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The Bayliss-Isaacson Algorithm and the Constraint Restoration Method are Equivalent

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With 2 Figures

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Summary

Bayliss and Isaacson (1975) method of modifying any given difference scheme so as to ensure total conservation of the appropriate physical invariants is shown to be equivalent to the constraint restoration method of Miele et al. (1968, 1969) subject to the requirement of least-square change of the state-vector coordinates.

Both methods are applied to enforce conservation of total energy and potential enstrophy in global shallow-water equations models. Some algorithmic differences between the methods are discussed as well as some implications of a posteriori enforcement of conservation of integral invariants on the performance of meteorological numerical weather prediction (NWP) models and the internal energy distribution.

1. Introduction

The long-term solution of the partial differential equations governing numerical weather prediction and climate models necessitates to employ numerical methods maintaining the conservation of the integral invariants satisfied by the continuous equations in order to inhibit nonlinear instability. Two types of approaches have been put forward towards solving this problem.

Arakawa (1966, 1970) and Arakawa and Lamb (1981) have developed a priori conserving difference schemes for specific NWP models. These methods have to be modified and developed anew for other models. Another way of looking at the problem was discovered simultaneously by Sasaki (1975, 1976, 1977) and by Bayliss and Isaacson (1975). See also Issacson and Turkel (1976) and Isaacson (1977). They found that it was possible to modify a posteriori any given difference scheme, so as to ensure conservation of its appropriate integral invariants. The method of Sasaki is a variational one, while that of Bayliss and Isaacson consits in linearizing the conservative constraints about the predicted values by means of a gradient method for modifying the predicted values at each time-step of the numerical integration.

The Bayliss-Isaacson method has been tested by Kalnay-Rivas et al. (1977) and Isaacson et al. (1979) while Navon (1981) tested both the variational method of Sasaki and the Bayliss-Isaacson method in long-term integrations of the nonlinear shallow-water equations on a β-plane limited-area domain. Navon and deVilliers (1983) proposed a new augmented Lagrangian method to enforce a posteriori conservation of integral invariants of the nonlinear shallow-water equations. Navon and deVilliers (1984, 1986) also tested a constraint restoration method due to Miele et al. (1969, 1971) and suggested to them by Prof. Angelo Miele (private communication). This method consists in satisfying the requirement that the integral constraints be restored with the least-square change in the field variables.

In a recent test of the constraint restoration method (CRM) it was suggested by E. Kalnay (private communication) that the the CRM method and the Bayliss-Issaacson method are equivalent.

In the present paper we will prove the equivalence between the two methods while detailing some differences in their algorithmic implementation.

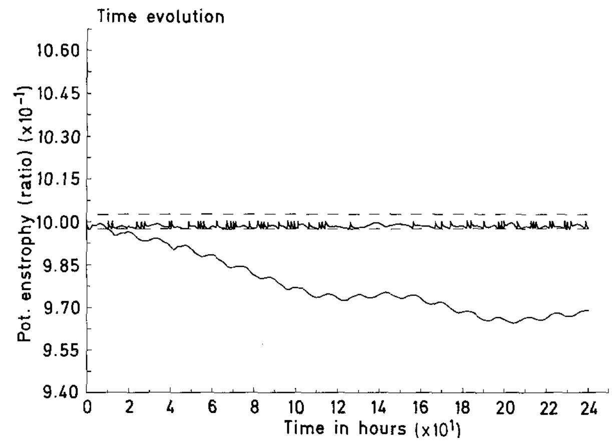

Fig. 1. Time variation of the potential enstrophy as function of its initial value without constraint restoration (continuous line) and with constraint restoration (quasi-constant spiky line)

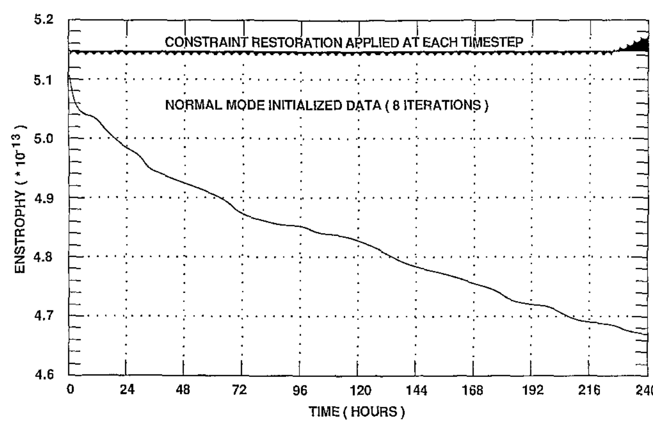

Fig. 2. Time variation of the potential enstrophy as a function of its initial value without application of constraint restoration and with constraint restoration (quasi-constant spiky line) for NASA/GLA fourth-order two layer global shallow-water model

2. The Bayliss-Isaacson Method

Bayliss and Isaacson (1975) presented a method making it possible to modify any given finite-difference scheme, so as to ensure the total conservation of the appropriate physical quantities. In what follows we shall describe the theoretical framework of the Bayliss-Isaacson conserving modification method.

Assume we have an initial-boundary value problem used for the partial differential equation for the vector $\boldsymbol{u}$:

$$u_t = B(u) \tag{1}$$

and that the solution $\boldsymbol{u}$ to (1) satisfies certain K integral invariants (conservation-laws)

$$g_k(u) = 0, \; k = 1, 2, \ldots, K. \tag{2}$$

by discretizing the integral invariants and representing the integrals as sums, we obtain then the approximating integral invariants

$$G_k[U_{ij}^n] = 0, \; k = 1, 2, \ldots, K, \tag{3}$$

where U_{ij}^n is a net function defined at the grid points (x_i, v_j, t_n) and $U(x_i, y_j, t_n)$ approximates $u(x_i, y_j, t_n)$. At time t_{n+1}, the difference operator solving for instance the shallow-water equations (i.e., solving for the vector $\boldsymbol{u}$ has the form:

$$W(n+1) = C[W(n), W(n-1), \ldots, W(n-s)] \equiv CW(n), \tag{4}$$

where $W(n)$ is a net function at time t_n.

We now wish to modify the given difference scheme (4) in such a way as to produce a net function $U(n+1)$ that will satisfy (3), the discrete approximation of the integral invariants (2). That is, a corrective net function $V(n+1)$ is to be found such that:

$$\begin{gathered} U(n+1) = CU(n) + V(n+1), \\ G_k[U(n+1)] = 0, \; k = 1, 2, \ldots, K \\ \min \| V(n+1) \| \end{gathered} \tag{5}$$

and such that the norm of the perturbation $V(n+1)$ is as small as possible i.e. $\min \| V(n+1) \|$.

The determination of $V(n+1)$ is a calculus problem for finding a net function that satisfies K simultaneous nonlinear equations (5) and is of minimum norm [Isaacson (1977)].

Bayliss and Isaacson (1975) propose to solve (5) by linearizing the discretized invariants $G_k[U(n$

+ 1)] about the predicted value $CU(n)$. This can be written as:

$$\begin{aligned} G_k[U(n+1) &= G_k[CU(n) + V(n+1)] \\ &\approx G_k[CU(n)] + \operatorname{grad} G_k \cdot V(n+1) \\ &= G_k[CU(n)] + \left.\frac{\partial G_k}{\partial U(n+1)}\right| \cdot V(n+1) \qquad (6) \\ &\equiv L_k(V(n+1)) \qquad U(n+1) = CU(n) \end{aligned}$$

Here $\operatorname{grad} G_k = \dfrac{\partial G_k}{\partial U(n+1)}$ is evaluated at $U(n+1) = CU(n)$ and the scalar product with $V(n+1)$ is taken, the resulting linear form L_k is set equal to zero. Since any vector V has a unique representation in the form

$$V(n+1) = \sum_{k=1}^{K} \alpha_k \operatorname{grad} G_k + P \qquad (7)$$

where P is an arbitrary vector orthogonal to the K gradients, it follows that any solution of the K simultaneous linear equation (6) is also of that form. If the Grammian matrix (grad $G_k \cdot$ grad G_r) is nonsingular, by substituting the expression (7) for $V(n+1)$ into (6), the K scalar coefficients α_k are determined by solving the K linear equations (6), i.e.

$$G_k[CU(n)] + \operatorname{gad} G_k \cdot \left(\sum_{r=1}^{K} \alpha_r \operatorname{grad} G_r \right) = 0, \qquad (8)$$
$$k = 1, \ldots, K.$$

Here we have used the orthogonality conditions

$$P \cdot \operatorname{grad} G_k = 0 \qquad (9)$$
$$k = 1, 2, \ldots, K.$$

If the norm $\| V(n+1) \|$ is the Euclidean norm then the arbitrary vector P must be zero, i.e.

$$P = 0 \qquad (10)$$

provides the solution of minimum norm. If we deal with a single integral constraint (for instance the potential enstrophy constraint for the shallow-water equations) and assume the correction:

$$V(n+1) = (U', V', H') \qquad (11)$$

is added to the predicted values of the velocity and height fields $\bar{U}, \bar{V}, \bar{H}$, then using (5) and (8) we get

$$(U', V', H') = \alpha \left(\frac{\partial G}{\partial U}, \frac{\partial G}{\partial V}, \frac{\partial G}{\partial H} \right)_{\bar{U}, \bar{V}, \bar{H}} \qquad (12)$$

$$\left(\frac{\partial G}{\partial U} \right)_{\bar{U}, \bar{V}, \bar{H}} \cdot U' + \left(\frac{\partial G}{\partial V} \right)_{\bar{U}, \bar{V}, \bar{H}} \cdot V' + \left(\frac{\partial G}{\partial H} \right)_{\bar{U}, \bar{V}, \bar{H}} \cdot H' = $$
$$= G(U, V_0, H_0) - G(\bar{U}, \bar{V}, \bar{H}) \qquad (13)$$

Using (12) and (13) in conjunction with (8) we find that α can now be determined as:

$$\alpha = \frac{G(U_0, V_0, H_0) - G(U, V, H)}{\left| \dfrac{\partial G}{\partial U} \right|^2 + \left| \dfrac{\partial G}{\partial V} \right|^2 + \left| \dfrac{\partial G}{\partial H} \right|^2}, \qquad (14)$$

Here $G(U, V, H)$ denotes a consistent approximation to the potential enstrophy and $G(V_0, V_0, H_0)$ is the initial (time $t = 0$) potential enstrophy.

3. The Constraint Restoration Method (CRM)

Angelo Miele, Heideman, and Damoulakis (1968, 1969) proposed a constraint restoration method based on a least-square change of the coordinates in the state-vector.

Their method starts by assuming that the vector $\boldsymbol{x}$

$$\boldsymbol{x} = (u_{11}^{\sim n} \ldots u_{N_x N_y}^{\sim n}, v_{11}^{\sim n} \ldots v_{N_x N_y}^{\sim n}, h_{11}^{\sim n} \ldots h_{N_x N_y}^{\sim n})^T \qquad (15)$$

at time $n \Delta t$, is in the vicinity of the optimal point $\boldsymbol{x}^*$ which satisfies exactly the discrete K equality constraints

$$\Phi(\boldsymbol{x}^*) = 0 \qquad (16)$$

$$\Phi(\boldsymbol{x}) = \begin{bmatrix} \Phi_1(\boldsymbol{x}) \\ \cdot \\ \cdot \\ \cdot \\ \Phi_K(\boldsymbol{x}) \end{bmatrix} \quad K < 3 N_x N_y = N. \qquad (17)$$

where N is the number of components of the vector $\boldsymbol{x}$. Suppose that a *nominal point* not consistent with (16) is available. Let $\tilde{\boldsymbol{x}}$ be a varied point related to the nominal point as follows:

$$\tilde{\boldsymbol{x}} = \boldsymbol{x} + \delta \boldsymbol{x}, \qquad (18)$$

$\delta \boldsymbol{x}$ being a perturbation of $\boldsymbol{x}$ about the nominal point. By using quasi-linearization Eq. (16) is approximated by

$$\Phi(\boldsymbol{x}) + A^T(\boldsymbol{x}) \delta \boldsymbol{x} = 0 \qquad (19)$$

where $A(\boldsymbol{x})$ denotes the $(N \times K)$ matrix:

$$A(\boldsymbol{x}) = \begin{bmatrix} \frac{\partial \Phi_1}{\partial x_1} & \frac{\partial \Phi_2}{\partial x_1} & \cdot\ \cdot & \frac{\partial \Phi_K}{\partial x_1} \\ \frac{\partial \Phi_1}{\partial x_2} & \frac{\partial \Phi_2}{\partial x_2} & \cdot\ \cdot & \frac{\partial \Phi_K}{\partial x_2} \\ \cdot & \cdot & & \cdot \\ \frac{\partial \Phi_1}{\partial x_N} & \frac{\partial \Phi_2}{\partial x_N} & \cdot\ \cdot & \frac{\partial \Phi_K}{\partial x_N} \end{bmatrix} \tag{20}$$

where the j-th column is the gradient of the integral constraint Φ_j with respect to the vector $\boldsymbol{x}$.

Here, the superscript T denotes the transpose of a matrix. In order to prevent the perturbation $\delta \boldsymbol{x}$ from becoming too large, it is convenient to imbed Eq. (19) into the one-parameter family of equations:

$$\alpha \Phi(\boldsymbol{x}) + A^T(\boldsymbol{x}) \delta \boldsymbol{x} = 0, \tag{21}$$

α being a prescribed scaling factor in the range

$$0 \leqslant \alpha \leqslant 1. \tag{22}$$

If the state vector $\boldsymbol{x}$ is an approximation to the described solution, we wish to restore the K constraints (16) while causing the least change in the components of vector $\boldsymbol{x}$. Therefore, we seek the minimum of the function

$$J = \tfrac{1}{2}\, \delta \boldsymbol{x}^T \delta \boldsymbol{x}, \tag{23}$$

subject to the linearized constraint (19). By using standard methods of the theory of maxima and minima one can show that the fundamental function of this problem is given by

$$\frac{1}{2} \delta \boldsymbol{x}^T \delta \boldsymbol{x} + \lambda^T [\Phi(\boldsymbol{x}) + A^T(\boldsymbol{x}) \delta \boldsymbol{x}] \tag{24}$$

where λ is the K component of the undetermined Lagrange multiplier vector

$$\lambda = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \cdot \\ \cdot \\ \lambda_K \end{bmatrix} \tag{25}$$

The optimum change $\delta \mathbf{x}$ is obtained when the gradient of the scalar function F with respect to the vector $\delta \mathbf{x}$ vanishes i.e. when

$$\delta \boldsymbol{x} = -A(\boldsymbol{x}) \lambda \tag{26}$$

(see also Appendix).

By using Eqs. (26) and (21) we obtain an explicit expression for the Lagrange multiplier vector of the form:

$$\alpha \Phi(\boldsymbol{x}) - B(\boldsymbol{x}) \lambda = 0 \tag{27}$$

where $B(\boldsymbol{x})$ denotes the $K \times K$ matrix

$$B(\boldsymbol{x}) = A^T(\boldsymbol{x}) A(\boldsymbol{x}). \tag{28}$$

Eq. (27) is linear in λ and admits the solution

$$\lambda = \alpha B^{-1}(\boldsymbol{x}) \Phi(\boldsymbol{x}). \tag{29}$$

When $\boldsymbol{x}$ is a large vector (typically for a numerical weather prediction model $3 N_x N_y > 10^4$) and K is the number of the constraints (for the shallow-water equations $K = 3$) we can easily calculate the vector of Lagrange multipliers.

From (29) and (26) we conclude that the optimum restoration correction is given by

$$\delta \boldsymbol{x} = -\alpha A(\boldsymbol{x}) B^{-1}(\boldsymbol{x}) \Phi(\boldsymbol{x}). \tag{30}$$

If we define a scalar performance index

$$P = \Phi^T(\boldsymbol{x}) \Phi(\boldsymbol{x}), \tag{31}$$

Clearly if $P = 0$, the vector $\boldsymbol{x}$ satisfies the discrete equality constraints $\Phi(\boldsymbol{x}) = 0$ and $P > 0$ otherwise. The first variation of the performance index is given by

$$\delta P = -2 \Phi^T(\boldsymbol{x}) A^T(\boldsymbol{x}) \delta \boldsymbol{x} \tag{32}$$

Using Eq. (21), then Eq. (32) reduces to:

$$\delta P = -2 \alpha \Phi^T(\boldsymbol{x}) \Phi(\boldsymbol{x}) = -2 \alpha P \tag{33}$$

Since $P > 0$, Eq. (33) shows that for $\alpha > 0$ the first variation of the performance index is negative, and hence for small enough α the decrease of the performance index is guaranteed. For a single constraint (say again potential enstrophy) and $\alpha = 1$, Eq. (21) reduces to

$$\Phi + \frac{\partial \Phi}{\partial u} \delta u + \frac{\partial \Phi}{\partial v} \delta v + \frac{\partial \Phi}{\partial h} \delta h = 0 \tag{34}$$

in which $\Phi, \frac{\partial \Phi}{\partial u}, \frac{\partial \Phi}{\partial v}, \frac{\partial \Phi}{\partial h}$ are computed at the nominal point.

The function J of (23) is:

$$J = \tfrac{1}{2} [(\delta u)^2 + (\delta v)^2 + (\delta h)^2] \tag{35}$$

subject to the linearized constraint (34). The fundamental function of this problem is given by:

$$F = \frac{1}{2} [(\delta u)^2 + (\delta v)^2 + (\delta h)^2] + \\ + \lambda \left[\left(\Phi + \frac{\partial \Phi}{\partial u} \cdot \delta u + \frac{\partial \Phi}{\partial v} \cdot \delta v + \frac{\partial \Phi}{\partial h} \cdot \delta h \right) \right] \tag{36}$$

where λ is an undetermined constant Lagrange multiplier. Optimum values of δu, δv, δh satisfy the relations:

$$\frac{\partial F}{\partial(\delta u)}=0,\ \frac{\partial F}{\partial(\delta v)}=0,\ \frac{\partial F}{\partial(\delta h)}=0 \tag{37}$$

whose explicit form is the following:

$$\delta u=-\lambda\frac{\partial\Phi}{\partial u},\ \delta v=-\lambda\frac{\partial\Phi}{\partial v},\ \partial h=-\lambda\frac{\partial\Phi}{\partial h} \tag{38}$$

From (38) and (34), the Lagrange multiplier is found to be

$$\lambda=\frac{\Phi}{\left(\frac{\partial\Phi}{\partial u}\right)^2+\left(\frac{\partial\Phi}{\partial v}\right)^2+\left(\frac{\partial\Phi}{\partial h}\right)^2} \tag{39}$$

For a given constraint G

$$\Phi=G_n-G_0=G(\bar u,\bar v,\bar h)-G(u_0,v_0,h_0) \tag{40}$$

i.e. (39) has the form

$$\lambda=\frac{G(\bar u,\bar v,\bar h)-G(u_0,v_0,h_0)}{\left|\frac{\partial\Phi}{\partial u}\right|^2+\left|\frac{\partial\Phi}{\partial v}\right|^2+\left|\frac{\partial\Phi}{\partial h}\right|^2} \tag{41}$$

4. Equivalence of the Bayliss-Isaacson and CRM Methods

In order to prove equivalence between the two methods we start by looking at the premises and assumptions adopted by both methods. Both the Bayliss-Isaacson and the CRM methods wish to satisfy the discretized constraints while minimizing the norm of the corrective perturbation. The quasilinearization of Eq. (16) gives Eq. (19) for the CRM which is equivalent to Eq. (16) for the Bayliss-Isaacson method which is also based on a linearization of the discretized constraints $G_{k(U(n+1))}$ about the predicted value $CU(n)$.

If we now identify the coefficients α_r in Eq. (8) of the CRM method with the Lagrange multipliers λ_k of the Lagrange multiplier vector λ of Eq. (27) for the CRM method we can see that Eq. (27) for the CRM method is identical to Eq. (8) for the Bayliss-Isaacson method (with $\alpha=1$). Also Eq. (8) for the Bayliss-Isaacson method and Eq. (29) of the CRM give the same expression for either α_r or the K components of the vector λ accordingly. This can be seen by taking $\alpha=1$ in Eq. (29) and then componentwise we have:

$$\lambda_k=[A^T{}_k(\mathbf{x})A_k(\mathbf{x})]^{-1}\Phi(\mathbf{x}) \tag{42}$$

or

$$A^T{}_k(\mathbf{x})A_k(\mathbf{x})\lambda_k=\Phi(\mathbf{x})=G_k[CU(n)] \tag{43}$$

where

$$A^T{}_k(\mathbf{x})A_k(\mathbf{x})\lambda_k=V-\text{grad}\,G_k\cdot\sum_{r=1}^{k}(\alpha_r\,\text{grad}\,G_k) \tag{44}$$

Finally the determination of the α_k or the λ_k gives the same functional terms according to Eq. (41) and (14), respectively. See additional proof of equivalence due to Prof. Isaacson (personal communication) in Appendix A.

5. Algorithmic Implementations of the Bayliss-Isaacson and CRM Methods

5.1. The Bayliss-Isaacson Method

As in Navon (1981) one obtains first the discrete finite-difference approximation of the integral invariant G_k (say for instance the potential enstrophy in a shallow-water equations method). The stages of the numerical algorithm implementing the Bayliss-Isaacson method are:

(i) Calculate

$$\frac{\partial G}{\partial u_{ij}},\frac{\partial G}{\partial v_{ij}},\frac{\partial G}{\partial h_{ij}}$$

(ii) Calculate α following Eq. (14).

(iii) Calculate the corrections to the predicted velocity and height fields, u'_{ij}, v'_{ij}, h'_{ij} using

$$u'_{ij}=\alpha\frac{\partial G'}{\partial u_{ij}},\ v'_{ij}=\alpha\frac{\partial G'}{\partial v_{ij}},\quad h'_{ij}=\alpha\frac{\partial G'}{\partial h_{ij}}; \tag{45}$$

(iv) Calculate the new potential enstrophy (say) using the corrected fields i.e.

$$G'(\bar u+u',\bar v+v',\bar h+h') \tag{46}$$

should satisfay up to truncation-error accuracy the constraint

$$G'(\bar u+u',\bar v+v',\bar h+h')=G(u_0,v_0,h_0) \tag{47}$$

(v) Use the new corrected fields $u^*=\bar u+u'$, $v^*=\bar v+v'$, $h^*=\bar h+h'$ as starting values for the new time-step integration of the numerical prediction model.

5.2. The CRM Method

1. Assume the nominal point $\boldsymbol{x}$ given by prediction at time t_n.

2. At the nominal point compute the constraint vector Φ, the gradient-matrix A with Eq. (20) and the $(K \times K)$ matrix $B = A^T(\boldsymbol{x}) A(\boldsymbol{x})$ with Eq. (28) as well as the performance index P [Eq. (31)].

3. Assume a restoration step-size $\alpha = 1$ and determine $\delta \boldsymbol{x} = \Delta \boldsymbol{x}$, the corrective net function using Eq. (30).

4. Compute the varied point $\tilde{x}$

$$\tilde{\boldsymbol{x}} = \boldsymbol{x} + \Delta \boldsymbol{x} \tag{48}$$

5. At the varied point compute the performance index $\tilde{P}$. If $\tilde{P} < P$ the first iteration is completed and the scaling factor $\alpha = 1$ is acceptable. Otherwise, if $\tilde{P} > P$ Miele et al. (1968, 1969) propose a bisection process i.e. α is bisected several times $\alpha = \frac{1}{2^n}$ until the condition $\tilde{P} < P$ is met, a fact guaranteed by the descent property.

6. After a value of α in the range $0 \leqslant \alpha \leqslant 1$ has been found such that $\tilde{P} < P$ the first iteration is completed. The new point $\tilde{\boldsymbol{x}} = \boldsymbol{x} + \Delta \boldsymbol{x}$ is used as a nominal point for a second iteration and the procedure repeated until a desired degree of accuracy is attained i.e. until

$$P \leqslant \varepsilon \tag{49}$$

where ε is a small number dictated by machine accuracy and truncation error of the difference scheme employed.

5.3. Application of the CRM Method for Enforcing Integral Invariants Conservation for the Shallow-Water Equations

We shall use the CRM to enforce conservation of total-mass, total energy and potential enstrophy for the shallow-water equations on limited-area domain on a β-plane. In this case the vector $\boldsymbol{x}$ is:

$$\boldsymbol{x} = (u_{11}^n \ldots, u_{N_x N_y}^n, v_{11}^n \ldots v_{N_x N_y}^n, h_{11}^n \ldots h_{N_x N_y}^n)^T \tag{50}$$

while $\Phi(\boldsymbol{x})$ is the 3-component equality constraints vector:

$$\Phi(\boldsymbol{x}) = \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{bmatrix} = \begin{bmatrix} H^n - H_0 \\ Z^n - Z_0 \\ E^n - E_0 \end{bmatrix} \tag{51}$$

where

$$\begin{aligned} \Phi_1 &= H^n - H^0 = \frac{1}{N_x N_y} \sum_i \sum_j h_{ij}^n \Delta x \Delta y - H^0 \\ \Phi_2 &= Z^n - Z^0 = \frac{\Delta x \Delta y}{2} \sum_i \sum_j \frac{1}{h_{ij}} \left[\frac{v_{i+1,j}^n - v_{i-1,j}^n}{2 \Delta x} - \frac{u_{i,j+1}^n - u_{i,j-1}^n}{2 \Delta y} + f_j \right]^2 - Z^0 \\ \Phi_3 &= E^n - E^0 = \frac{\Delta x \Delta y}{2} \sum_i \sum_j (u_{ij}^{n2} + v_{ij}^{n2} + g h_{ij}^n) h_{ij}^n. \end{aligned} \tag{52}$$

Here H^n, Z^n, E^n are the values of the discrete integral invariants of total mass, potential enstrophy and total energy at time $t_n = n \Delta t$, while H^0, Z^0, and E^0 are the values of the same integral invariants at the initial time $t = 0$. The next stage in the application of the CRM method is the calculation of the $(N \times 3)$ gradient matrix $A(\boldsymbol{x})$ which corresponds to $\Phi_x(\boldsymbol{x})$. If we denote

$$q_{ij} = \frac{1}{h_{ij}} \left[\frac{v_{i+1,j}^n - v_{i-1,j}^n}{2 \Delta x} - \frac{u_{i,j+1}^n - u_{i,j-1}^n}{2 \Delta y} + f_j \right] \tag{53}$$

and if we omit the superscript n for simplicity sake, we obtain

$$\begin{aligned} &\frac{\partial \Phi_1}{\partial u_{ij}} = 0 \qquad \frac{\partial \Phi_2}{\partial u_{ij}} = \frac{\Delta x}{2} (q_{i,j+1} - q_{i,j-1}) \\ &\frac{\partial \Phi_3}{\partial u_{ij}} = \Delta x \Delta y \, u_{ij} h_{ij} \\ &\frac{\partial \Phi_1}{\partial v_{ij}} = 0 \qquad \frac{\partial \Phi_2}{\partial v_{ij}} = \frac{\Delta y}{2} (-q_{i+1,j} + q_{i-1,j}) \\ &\frac{\partial \Phi_3}{\partial v_{ij}} = \Delta x \Delta y \, v_{ij} h_{ij} \\ &\frac{\partial \Phi_1}{\partial h_{ij}} = \Delta x \Delta y \qquad \frac{\partial \Phi_2}{\partial h_{ij}} = \frac{-\Delta x \Delta y}{2} q_{ij}^2 \\ &\frac{\partial \Phi_3}{\partial h_{ij}} = \frac{\Delta x \Delta y}{2} (u_{ij}^2 + v_{ij}^2 + 2 g h_{ij}) \end{aligned} \tag{54}$$

Having the matrix $A(x)$ we can calculate the 3×3 matrix $B(\boldsymbol{x})$

$$B(\boldsymbol{x}) = A^T(\boldsymbol{x})\, A(\boldsymbol{x}) \tag{55}$$

where

$$B(\boldsymbol{x}) = \tag{56}$$

$$\begin{matrix}
\sum_i \sum_j \left(\frac{\partial \Phi_1}{\partial h_{ij}}\right)^2; & \sum_i \sum_j \frac{\partial \Phi_1}{\partial h_{ij}} \frac{\partial \Phi_2}{\partial h_{ij}}; & \sum_i \sum_j \frac{\partial \Phi_1}{\partial h_{ij}} \frac{\partial \Phi_3}{\partial h_{ij}}; \\
\sum_i \sum_j \frac{\partial \Phi_1}{\partial h_{ij}} \frac{\partial \Phi_2}{\partial h_{ij}}; & \sum_i \sum_j \left[\left[\frac{\partial \Phi_2}{\partial u_{ij}}\right]^2 + \left[\frac{\partial \Phi_2}{\partial v_{ij}}\right]^2 + \left[\frac{\partial \Phi_2}{\partial h_{ij}}\right]^2\right]; & \sum_i \sum_j \left[\frac{\partial \Phi_2}{\partial u_{ij}} \frac{\partial \Phi_3}{\partial u_{ij}} + \frac{\partial \Phi_2}{\partial v_{ij}} \frac{\partial \Phi_3}{\partial V_{ij}} + \frac{\partial \Phi_2}{\partial h_{ij}} \frac{\partial \Phi_3}{\partial h_{ij}}\right] \\
\sum_i \sum_j \frac{\partial \Phi_1}{\partial h_{ij}} \frac{\partial \Phi_3}{\partial h_{ij}}; & \sum_i \sum_j \left[\frac{\partial \Phi_2}{\partial u_{ij}} \frac{\partial \Phi_3}{\partial u_{ij}} + \frac{\partial \Phi_2}{\partial v_{ij}} \frac{\partial \Phi_3}{\partial v_{ij}} + \frac{\partial \Phi_2}{\partial h_{ij}} \frac{\partial \Phi_3}{\partial h_{ij}}\right]; & \sum_i \sum_j \left[\left[\frac{\partial \Phi_3}{\partial u_{ij}}\right]^2 + \left[\frac{\partial \Phi_3}{\partial v_{ij}}\right]^2 + \left[\frac{\partial \Phi_3}{\partial h_{ij}}\right]^2\right]
\end{matrix}$$

Assuming $\alpha = 1$ we can then calculate the Lagrange multiplier vector (3 components) λ using Eq. (29) i.e.

$$\lambda = B^{-1}(\boldsymbol{x})\, \Phi(\boldsymbol{x}) = (\Phi_x^T \Phi_x)^{-1}\, \Phi(\boldsymbol{x}) \tag{57}$$

We then determine the restorative correction $\Delta \mathbf{x}$ by calculating the $3 N_x N_y = N$ vector $\delta \boldsymbol{x}$:

$$\delta \boldsymbol{x} = p = -A(\boldsymbol{x})\, \lambda = -\Phi_x(\mathbf{x})\, \lambda \tag{58}$$

$$\delta x = p = \tag{59}$$

$$\begin{bmatrix}
0 & -\lambda_2 \frac{\partial \Phi_2}{\partial u_{11}} & -\lambda_3 \frac{\partial \Phi_3}{\partial u_{11}} \\
0 & -\lambda_2 \frac{\partial \Phi_2}{\partial V_{11}} & -\lambda_3 \frac{\partial \Phi_3}{\partial V_{11}} \\
-\lambda_1 \frac{\partial \Phi_1}{\partial h_{11}} & -\lambda_2 \frac{\partial \Phi_2}{\partial h_{11}} & -\lambda_3 \frac{\partial \Phi_3}{\partial h_{11}} \\
\vdots & \vdots & \vdots \\
0 & -\lambda_2 \frac{\partial \Phi_2}{\partial u_{N_x N_y}} & -\lambda_3 \frac{\partial \Phi_3}{\partial u_{N_x N_y}} \\
0 & -\lambda_2 \frac{\partial \Phi_2}{\partial V_{N_x N_y}} & -\lambda_3 \frac{\partial \Phi_3}{\partial V_{N_x N_y}} \\
-\lambda_1 \frac{\partial \Phi_1}{\partial h_{N_x N_y}} & -\lambda_2 \frac{\partial \Phi_2}{\partial h_{N_x N_y}} & -\lambda_3 \frac{\partial \Phi_3}{\partial h_{N_x N_y}}
\end{bmatrix}$$

6. Numerical Results

The Bayliss-Isaacson method has been applied by Kalnay (1976) and by Kalnay et al. (1977) to enforce potential enstrophy in the 4th order dry-adiabatic version of the GISS general circulation model. Navon (1981) applied the same method to enforce conservation of potential enstrophy in a limited area shallow-water equations model. Isaacson et al. (1979 a) and Isaacson et al. (1979 b) have implemented the same technique in terms of simultaneous conservation of integral constraints for the shallow-water equations over a sphere taking into account orography effects.

Navon and deVilliers (1984, 1986) have implemented the CRM method for simultaneous conservation of the integral invariants of the shallow-water equations on both a limited area β-plane domain as well as an hemispheric domain when using a Turkel-Zwas large-time-step explicit difference scheme. Fig. 1 depicts the effect of the CRM method on the conservation of potential enstrophy. The CRM method was applied here at those time-steps of the numerical integration where a constraint violation, defined in terms of a predetermined relative change i.e. of the relation

$$\left|\frac{Z_n - Z_0}{Z_0}\right| < \delta_Z \tag{60}$$

was detected.

Fig. 2 shows the effect of applying the CRM method for enforcing conservation of potential enstrophy in the NASA/GLA model [see Takacs (1986)] which uses a Matsuno explicit time integration scheme and 4th order space-differencing.

7. Discussion of the Numerical Results

While the CRM method restores conservation of potential enstrophy and total energy some open questions still remain.

The first one is to what degree is this a posteriori restoration of integral invariants affecting the process of geostrophic adjustment of the shallow-water equations model? A more involved question related to the first is how are the a posteriori methods of the constraint restoration type affecting the nonlinear enstrophy and energy transfers in the resolved spectrum.

In other words, we know that a potential enstrophy conserving finite-difference model of the nonlinear shallow-water equations is characterized by an equipartition of enstrophy among higher wave numbers. In general an equipartition in an inviscid, truncated (discretized) flow would correspond to a cascade in the original continuous system (see Sadourny, 1975, 1980; Fairweather and Navon, 1980). One should also parameterize subgrid scales so that the enstrophy cascade and a different cascade towards the dissipation range should be conserved (Smagorinsky et al., 1965).

Preliminary experiments (L. Takacs, private communication) show that while the restoration method successfully conserves total energy and potential enstrophy it introduces a distortion in the energy spectra transfers evidenced by an increase in eddy energy when one omits the Shapiro filtering and relies only on constraint restoration when integrating the 4th order A-grid (nonstaggered) NASA/GLA global shallow-water equations model with orography. The results of using an Arakawa conservative C-grid formulation are not being matched by the results on a A-grid with constraint-restoration. To understand this one should consider the effect of the A and C grids respectively on geostrophic adjustment using the transfer function approach (Schoenstadt, 1977, 1980). Schemes using unstaggered grid points like the A-scheme have a tendency to be noisier and to produce solution separation-coupled with aliasing near the $2\Delta x$ resolution cutoff.

The staggered-grid Scheme C not only has better phase propagation characteristics—but also tends to window out much of the high-frequency noise in the discretized model (Schoenstadt, 1980). Thus, the conservation of the 3 integral invariants cannot affect all the degrees of freedom of the model which are depending on the full range of the discrete frequency and group velocity parameters. Group velocity is determining the velocity at which energy in the different frequencies propagates.

One should therefore not expect a posteriori enforcement of integral invariants conservation to have more effect than the particular grid point distribution, which controls a much larger number of degrees of freedom of the model.

Further studies should concentrate on studying the effect of constraint restoration methods on the model energy and enstrophy spectra in a given spectral band as well as its effect on the geostrophic adjustment process. Another application would be the use of constraint restoration methods in Arakawa C grids using the Arakawa-Lamb (1981) conserving scheme to correct for variations due to time-differencing.

8. Conclusion

The Bayliss-Isaacson (1975) method has been shown to be equivalent to the constraint restoration method of Miele et al. (1968, 1969). In its algorithmic implementation the CRM method corresponds to an iterated Bayliss-Isaacson method. As a matter of fact the Bayliss-Isaacson method itself can in some instances be iterated. Battifaranno (1984) has studied the problem of a conservative modification of upwind differencing for a scalar wave equation allowing him to use time-steps Δt, larger than the CFL condition. If Δt was larger than the CFL condition permitted, a constraint involving derivatives was imposed and the Bayliss-Isaacson method had to be iterated a number of times depending on how big Δt was (E. Isaacson, personal communication). A similar situation arose in the application of the CRM method to a large-time step Turkel-Zwas Scheme (Navon and deVilliers, 1984) where we found the number of CRM iterations increasing when we used a time-step larger than allowed by the CFL condition. Both methods have successfully been tested for enforcing conservation of integral invariants in limited-area and global shallow-water equations models.

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Appendix

Additional proof of equivalence between the Bayliss-Isaacson and the CRM methods (Isaacson).

When minimizing $\frac{1}{2}\,\delta\boldsymbol{x}^T\delta\boldsymbol{x}$ subject to constraints (16) then Lagrange multipliers appear in Eq. (24) which can be written as:

$$\min_{\delta_{x},\lambda}\left[\tfrac{1}{2}\,\delta\boldsymbol{x}^T\delta\boldsymbol{x}+\lambda^T\Phi(\boldsymbol{x}+\delta\boldsymbol{x})\right] \tag{A 1}$$

Taking the minimum w.r.t. the Lagrange multipliers results in

$$\frac{\partial}{\partial_{\lambda_l}}[(A_l)]=\Phi_l(\boldsymbol{x}+\delta\boldsymbol{x})=0 \quad 1\leqslant l\leqslant K \tag{A 2}$$

and the minimum w.r.t. $\delta\boldsymbol{x}$ yields

$$\frac{\partial}{\partial\,\delta x_K}[(A_1)]=$$

$$=\delta x_K+\sum_{r=1}^{K}\lambda_r\frac{\partial\Phi_r}{\partial\,\delta x_K}(\boldsymbol{x}+\delta\boldsymbol{x})=0 \tag{A 3}$$

$$1\leqslant K\leqslant N$$

Equation (A 3) is approximated by expanding about $\delta\boldsymbol{x}=0$ yielding:

$$\begin{bmatrix}\delta x_1\\ \delta x_2\\ \cdot\\ \cdot\\ \cdot\\ \delta x_N\end{bmatrix}+\sum_{r=1}^{K}\lambda_r\begin{bmatrix}\dfrac{\partial\Phi_r}{\partial x_1}(\boldsymbol{x})\\ \dfrac{\partial\Phi_r}{\partial x_2}(\boldsymbol{x})\\ \cdot\\ \cdot\\ \cdot\\ \dfrac{\partial\Phi_r}{\partial x_N}(\boldsymbol{x})\end{bmatrix}=0 \tag{A 4}$$

If we identify the perturbation vector $V(n+1)$ with $\delta\boldsymbol{x}$ we find that Eq. (A 4) is the same as Eq. (7) with $P=0$, if $\alpha_r=-\lambda_r$ for $1\leqslant r\leqslant K$. This proves equivalence between the Bayliss-Isaacson and the C.R.M. method.

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