n-1])$, and use the inequality (73) then we obtain

$$\| \vec{T}[n-\frac{1}{2}] \|_h < \| \vec{T}[n-1] \|_h$$

where $\| \vec{T} \|_h \equiv <\vec{T}, \vec{T}>_h^{1/2}$. Similar procedure as applied to the rest homogeneous equations of the schemes (83) and (84) results in the inequalities

$$\| \vec{T}[n+1] \|_h < \| \vec{T}[n-1] \|_h \tag{85}$$

and

$$\| \vec{g}[n-1] \|_h < \| \vec{g}\,[n+1] \|_h \tag{86}$$

which are valid for each n. Thus the schemes (83) and (84) are stable to any initial errors regardless of the choice of the scheme time step τ, or absolutely stable. Therefore τ should be chosen only for reasons of getting a good approximation of the original unsplit differential problems.

Let us now take the inner product (71) of each of the three equations (83) with the vectors $\frac{1}{2}(\vec{g}\,[n-\frac{1}{2}] + \vec{g}\,[n-1])$, $\frac{1}{2}(\vec{g}\,[n+\frac{1}{2}] + \vec{g}\,[n-\frac{1}{2}])$ and $\frac{1}{2}(\vec{g}\,[n+1] + \vec{g}\,[n+\frac{1}{2}])$ respectively. Similarly, let us take the inner product (71) of the vectors $\frac{1}{2}(\vec{T}[n+\frac{1}{2}] + \vec{T}[n+1])$, $\frac{1}{2}(\vec{T}[n+\frac{1}{2}] + \vec{T}[n-\frac{1}{2}])$ and $\frac{1}{2}(\vec{T}[n-1] + \vec{T}[n-\frac{1}{2}])$ with the first, second and the third equation of the system (84) respectively. Then the Lagrange identity (72) leads to the formula

$$<\vec{T}[n+1], \vec{g}[n+1]>_h - <\vec{T}[n-1], \vec{g}[n-1]>_h$$

$$= 2\tau <\vec{f}[n], \frac{1}{2}(\vec{g}[n+\frac{1}{2}] + \vec{g}[n-\frac{1}{2}])>_h$$

$$-2\tau <\frac{1}{2}(\vec{T}[n+\frac{1}{2}] + \vec{T}[n-\frac{1}{2}]), \vec{R}[n]>_h \tag{87}$$

which is the second order difference approximation of the identity (43) written for a small time interval $(t-\tau, t+\tau)$. Thus the main and adjoint numerical schemes are not only absolutely stable , but also balanced and compatible to each other.

Under the conditions (74), and $\vec{f}[n] \equiv 0$ and $\vec{R}[n] \equiv 0$, each of the schemes (83) and (84) has the conservation law

$$\| \vec{T}[n+1] \|_h = \| \vec{T}[n-1] \|_h \tag{88}$$

and

$$\| \vec{g}[n-1] \|_h = \| \vec{g}[n+1] \|_h \tag{89}$$

The second conservation law under the same conditions is

$$\sum_{i,j} T_{ij} \sin \vartheta_j = \text{ Const}, \ \sum_{i,j} g_{ij} \sin \vartheta_j = \text{ Const} \tag{90}$$

Each equation of the schemes (83) and (84) represents a simple three-point equation that is easily solved by the routine factorization method (Skiba and Adem, 1995).

11. Concluding remarks

The Adem Thermodynamic Model and its adjoint are shown to be well posed in closed and open oceanic basins. Balanced, compatible in the sense of the discrete Lagrange identity, and absolutely stable main and adjoint finite-difference schemes of the second order approximation in space and time are constructed for the sensitivity study of the Adem Thermodynamic Model in closed and open oceanic basins. In the absence of dissipation and forcing the schemes have two conservation laws each.

Specially formulated boundary conditions for the open basin permitted to conserve the property of the positive definiteness for the discrete split operators of both the models, and apply the splitting method for their solution.

In spite of the fact that the schemes are implicit, the symmetric splitting method makes it possible to reduce the original two-dimensional problem to the solution of three simple one-dimensional problems. As a result, the implicit numerical algorithm is economical, and can be realized exactly (without iterations) by the factorization.

The method is readily generalized to three dimension problems.

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