

The Double Fourier Model: A Faster Spectral Dynamical Core

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1 Introduction

We propose a new spectral dynamical core for atmospheric models which uses a double Fourier expansion [1, 2] rather than the standard spherical harmonics. The obvious advantage to such an approach is that fast Fourier transforms can be used in both the longitude *and* latitude directions, rather than the slower associated Legendre transforms used by the standard approach in the latitude direction. Unfortunately, the double Fourier expansion permits discontinuities at the poles and non-isotropic waves which lead to prohibitive time step restrictions. We remedy this by performing a least-squares projection of the prognostic variables onto the spherical harmonics at the end of every time step. Aliasing in Eulerian models is controlled by choosing a 2/3 truncation for the projection. This reintroduces associated Legendre transforms into the dynamics, but reduces the Legendre transform operation count by 42% for Eulerian models (67% for semi-Lagrangian), and reduces the memory requirement from $\mathcal{O}(N^3)$ to $\mathcal{O}(N^2)$ [3] (where N is a measure of the resolution) without requiring the computation of Legendre functions on-the-fly, which in turn results in additional savings from improved cache utilization [4].

2 The Double Fourier Model

To demonstrate the method, we will apply the double Fourier expansion to the Eulerian form of the spherical shallow water equations, in longitude $0 \leq \lambda < 2\pi$ and colatitude $0 \leq \theta \leq \pi$. As with the standard approach, we can minimize the required number of transposes in a distributed memory implementation by solving the absolute-vorticity/divergence (η, δ) form of the governing equations, and we use the spherical scalar form of the velocity components $U = u \sin \theta$, $V = v \sin \theta$, to avoid velocity components which are multi-valued at the poles. The absolute vorticity $\eta = \zeta + f$, where ζ is the relative vorticity $\zeta = \mathbf{k} \cdot \nabla \times (u, v)$, where \mathbf{k} is the outward normal vector and f is the Coriolis parameter with $f = -2\Omega \cos \theta$, where Ω is the rotational rate of the earth. The third prognostic variable is the geopotential, $\phi = gh$, where g is gravitational acceleration at the

surface of the earth and h is the height of the atmosphere. This is decomposed into $\phi = \phi' + \bar{\phi}$, where $\bar{\phi}$ is the global mean geopotential and ϕ' is the geopotential deviation.

It is convenient to define nonlinear terms $A = U\eta$, $B = V\eta$, $C = U\phi'$, $D = V\phi'$ and $E = (U^2 + V^2)/(2\sin^2\theta)$. With these definitions, we can write the governing equations as

$$\sin^2\theta \frac{\partial\eta}{\partial t} = -\frac{1}{a} \frac{\partial A}{\partial\lambda} - \frac{\sin\theta}{a} \frac{\partial B}{\partial\theta}, \quad (1)$$

$$\sin^2\theta \frac{\partial\delta}{\partial t} = \frac{1}{a} \frac{\partial B}{\partial\lambda} - \frac{\sin\theta}{a} \frac{\partial A}{\partial\theta} - \sin^2\theta \nabla^2 (\phi' + E), \quad (2)$$

$$\sin^2\theta \frac{\partial\phi'}{\partial t} = \frac{1}{a} \frac{\partial C}{\partial\lambda} - \frac{\sin\theta}{a} \frac{\partial D}{\partial\theta} - \bar{\phi}\delta \sin^2\theta, \quad (3)$$

where a is the radius of the earth and ∇^2 is the spherical Laplacian operator given by

$$\nabla^2 = \frac{1}{a^2 \sin^2\theta} \frac{\partial^2}{\partial\lambda^2} + \frac{1}{a^2 \sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right).$$

Note that equations (1)–(3) differ from the standard form in that they are scaled by $\sin^2\theta$. This prevents $\sin\theta$ from appearing in the denominator of any terms and facilitates the use of standard trigonometric identities when the double Fourier expansions are utilized.

The velocity components U and V can be obtained from vorticity and divergence by first computing the stream function ψ and velocity potential χ from

$$\sin^2\theta \nabla^2 \psi = \zeta \sin^2\theta, \quad (4)$$

$$\sin^2\theta \nabla^2 \chi = \delta \sin^2\theta, \quad (5)$$

and then utilizing the diagnostic equations

$$U = \frac{1}{a} \frac{\partial\chi}{\partial\lambda} - \frac{\sin\theta}{a} \frac{\partial\psi}{\partial\theta}, \quad (6)$$

$$V = \frac{1}{a} \frac{\partial\psi}{\partial\lambda} + \frac{\sin\theta}{a} \frac{\partial\chi}{\partial\theta}. \quad (7)$$

To solve equations (1)–(7), we expand all the scalar functions in a double Fourier series,

$$\xi(\lambda, \theta) = \sum_{m=-N}^N \xi_m(\theta) e^{im\lambda}, \quad (8)$$

$$\xi_m(\theta) = \begin{cases} \sum_{n=0}^N \xi_{m,n} \cos n\theta, & m \text{ even,} \\ \sum_{n=0}^N \xi_{m,n} \sin n\theta, & m \text{ odd,} \end{cases} \quad (9)$$

where ξ is some arbitrary spherical scalar, m is the longitudinal (or zonal) wave number, n is the latitudinal (or meridional) wave number, and $i = \sqrt{-1}$. As with spherical harmonics, transformation between grid space, $\xi(\lambda_i, \theta_j)$ for $i = 1 \dots N_{\text{lon}}$, $j = 1 \dots N_{\text{lat}}$, and double Fourier space $\xi_{m,n}$ is facilitated by the introduction of single Fourier space $\xi_m(\theta)$.

This expansion was first proposed explicitly by Yee [5], based on the ideas of Orszag [1]. It has been avoided in operational models in the past because it permits discontinuities at the poles and non-isotropic waves which lead to prohibitive time-step restrictions. By projecting $\eta_{m,n}$, $\delta_{m,n}$ and $\phi'_{m,n}$ onto the space of spherical harmonics after each is advanced forward in time, these problems are avoided and the numerical results are the same as the standard approach to within roundoff, while still providing a savings in operation count.

The governing equations in this form are now suitable for expansion in terms of double Fourier series. For example, equations (4) and (5) are in the same form as in Yee [5]. Further, if we denote the double Fourier coefficients of $\frac{\partial \xi}{\partial \lambda}$ by $\left(\frac{\partial \xi}{\partial \lambda}\right)_{m,n}$, it is trivial to show that

$$\left(\frac{\partial \xi}{\partial \lambda}\right)_{m,n} = im\xi_{m,n}. \quad (10)$$

Similarly, we can utilize simple trigonometric identities to obtain

$$\left(\sin \theta \frac{\partial \xi}{\partial \theta}\right)_{m,n} = r\xi_{m,n-1} - s\xi_{m,n+1}, \quad (11)$$

where

$$(r, s) = \begin{cases} (0, \frac{1}{2}), & n = 0, \\ (\frac{n-1}{2}, \frac{n+1}{2}), & 0 < n < N, \\ (\frac{N-1}{2}, 0), & n = N, \end{cases}$$

and

$$(\xi \sin^2 \theta)_{m,n} = x\xi_{m,n-2} + y\xi_{m,n} + z\xi_{m,n+2}, \quad (12)$$

where

$$(x, y, z) = \begin{cases} (0, \frac{1}{2}, -\frac{1}{4}), & n = 0, \\ (0, \frac{(1+2\ell)}{4}, -\frac{1}{4}), & n = 1, \\ (\frac{2\ell-2}{4}, \frac{1}{2}, -\frac{1}{4}), & n = 2, \\ (-\frac{1}{4}, \frac{1}{2}, -\frac{1}{4}), & 2 < n < N-1, \\ (-\frac{1}{4}, \frac{1}{2}, 0), & n = N-1, N, \end{cases}$$

and $\ell = 0$ (1) if m is even (odd). The coefficients for the $\sin^2 \theta \nabla^2$ operator are obtained in the same manner as in [5].

All the pieces are now in place to develop an algorithm for advancing the shallow water equations forward in time using leapfrog time stepping. Let R^η , R^δ and R^ϕ equal the right hand sides of equations (1)–(3), respectively. We begin at an arbitrary time step level given current grid point values of η , ϕ' , U

and V , as well as double Fourier coefficients $\eta_{m,n}$, $\delta_{m,n}$ and $\phi'_{m,n}$, either from the previous time step or initialization. The following steps will advance the solution forward in time by one time step.

1. From η , ϕ' , U and V , compute the nonlinear terms A , B , C , D and E in grid space.
2. Transform A , B , C , D and E from grid space to double Fourier space. This introduces five transposes to a parallel implementation.
3. Compute $R_{m,n}^\eta$, $R_{m,n}^\delta$ and $R_{m,n}^{\phi'}$ using the double Fourier differentiation and Laplace operator rules, and advance $\eta_{m,n}$, $\delta_{m,n}$ and $\phi'_{m,n}$ forward in time using leapfrog time stepping and (12).
4. Project $\eta_{m,n}$, $\delta_{m,n}$ and $\phi'_{m,n}$ onto the space of spherical harmonics using an associated Legendre projection.
5. Compute $\zeta_{m,n}$ by adding 2Ω to $\eta_{0,1}$. Solve (4) and (5) for $\psi_{m,n}$ and $\chi_{m,n}$ using Yee's method, and compute $U_{m,n}$ and $V_{m,n}$ from (6) and (7) using the differentiation rules (10) and (11).
6. Transform $\eta_{m,n}$, $\phi'_{m,n}$, $U_{m,n}$ and $V_{m,n}$ from double Fourier space back to grid space. This introduces an additional four transposes to a parallel implementation, for a total of nine.

This puts the model in an appropriate state for grid-point based physics.

3 The Associated Legendre Projection

The motivation for proposing the double Fourier method is to increase the speed of the dynamics of atmospheric models. The associated Legendre transform is the only $\mathcal{O}(N^3)$ algorithm in either the standard or proposed methods, and the proposed method reduces the number of required transforms from nine to six. Additional savings are possible because the projection can be made more efficient in ways the individual transforms cannot. Jakob and Alpert [6] developed an asymptotically $\mathcal{O}(N^2)$ projection based on the fast multipole method which was improved by Yarvin and Rokhlin [7]. Swarztrauber and Spatz [3] developed a projection based on the weighted orthogonal complement to the associated Legendre functions, which provides a 50% and 12.5% reduction in operation count versus standard transforms for untruncated and 2/3 truncated projections, respectively.

The performance of these projections were compared recently [4], where it was found that the weighted orthogonal complement (WOC) projection has the best overall performance. The fast multipole method provides some savings over the standard method for performing associated Legendre transforms, but requires too much overhead to run faster than the WOC at resolutions of current interest. Furthermore, the WOC functions require only $\mathcal{O}(N^2)$ storage, as opposed to $\mathcal{O}(N^3)$, which leads to cache reutilization and additional savings.

The overall savings of the WOC projection compared to a forward and backward associated Legendre transform is roughly 80% and 60% for untruncated and 2/3 rule truncations, respectively. Combined with the fact that within a shallow water model fewer transforms are needed, this translates roughly to spending 13% and 26% the amount of time performing Legendre transforms compared to the standard approach.

4 Overhead

The savings obtained by using the projection instead of standard transforms are reduced by the addition of overhead incurred by the double Fourier model. For example, the Poisson equation reduces to an explicit calculation for a spherical harmonics expansion. For the double Fourier method, the Poisson solver reduces to a series of $2N$ tridiagonal systems of rank N . The same is true of the time derivative terms, which are scaled by $\sin^2 \theta$ and result in a tridiagonal system as in (12). Also, double Fourier series employ a rectangular truncation as compared to a triangular truncation, effectively doubling any calculation involving spectral coefficients, such as derivatives or building the right-hand side terms. Finally, the 15 sin and cos transforms in θ (nine for the transforms to and from grid space and six for the projection) have to be completely regarded as overhead when compared to the spherical harmonic method. Thus the double Fourier method will break even with the spherical harmonics method when the overhead (proportional to N^2 and $N^2 \log N$) equals the savings provided by the projection algorithm. Our current goal is to achieve break-even timings between T85 and T170 resolutions.

5 Future Work

The double Fourier method, combined with an associated Legendre projection, provides an attractive alternative to the standard spherical harmonic approach. It provides the same accuracy and stability as the spherical harmonics, while providing a reduced operation count at moderate resolutions. The discussion here has been for an Eulerian formulation, but the associated Legendre projection savings are even greater for a semi-Lagrangian formulation. Furthermore, research continues on the projection algorithm. The ideas of Dilts [8] may be used to eliminate six $\sin \theta$ and $\cos \theta$ transforms. Perhaps the weighted orthogonal complement ideas can be combined with the fast multipole method in a manner which takes advantage of the efficiencies of both. Finally, the triangular UTV decomposition is being explored to exploit additional optimizations.

References

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