A Lagrange multiplier approach for the metric terms of semi-Lagrangian models on the sphere

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SUMMARY

The horizontal momentum equation of the shallow-water equations on the sphere is written in 3-D vector form using the undetermined Lagrange multiplier method. The direct time discretization of this equation is proposed as an alternative to the usual approach, i.e. time discretization after explicit removal of the constraint by the use of generalized coordinates. The proposed procedure is applicable to any coordinate system and eliminates an instability associated with the metric term in a spherical grid spectral semi-Lagrangian model. For a polar-stereographic grid finite-element model, equivalent results and a gain in efficiency are obtained. The formalism can be extended to multilevel models.

1. INTRODUCTION

In primitive equation models the metric (or curvature) terms in the momentum equations are small but are retained to preserve the transformation properties of the equations. However, in the course of developing a semi-Lagrangian spectral model of the shallow-water equations, an instability occurred which was traced back to these terms by Robert (Ritchie 1988). One way of stably handling these terms is given by Ritchie.

In this paper we present an alternative solution to the problem. First we look on horizontal motion on the sphere as constrained motion and introduce the force of constraint using the undetermined Lagrange multiplier method. Then the metric term in spherical coordinates is identified as the force of constraint, where the multiplier has been determined a priori, i.e. before time discretization. Our solution consists of using a multiplier determined after the time discretization. The method is also applicable to semi-Lagrangian models using other coordinates and we give numerical results obtained using a finite-element model on a polar-stereographic grid. We also indicate the extension to multilevel models.

2. THEORY

We write the shallow-water equations on a sphere of unit radius in 3-D vector form and standard notation as

\[ \frac{d\mathbf{V}}{dt} = \mathbf{F} + \mu \mathbf{r} \quad (1) \]
\[ \frac{d\phi}{dt} + \phi \nabla \cdot \mathbf{V} = 0 \quad (2) \]

where

\[ \mathbf{V} = \frac{d\mathbf{r}}{dt} \quad (3) \]
\[ \mathbf{F} = -f \mathbf{r} \times \mathbf{V} - \nabla \phi \quad (4) \]

and \( \mu \) is a Lagrange multiplier determined by requiring that the constraint

\[ \mathbf{r} \cdot \mathbf{r} = 1 \quad (5) \]

be satisfied for all time.
The horizontal momentum equation (1) is written using the undetermined Lagrange multiplier method. In this method (Goldstein 1965; Lanczos 1970) we solve a higher-dimension equation, one in 3-D rather than the usual 2-D, and the undetermined multiplier term \((\mu r)\) represents the supplementary force to be applied on the fluid elements to keep them on the sphere. This force of constraint is along \(r\), the normal to the surface defined by (5). The unknowns \(V\) and \(\mu\) are obtained simultaneously from the momentum equation (1) and the constraint condition (5).

We now show that this is equivalent to the more usual formulation that uses generalized coordinates, such as spherical or polar–stereographic coordinates, where the constraint is trivially satisfied. We first determine the Lagrange multiplier by taking the scalar product of (1) with \(r\). Thus

\[
\mu = -V \cdot V
\]

(6)

where we have used the fact that for constrained motion \(\nabla \phi\) has no radial component, and

\[
r \cdot V = 0
\]

(7)

by virtue of (5).

Let us briefly examine the physical significance of (6). The force of constraint is always directed towards the centre of the sphere and its functional value is independent of the other force \((F)\). If we set \(F\) to zero we recover a classical result: \(\mu\) is constant in time and the position vector \(r\) rotates at a constant angular velocity \(|V|\) and therefore the trajectories are great circles as opposed to straight lines in the absence of constraint (where \(\mu = 0\)). In the more general case \(\mu\) is no longer independent of time but its value is such as to instantaneously balance the inertial centrifugal acceleration.

Introducing the spherical wind images, i.e. the horizontal wind components multiplied by \(\cos \theta\) as in (A.3), we project the equation of motion (1) to obtain

\[
\begin{align*}
\frac{dV_A}{dt} = \frac{d}{dt} (r \times V)_z & = \left(r \times \frac{dV}{dt}\right)_z = F_A, \\
\frac{dV_\theta}{dt} = \frac{dV_z}{dt} & = F_z + \mu z = F_\theta - \frac{V_\theta^2 + V_\phi^2}{\cos^2 \theta} \sin \theta.
\end{align*}
\]

(8)

Equation (8) is indeed the advective form of the momentum equation in spherical coordinates and the metric term can now be identified as the projection of the force of constraint. The singular behaviour of the metric term near the poles was the source of an instability that prevented the use of (8) in a spherical grid semi-Lagrangian spectral model.

The momentum equation can also be projected onto a polar–stereographic domain by using the decomposition (A.8) yielding

\[
\frac{1}{m} \frac{dV}{dt} = \frac{dV_X}{dt} + \frac{1}{2}(V_X^2 + V_Y^2) \frac{\partial m^2}{\partial X} = F_X
\]

(9)

for the \(X\) direction and a similar expression for the \(Y\) direction.

Equations (2) and (9) have been the starting point for the semi-Lagrangian discretization of the shallow-water equations on a polar–stereographic grid in Staniforth and Temperton (1986) and Temperton and Staniforth (1987).

To arrive at (8) or (9) we have used exact relations for the time derivatives and a Lagrange multiplier that corresponds to the exact solution. A natural alternative that
should give a solution of the same accuracy is first to time discretize the momentum equation (1) and then determine the Lagrange multiplier afterwards rather than the converse. It is essential that the Lagrange multiplier be determined anew. Physically this is because the discretized constraint must be in balance with the discretized motion. If we insisted on using the a priori value (6) we would then have three unknowns to be determined from four equations.

Suppose that we know the trajectory of the fluid element that is at position \( r \) at forecast time \( t \), then a semi-implicit time discretization of (1) over a time interval \( \Delta t \) is

\[
\frac{V(r, t) - V(r^-, t - \Delta t)}{\Delta t} = \tfrac{1}{2} [G(r, t) + G(r^-, t - \Delta t)] + \mathbf{E}(r^0, t - \Delta t/2) + \mu (r + r^-)/2
\]

(10)

where \( r^0 \) and \( r^- \) are the upstream positions of the fluid element at times \( t - \Delta t/2 \) and \( t - \Delta t \) respectively and \( F \) has been partitioned as \( E + G \). Regrouping the terms with the same arguments we have

\[
\mathbf{R} = \mathbf{R}^- + \mathbf{R}^0 + \mu \Delta t \mathbf{c}
\]

(11)

with

\[
\mathbf{R} = \left[ \mathbf{V} - \frac{\Delta t}{2} \mathbf{G} \right]_{(r, t)}
\]

\[
\mathbf{R}^- = \left[ \mathbf{V} + \frac{\Delta t}{2} \mathbf{G} \right]_{(r^-, t - \Delta t)}
\]

\[
\mathbf{R}^0 = \Delta t \mathbf{E}(r^0, t - \Delta t/2)
\]

\[
\mathbf{c} = \tfrac{1}{2} (r + r^-).
\]

The Lagrange multiplier \( \mu \) is determined by requiring that \( \mathbf{R} \) be a horizontal vector at the point \( r \), so

\[
r \cdot \mathbf{R} = r \cdot (\mathbf{R}^- + \mathbf{R}^0) + \mu \Delta t r \cdot \mathbf{c} = 0
\]

which substituted in (11) gives

\[
\mathbf{R} = \mathbf{R}^- - \frac{r \cdot \mathbf{R}^-}{r \cdot \mathbf{c}} \mathbf{c} + \mathbf{R}^0 - \frac{r \cdot \mathbf{R}^0}{r \cdot \mathbf{c}} \mathbf{c}
\]

(12)

We then project the images of \( \mathbf{R} \) with (A.5) or (A.10) and the rest of the semi-Lagrangian algorithm proceeds as usual. Since the 3-D vectors can be constructed from their images it is not necessary to compute them explicitly and the whole procedure is a linear transformation of the right-hand side images computed at the upstream points \( r^0 \) and \( r^- \) to yield the images of \( \mathbf{R} \) at the grid point \( r \).

For example in the case of spherical coordinates one obtains

\[
R_\lambda = c_{\lambda \lambda}^0 R_\lambda + c_{\lambda \theta}^0 R_\theta + c_{\lambda \phi}^0 R_\phi + c_{\lambda \rho}^0 R_\rho
\]

(13)

\[
R_\theta = c_{\theta \lambda}^0 R_\lambda + c_{\theta \theta}^0 R_\theta + c_{\theta \phi}^0 R_\phi + c_{\theta \rho}^0 R_\rho
\]

(14)

with

\[
c_{\rho \rho}^\delta = k \cdot r \times \left[ A_\rho^\delta - \frac{r \cdot A_\rho^\delta}{r \cdot \mathbf{c}} \mathbf{c} \right] \quad c_{\rho \phi}^\delta = k \cdot \left[ A_\rho^\delta - \frac{r \cdot A_\rho^\delta}{r \cdot \mathbf{c}} \mathbf{c} \right]
\]

where \( \rho = \lambda \) or \( \theta \), \( \delta = - \) or \( \phi \),

\[
\rho = \lambda \text{ or } \theta, \quad \delta = - \text{ or } \phi,
\]
\[ A_\lambda^\delta = \frac{1}{\cos \theta^\delta} \left( -\sin \lambda^\delta \mathbf{i} + \cos \lambda^\delta \mathbf{j} \right) \]

\[ A_\theta^\delta = \frac{1}{\cos \theta^\delta} \left( -\cos \lambda^\delta \sin \theta^\delta \mathbf{i} - \sin \lambda^\delta \sin \theta^\delta \mathbf{j} + \cos \theta^\delta \mathbf{k} \right). \]

In the above \( \lambda^\delta, \theta^\delta \) are the longitude and latitude respectively of the upstream point \( r^\delta \).

One can readily identify the components of \( A_\lambda^\delta \) and \( A_\theta^\delta \) in the linear relation (A.4) applied at \( r^\delta \).

When the Coriolis force is treated implicitly then

\[ V_\lambda - \frac{\Delta t}{2} fV_\theta + \frac{\Delta t}{2} \frac{\partial \phi}{\partial \lambda} = R_\lambda \]

(15)

\[ V_\theta + \frac{\Delta t}{2} fV_\lambda + \frac{\Delta t}{2} \cos \theta \frac{\partial \phi}{\partial \theta} = R_\theta \]

(16)

otherwise \( f \) is set to zero in the left-hand sides of (15) and (16).

Equations (15) and (16) together with the discretized continuity equation form a set of three equations from which \( V_\lambda, V_\theta \) and \( \phi \) are predicted. Similar expressions are obtained for polar–stereographic coordinates.

The right-hand sides of Eqs. (42) and (43) of Ritchie (1988) can be recast in the form of our Eqs. (13) and (14) and the coefficients \( c_{\rho\rho'} \) compared. After some lengthy algebra it turns out that the \( c_{\rho\rho'} \) coefficients are identical whereas the \( c_{\rho'\rho} \) coefficients differ by \( O(\Delta t^2) \).

3. Results

The algorithm described above has been implemented in semi-Lagrangian spectral and finite-element models of the shallow-water equations.

As mentioned in the introduction, it was necessary in the spectral model to find an alternative treatment of the metric term, since it was the source of a numerical instability. The algorithm proposed in this work solves the problem. The results one obtains are nearly identical to those obtained by Ritchie (1988). In fact the treatment of the \( \mathbf{R}^- \) term is identical while there is a small \( O(\Delta t^2) \) difference for the \( \mathbf{R}^\delta \) term. This results in r.m.s. height differences of less than half a millimetre after a five-day global integration at T126 with a timestep \( (\Delta t) \) of 2h.

Problems with the metric terms have not been observed in Cartesian polar–stereographic grid semi-Lagrangian models since the singular point of the transformation is outside the computational domain. To illustrate the equivalence of the proposed treatment and the usual formulation we have used the two-time-level semi-Lagrangian semi-implicit finite-element barotropic model of Temperton and StanifORTH (1987). In the context of this model we expect integrations of similar accuracy and some gain in efficiency since the metric term in (9) is nonlinear and involves a derivative.

The experimental procedure is the same as in Temperton and Staniforth, the only difference being the use of an improved second-order implicit normal mode initialization (Temperton 1988). The results are summarized in Table 1 where we display the r.m.s. height differences over the area of interest between two variable resolution semi-Lagrangian runs and a uniform resolution Eulerian control run. The only difference between the two semi-Lagrangian formulations is a different treatment of the metric terms. It is clear that the two methods give similar accuracy. The efficiency gain that we observe when using the new algorithm is about 17% of the total semi-Lagrangian integration time.
TABLE 1. Root mean square height differences at 48 hours

<table>
<thead>
<tr>
<th>$\Delta t$ (min)</th>
<th>r.m.s. 'old' (m)</th>
<th>r.m.s. 'new' (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>3.258</td>
<td>3.250</td>
</tr>
<tr>
<td>60</td>
<td>2.508</td>
<td>2.501</td>
</tr>
<tr>
<td>90</td>
<td>2.695</td>
<td>2.704</td>
</tr>
<tr>
<td>120</td>
<td>3.344</td>
<td>3.335</td>
</tr>
<tr>
<td>180</td>
<td>5.842</td>
<td>5.827</td>
</tr>
</tbody>
</table>

4. CONCLUSION

We have proposed an alternative treatment of the metric terms in semi-Lagrangian models of the shallow-water equations. In a spectral model this treatment eliminates an instability, and gives results that are nearly identical to the stable scheme presented in Ritchie (1988). In a polar–stereographic finite-element model it gives results of the same accuracy as before with a gain in efficiency.

The extension to multilevel models is straightforward. The Lagrange multiplier $\mu$ and the right-hand side of the momentum equation are then dependent on the vertical coordinate and Eq. (12) is used at all levels.

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APPENDIX

Relations between the 3-D Cartesian components of a horizontal vector and its spherical and polar–stereographic images

Let $i$, $j$ and $k$ be the unit vectors of a Cartesian system of reference fixed at the centre of the sphere. The position vector of a point on the sphere is

$$
r = xi + yj + zk
$$

(A.1)

where

$$
x = \cos \lambda \cos \theta, \quad y = \sin \lambda \cos \theta, \quad z = \sin \theta
$$

(A.2)

and $\lambda$ is the longitude and $\theta$ the latitude. A horizontal vector $h$ tangent to the sphere at the point $r$ can be written (except at the poles) as

$$
h = (1/\cos \theta)(h_\lambda \lambda + h_\theta \theta)
$$

(A.3)

where $\lambda$ and $\theta$ are unit vectors along $\partial r/\partial \lambda$ and $\partial r/\partial \theta$ respectively and $h_\lambda$ and $h_\theta$ are the spherical images of the vector. Using (A.1) and (A.2) in (A.3) we get the Cartesian components

$$
\begin{align*}
h_x &= h \cdot i = (-1/\cos \theta)(h_\lambda \sin \lambda + h_\theta \cos \lambda \sin \theta) \\
h_y &= h \cdot j = (1/\cos \theta)(h_\lambda \cos \lambda - h_\theta \sin \lambda \sin \theta) \\
h_z &= h \cdot k = h_\theta.
\end{align*}
$$

(A.4)
We have the inverse relations

\[ h_x = (r \times h)_z = x h_y - y h_z \]
\[ h_y = h_z. \]  \hspace{1cm} (A.5)

The polar–stereographic coordinates are defined by

\[ X = mx, \quad Y = my \]
\[ m = m_0/(1 + z) = (m_0^2 + X^2 + Y^2)/(2m_0), \quad 2 \geq m_0 > 0 \]  \hspace{1cm} (A.6)

which can be inverted to give \( x, y, z \) in terms of \( X \) and \( Y \). We introduce \( I \) and \( J \) the unit vectors along \( \partial r/\partial X \) and \( \partial r/\partial Y \) respectively, so that

\[ I = m\partial r/\partial X = i - \{x/(1 + z)\}(r + k) \]
\[ J = m\partial r/\partial Y = j - \{y/(1 + z)\}(r + k). \]  \hspace{1cm} (A.7)

\( I, J \) and \( r \) form a right-handed system with \( I \times J = r \) and cyclic permutations. A horizontal vector can then be written (except at the south pole) as

\[ h = m(h_x I + h_y J) \]  \hspace{1cm} (A.8)

which defines \( h_x \) and \( h_y \) the polar–stereographic images of \( h \). We obtain the Cartesian components of \( h \) by taking the scalar product of (A.8) with \( i, j \) and \( k \) successively, so

\[ h_x = \{m/(1 + z)\}\{(1 + z - x^2)h_x - xy h_y\} \]
\[ h_y = \{m/(1 + z)\}\{-xy h_x + (1 + z - y^2)h_y\} \]
\[ h_z = -m(x h_x + y h_y). \]  \hspace{1cm} (A.9)

The inverse relations are given by

\[ h_x = \frac{1}{m} \cdot h = \frac{1}{m} \left( h_z - \frac{x}{1 + z} h_z \right) \]
\[ h_y = \frac{1}{m} \cdot h = \frac{1}{m} \left( h_y - \frac{y}{1 + z} h_z \right). \]  \hspace{1cm} (A.10)

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