A mass and energy conserving spectral element atmospheric dynamical core on the cubed-sphere grid

M. A. Taylor\textsuperscript{1}, J. Edwards\textsuperscript{2}, S. Thomas\textsuperscript{2} and R. Nair\textsuperscript{2}

\textsuperscript{1}Sandia National Laboratories, Albuquerque NM 87185
\textsuperscript{2}National Center for Atmospheric Research, Boulder CO 80303

E-mail: mataylo@sandia.gov

Abstract. We present results from a conservative formulation of the spectral element method applied to global atmospheric circulation modeling. Exact local conservation of both mass and energy is obtained via a new compatible formulation of the spectral element method. Compatibility insures that the key integral property of the divergence and gradient operators required to show conservation also hold in discrete form. The spectral element method is used on a cubed-sphere grid to discretize the horizontal directions on the sphere. It can be coupled to any conservative vertical/radial discretization. The accuracy and conservation properties of the method are illustrated using a baroclinic instability test case.

1. Introduction

The spectral element method is a finite element method which relies on polynomial basis functions and quadrilateral elements. The equations of interest are solved in integral formulation and the integrals are evaluated with Gauss-Lobatto quadrature within each element. The Gauss-Lobatto quadrature leads to a diagonal mass matrix, which allows the method to obtain spectral accuracy while retaining both parallel efficiency and the geometric flexibility of unstructured finite elements grids. The method has proven accurate and efficient for a wide variety of geophysical problems, including global atmospheric circulation modeling [1, 2, 3, 4] ocean modeling [5, 6, 7] and planetary scale seismology [8]. The method has unsurpassed parallel performance; it was used for earthquake modeling by the 2003 Gordon Bell Best Performance winner [8] and for climate modeling by a 2002 Gordon Bell Award honorable mention [9].

In this work, we use a modified version of the spectral element component of HOMME, the High Order Multiscale Modeling Environment [10], which we refer to as HOMME-SE. HOMME-SE models the global circulation of the Earth’s atmosphere using the three-dimensional hydrostatic primitive equations. The formulation of the equations is taken from [11]. Spectral elements on a cubed-sphere grid are used to discretize the horizontal directions (the surface of the Earth). In the radial direction, HOMME-SE uses the hybrid $\eta$ pressure vertical coordinate system [12, 11]. We made several modifications to HOMME-SE in order to make the method locally conservative: we implemented the compatible spectral element formulation from [13], which involved slightly different forms of the metric terms in the discrete integrals, divergence, gradient and vorticity operators, and we switched from advection of $\log(p_s)$ to surface pressure $p_s$. 

© 2007 IOP Publishing Ltd
The conservation properties of the original formulation of HOMME-SE were good, but relied on the high accuracy of the method and thus only held to truncation error levels. In our new formulation, the conservation of mass and energy is semi-discrete, meaning the conservation is exact (to round off error levels) with exact time stepping. With the leapfrog time stepping scheme used in HOMME-SE, the conservation of linear and quadratic terms such as mass and tracer mass is exact, but the conservation of cubic terms such as energy has an error proportional to $\Delta t^2$.

2. Compatible Spectral Elements

The compatible formulation of the spectral element method obeys several discrete versions of the integral properties of the differential operators. For conservation, the key property is

$$\int_\Omega h \nabla \cdot \mathbf{v} \, dA + \int_\Omega \mathbf{v} \cdot \nabla h \, dA = \oint_{\partial \Omega} h \mathbf{v} \cdot \mathbf{n} \, ds$$

where $\Omega$ is a small control volume on the surface of the sphere, $dA$ is the area measure, $ds$ is the arc length measure, $h$ is a scalar and $\mathbf{v}$ is a vector field. In the compatible formulation of the spectral element method, taking $\Omega$ to be a single element and approximating the integrals by Gauss-Lobatto quadrature, we can show

$$\sum_\Omega h \text{DIV}(\mathbf{v}) + \sum_\Omega \mathbf{v} \cdot \text{GRAD}(h) = \sum_{\partial \Omega} h \mathbf{v} \cdot \mathbf{n}$$

where DIV and GRAD are the divergence and gradient operators used by the spectral element method. The left hand side of Eq. 2 is the usual flux contour integral. This identity is the key to showing the local conservation of the spectral element method, as it is used to show that the change in a conserved quantity within a single element is given exactly by the flux out of that element. Here we will focus on global conservation, which is shown by summing Eq. 2 over all elements. Because the spectral element uses globally continuous basis functions, the discrete flux out of one element through an edge is equal and opposite to the discrete flux through that edge into the adjacent element. Over the surface of the sphere, the sum of all flux terms will exactly cancel and the method will obey a discrete version of

$$\int h \nabla \cdot \mathbf{v} \, dA + \int \mathbf{v} \cdot \nabla h \, dA = 0$$

where the unlabeled integral represents integration over the entire surface of the sphere.

3. Mass conservation via compatibility

In the hybrid $\eta$ pressure vertical coordinate system, total air mass is given by

$$M = \int \int \frac{\partial p}{\partial \eta} \, dA \, d\eta$$

where $p$ is the pressure and $\eta$ is the vertical coordinate. The volume integral is decomposed into a radial component, $\int d\eta$, which is the integral from the top of the atmosphere ($\eta = 0$) to the surface ($\eta = 1$), and $\int dA$, the area weighted integral over the surface of the sphere. In pressure coordinates, the continuity equation has the form

$$\frac{\partial \frac{\partial p}{\partial \eta}}{\partial t} + \nabla \cdot \left( \frac{\partial p}{\partial \eta} \mathbf{u} \right) + \frac{\partial}{\partial \eta} \left( \frac{\partial p}{\partial \eta} \dot{\eta} \right) = 0$$
where \( \frac{\partial p}{\partial \eta} \) is the prognostic variable and \( \mathbf{u} \) is the horizontal velocity vector, \( \nabla \cdot \) is the two-dimensional divergence operator on the sphere and \( \dot{\eta} \) plays the role of a vertical velocity. (Note that for efficiency, this equation is usually replaced by an equivalent prognostic equation for surface pressure \( p_s \) and a diagnostic equation for the pressure surface vertical velocity \( \omega \).) Integrating this equation, we have that

\[
\frac{dM}{dt} = - \int \int \nabla \cdot \left( \frac{\partial p}{\partial \eta} \mathbf{u} \right) dA d\eta - \int \int \frac{\partial}{\partial \eta} \left( \frac{\partial p}{\partial \eta} \dot{\eta} \right) dA d\eta
\]

A conservative vertical discretization (coupled with the usual boundary conditions on \( \frac{\partial p}{\partial \eta} \dot{\eta} \)) will guarantee that the appropriate discrete version of

\[
\int \frac{\partial}{\partial \eta} \left( \frac{\partial p}{\partial \eta} \dot{\eta} \right) d\eta = 0.
\]

The compatible spectral element method, taking \( h = 1 \) and \( \mathbf{v} = \frac{\partial p}{\partial \eta} \mathbf{u} \) in Eq. 3 will guarantee that the appropriate discrete version of

\[
\int \nabla \cdot \left( \frac{\partial p}{\partial \eta} \mathbf{u} \right) dA = 0,
\]

and thus we have that \( \frac{dM}{dt} = 0 \) and mass is conserved.

4. Energy conservation via compatibility

In the hybrid \( \eta \) pressure vertical coordinate system, the equations are written \( \mathbf{u} \) and \( T \) as the prognostic variables. This allows the equations to be formulated with at most quadratic nonlinearities, but does mean that the equations cannot be written in conservation form. However, a compatible method does not require conservation form and instead obtains conservation by using an advection scheme with DIV and GRAD operators which satisfy Eq. 2.

The algebra needed to show conservation of energy is similar to that used to show conservation of mass and is given in [11]. The energy is a sum of kinetic (KE), internal (IE) and potential (PE) energy. For simplicity of this exposition, we write the equations assuming no topography which allows us to neglect the PE term (this term is included in the actual simulations). The energies are given by

\[
\text{KE} = \frac{1}{2} \int \int \frac{\partial p}{\partial \eta} \mathbf{u}^2 dA d\eta \quad \text{IE} = C_p \int \int \frac{\partial p}{\partial \eta} T dA d\eta
\]

and the energy evolution equations are

\[
\frac{d}{dt} \text{KE} = A_{KE} + T_1 \quad \frac{d}{dt} \text{IE} = A_{IE} + T_2
\]

with

\[
A_{KE} = - \int \int \left( \frac{\partial p}{\partial \eta} \mathbf{u} \cdot \nabla \frac{1}{2} \mathbf{u}^2 + \frac{1}{2} \mathbf{u}^2 \nabla \cdot \left( \frac{\partial p}{\partial \eta} \mathbf{u} \right) \right) dA d\eta - \int \int \left( \frac{\partial p}{\partial \eta} \mathbf{u} \cdot \nabla \dot{\eta} + \frac{1}{2} \mathbf{u}^2 \frac{\partial}{\partial \eta} \left( \frac{\partial p}{\partial \eta} \dot{\eta} \right) \right) dA d\eta
\]

\[
A_{IE} = - \int \int \left( \frac{\partial p}{\partial \eta} \mathbf{u} \cdot \nabla T + T \nabla \cdot \left( \frac{\partial p}{\partial \eta} \mathbf{u} \right) \right) dA d\eta - \int \int \left( \frac{\partial p}{\partial \eta} \dot{\eta} \frac{\partial T}{\partial \eta} + T \frac{\partial}{\partial \eta} \left( \frac{\partial p}{\partial \eta} \dot{\eta} \right) \right) dA d\eta
\]

\[
T_1 = \int \int \left( RT \mathbf{u} \cdot \nabla \frac{\partial p}{\partial \eta} + \frac{\partial p}{\partial \eta} \mathbf{u} \cdot \nabla \phi \right) dA d\eta
\]

\[
T_2 = - \int \int \frac{\partial p}{\partial \eta} \frac{RT \omega}{p} dA d\eta
\]
In the hybrid pressure vertical coordinate system, with a conservative vertical discretization, the hydrostatic relation, and a spatial discretization that obeys Eq. 2, we can show that the discrete versions of the terms in Eq. 4 satisfy

\[ A_{KE} = A_{IE} = 0 \]

so that

\[ E = KE + IE \]

\[
\frac{dE}{dt} = 0.
\]

Thus the energy conservation in HOMME-SE is obtained because the change in KE and IE due to advection \(A_{KE}, A_{IE}\) is exactly zero and the net internal transfer between KE and IE \(T_1 + T_2\) is exactly zero.

5. Results and conclusions

To demonstrate the conservation properties of HOMME-SE we use the Jablonowski and Williamson primitive equation test case [14]. It is an unforced problem were a quasi-realistic initial state is perturbed to trigger the growth of a baroclinic instability over several days. We first run the problem without any viscosity to verify the energy conservation properties of HOMME-SE. The results are shown in Table 1. The dissipation due to advection and the internal transfer terms is zero to machine precision, as expected. The only dissipation is from the leapfrog time stepping scheme, and this term decays as \(\Delta t^2\), also as expected. It is near machine precision at \(\Delta t = 15\). For this problem, a machine precision change in the energy over one time step is a dissipation rate of \(10^{-9}\) W/m\(^2\).

Table 1. Instantaneous values, in W/m\(^2\), of the terms in the energy equations at \(t = 7\) days of an inviscid simulation.

| \(\Delta t\) | \(A_{KE}\) | \(A_{IE}\) | Transfer | Leapfrog KE |
|-------------|-----------|-----------|----------|-------------|
| 200         | \(-2.9 \times 10^{-14}\) | \(-2.9 \times 10^{-14}\) | \(1.2 \times 10^{-13}\) | \(1.9 \times 10^{-6}\) |
| 60          | \(-1.0 \times 10^{-13}\) | \(-1.0 \times 10^{-13}\) | \(1.2 \times 10^{-13}\) | \(1.1 \times 10^{-7}\) |
| 15          | \(-2.6 \times 10^{-14}\) | \(9.9 \times 10^{-17}\) | \(9.9 \times 10^{-14}\) | \(8.1 \times 10^{-9}\) |

For realistic simulations some dissipation is needed to control the pileup of enstrophy at small scales. We use a traditional hyperviscosity modeled after that used in [11]. With a conservative
scheme such as HOMME-SE, the only KE dissipation will be only what we explicitly add via hyperviscosity and the small amount due to the leapfrog scheme. The convergence of the method with hyperviscosity is shown in Figure 1. This figure should be compared with Figure 11 in [14].

Our highest resolution solution is used as the reference solution, after first establishing that it is accurate to within the uncertainty level of the test case [14]. Contour plots of the surface pressure are shown in Figure 2, at four different resolutions. This figure should be compared with Figure 6 in [14]. These figures show that the HOMME-SE method requires an average grid spacing of 1.25° to converge to the reference solution uncertainty. In terms of accuracy per resolution HOMME-SE thus falls somewhere between the spectral Eulerian (requiring 1.4° resolution) and finite volume dynamical cores (1.0° resolution). We note however that because of the more uniform spacing of grid points on the cubed-sphere grid, at these resolutions the HOMME-SE grid will have 60% less grid points than that used by the spectral Eulerian model.

References
[1] Taylor M, Tribbia J and Iskandarani M 1997 J. Comput. Phys. 130 92–108
[2] Giraldo F X 2001 International Journal for Numerical Methods in Fluids 35 869–901
[3] Thomas S and Loft R 2002 Journal of Scientific Computing 17 339–350
[4] Wang H, Tribbia J J, Baer F, Fournier A and Taylor M A 2007 Monthly Weather Review To appear
[5] Haidvogel D, Curchitser E N, Iskandarani M, Hughes R and Taylor M A 1997 Atmosphere-Ocean Special 35 505–531
[6] Iskandarani M, Haidvogel D, Levin J, Curchitser E N and Edwards C A 2002 Computing in Science and Engineering 4
[7] Molcard A, Pinardi N, Iskandarani M and Haidvogel D 2002 Dynamics of Atmospheres and Oceans 35 97–130
[8] Komatitsch D, Tsuboi S, Ji C and Tromp J 2003 Proceedings of the ACM / IEEE Supercomputing SC’2003 conference
[9] Loft R, Thomas S and Dennis J 2001 Proceedings of the ACM / IEEE Supercomputing SC’2001 conference
[10] Thomas S and Loft R 2005 J. Sci. Comput. 25 307–322
[11] Collins W D, Rasch P J, Boville B A, Hack J J, Mccaa J R, Williamson D L, Kiehl J T, Brriegleb B, Bitz C, Lin S J, Zhang M and Dai Y 2004 Description of the ncar community atmosphere model (CAM 3.0) Tech. Rep. TN–464+STR NCAR
[12] Simmons A J and Burridge B M 1981 Mon. Wea. Rev. 109 758–766
[13] Taylor M A and Fournier A 2007 In preperation
[14] Jablonowski C and Williamson D L 2006 Q. J. R. Meteorol. Soc. 132 doi:10.1256/qj.06.n