THE SPECTRAL METHOD (draft-version 1)

Introduction
When using finite difference techniques for evolutionary problems, we only consider grid-point values of the dependent variables; no assumption is made about how the variables behave between grid points. An alternative approach is to expand the dependent variables in terms of a finite series of smooth orthogonal functions. The problem is then reduced to solving a set of ordinary differential equations which determine the behaviour in time of the expansion coefficients.

As an example consider the linear one-dimensional evolutionary problem

$$\partial_t \varphi = H(\varphi) \tag{1}$$

where H is a linear differential operator. Expanding in terms of a set of orthogonal functions
$$e_m(x), m = m_1, m_2, m_{3.} \dots\dots\dots\dots\dots \tag{2}$$
so that φ is written as
$$\varphi = \sum_m \varphi_m(t)\, e_m(x) \tag{3}$$
the sum is taken over all possible wave numbers $(-\infty, +\infty)$
The expansion functions are orthonormal so that

$$\int_x e_l^*(x) e_m(x) dx = \begin{cases} 1, & l = m \\ 0, & l \neq m \end{cases} \tag{4}$$

where $e_l^*(x)$ is the complex conjugate of $e_l(x)$

The $\varphi_m(t)$ are the expansion coefficients whose behaviour we want to determine. Eq. (1) is multiplied by $e_l^*(x)$ and we integrate over all possible x-values. This give,
$$\int_x \partial_t \varphi\, e_l^*(x)\, dx = \int_x H(\varphi)\, e_l^*(x)\, dx \tag{5}$$
The procedure is valid for all possible values of l.

Since $\int_x \partial_t \varphi\, e_l^*(x)\, dx = \int_x (\sum_m \partial_t (\varphi_m(t)) e_m(x))\, e_l^*(x)\, dx$, we only get contributions from wave number $m=l$, so that
$$\partial_t \varphi_m = \sum_m \varphi_m(x) \int_x e_l^*(x) H(e_m) dx \tag{6}$$
That is, we have a set of ordinary differential equations for the rate of change with time of the expansion coefficients.

It is now interesting to consider how our choice of expansion functions can greatly simplify the problem

(a) If the expansion functions are eigenfunctions of H, we have $H(e_m) = \lambda_m e_m$ where the λ_m are the eigenvalues; Eq. (6) then becomes

$$\partial_t \varphi_m = \sum_m \varphi_m(x) \int_x e_l^*(x) \lambda_m e_m(x) dx = \lambda_m \varphi_m, \quad \text{for all m} \tag{7}$$

The equations have become decoupled.

(b) If the original equation is

$$L(\partial_t \varphi) = H(\varphi) \tag{8}$$

where *L* is a linear operator, then our problem is simplified by using expansion functions that are eigenfunctions of *L* with eigenvalues λ_m; we then have,

$$\lambda_m \, \partial t(\varphi_m) = \sum_m \varphi_m \int_x e_l^* H(e_m) dx \tag{9}$$

The one-dimensional linear advection equation
We demonstrate the method for the one dimensional advection equation on the globe, e.g. along a latitude where with cyclic boundary conditions
$$\partial_t \varphi = -c \partial \varphi_x \tag{10}$$
It is convenient to write the advection equation in terms of the longitude and the angular velocity.
We therefore change coordinates to $\lambda = \dfrac{2\pi x}{L}$ where L is the cicumference around the globe at the particular latitude $L = 2\pi r = 2\pi a \cos(latitude)$, where a is the radius of the earth.
Since $\partial_x = (\partial_x \lambda) \partial_\lambda = \dfrac{2\pi}{L} \partial_\lambda$ we get
$$\partial_t \varphi = -(c2\pi/L) \partial_\lambda \varphi \equiv -\gamma \partial_\lambda \varphi$$
i.e.

$$\partial_t \varphi = -\gamma \partial_\lambda \varphi \tag{11}$$

with boundary conditions: $\varphi(\lambda,t) = \varphi(\lambda + 2\pi p, t)$ (p is a natural number), and initial conditions: $\varphi(\lambda,0) = f(\lambda)$. For any reasonable function $f(\lambda)$, the analytical solution of (11) is

$$f(\lambda - \gamma t) \tag{12}$$

We must now choose suitable expansion functions. The obvious choice is the finite Fourier series

$$\varphi(\lambda,t) = \sum_m \varphi_m(t) e^{im\lambda}, \text{ (i.e. a Fourier series)} \tag{13}$$

because the expansion functions are then eigenfunctions of the differential space operator.

Using grid points rather than a continuous representations, we need to use a truncated series, i.e.

$$\varphi(\lambda,t) = \sum_{m=-M}^{m=+M} \varphi_m(t) e^{im\lambda} \tag{14}$$

Here M is the maximum wave number and the $\varphi_m(t)$ are the complex expansion coefficients. Since $\varphi_{-m}(t) = \varphi_m^*(t)$, we need only be concerned with φ_m for $0 \leq m \leq M$, rather than the full set of expansion coefficients.

We now substitute into (11) and equate coefficients of the expansion functions. This yield

$$\partial_t(\varphi_m) + \gamma i m \varphi_m = 0, \quad m = -M, M \tag{15}$$

giving 2M+1 equations for the φ_m's. For this particular case (15) can be integrated exactly to give

$$\varphi_m(t) = \varphi_m(0) e^{-i\gamma t} \tag{16}$$

If $f(\lambda)$ is also represented by a truncated Fourier series $f(\lambda) = \sum_m a_m e^{im\lambda}$, the complete solution is

$$\varphi(\lambda,t) = \sum_{-m}^{m} a_m e^{im(\lambda - \gamma t)} \tag{17}$$

which is the same as the exact (analytical) solution of (11). There is no dispersion due to the space discretization, unlike in the finite differences method. This fact is due to the space derivatives being computed analytically while they were approximated in the finite difference method.

Scalarly multiplying (14)

$$\varphi(\lambda,t) = \sum_{m=-M}^{m=+M} \varphi_m(t) e^{im\lambda}, \text{ by each of the basis functions } (e^{-il\lambda}, l = -M, M)$$

and using the orthogonality property of the Fourier basis we get at the initial time

$$\varphi_m(0) = A_m \int_0^{2\pi} \varphi(\lambda,0) e^{-im\lambda} d\lambda \tag{18}$$

where A_m are the normalization factors (which is known as the direct Fourier transform).

$$\varphi_m(0) = A_m \int_0^{2\pi} \varphi(\lambda,0) e^{-im\lambda} d\lambda \tag{19}$$

In the practice the initial conditions can be given in the form of grid-point data (N+1 points with spacing say). Therefore, we think of the truncated Fourier series as representing an interpolating function which exactly fits the values of at the grid points. Eq. (18) must then be computed as a finite sum, i,e,

$$\varphi_m(0) = A'_m \sum_{j=1}^{K} \varphi(\lambda_j,0)e^{-im\lambda_j} \qquad (20)$$

which is known as discrete direct Fourier transform. The corresponding discrete inverse Fourier transform is

$$\varphi(\lambda_j,0) = \sum_{m=-M}^{M} \varphi_m(0)e^{im\lambda_j} \qquad (21)$$

Both of them can be computed with the Fast Fourier Transform (FFT) algorithm. It can be shown that, starting from the set of $\varphi_m(0)$, going to the set $\varphi(\lambda_j,0), j=1,.....,K$, and returning to $\varphi_m(0)$, we recover exactly the original values (the transforms are exact) as long as $K \geq 2M+1$ and the points are equally spaced in λ. This distribution of points with $K = 2M+1$ is known as the linear grid. On the other hand it can be shown also that the product of two functions can be computed without aliassing by the transform method of transforming both functions to grid-point space, multiplying together the functions at each grid-point and transforming back the product to Fourier space, as long as $K \geq 3M+1$. The distribution of points for which $K = 3M+1$ is known as the quadratic grid.

Having derived the initial conditions in terms of the spectral coefficients we must now integrate the ordinary differential equations for the expansion coefficients at some future time. Normally this has to be done using a timestepping procedure such as the leapfrog scheme, i.e. $\partial_t(\varphi_m) = F_m$, which we for instance solve by,

$$\varphi_m^{n+1} = \varphi_m^{n-1} + 2\Delta t\, F_m^n$$

In our case,

$$\varphi_m^{n+1} = \varphi_m^{n-1} - i\gamma m 2\Delta t\, \varphi_m^n$$

A standard stability analysis shows that the scheme is stable if $G^2 + 2im\gamma\Delta t G - 1 = 0$, i.e. $G = im\gamma\Delta t \pm \sqrt{1 - m^2\gamma^2\Delta t^2}$ so that as long as $|1 - m^2\gamma^2\Delta t^2| \leq 1$ the scheme is stable. But since the maximum value of $m=M$, we require $M\gamma\Delta t \leq 1$.

Utilizing that $\lambda = \dfrac{2\pi x}{L}$ this means that $\dfrac{Mc2\pi\Delta t}{L} \leq 1$. We further introduce that $L = 2M\Delta x$ and

obtain $\dfrac{c\Delta t}{\Delta x} \leq \dfrac{1}{2}$ \qquad (22)

This shows that the stability criterion is more restrictive than for conventional explicit finite difference schemes. However, the spectral scheme has the great advantage that it has only very small phase errors which are not significant even for two grid length waves.

Non-linear terms
In practice there are two approaches to the problem of calculating non-linear terms in the context of the spectral method—using interaction coefficients or the transform method. The transform is normally used for purposes where the numbers of grid points is not trivially small.

Using Fast Fourier Transforms (FFTs) it is easy to move from the spectral representation (spectral space) to a grid-point representation (physical space). Therefore, the essence of the transform method is to calculate derivatives in spectral space, but to transform to physical space using FFTs whenever a product is required. Once all the products have been computed at grid points, the spectral coefficients of this product field are calculated—that is we use FFTs to return to spectral space. Now, consider how we apply this to the non-linear advection equation. Given the we want to compute the spectral coefficients of the non-linear term $u\partial_x u$ (i.e. the on the right-hand side of $\partial_t u = -u\partial_x u = F$ The following three steps are required to do this:
(i) Calculate and at grid points by using the spectral coefficients
$$u(\lambda_j) = \sum_m u_m e^{im\lambda_j} \ , \quad D(\lambda_j) = \sum_m im u_m e^{im\lambda_j}$$
(ii) Calculate the advection term at each grid point in physical space
$$F(\lambda_j) = -u(\lambda_j) \cdot D(\lambda_j)$$

(iii) Return to spectral space by calculating the Fourier coefficients
$$F_m = \frac{1}{2\pi} \sum F(\lambda_j) e^{-im\lambda_j} \tag{23}$$

In practice this procedure has to be employed to calculate the spectral coefficients of the non-linear term at every time level. As the product of the two functions is computed in grid-point space and not in spectral space, we get aliasing unless the number of grid-points corresponds to the quadratic grid. Even so, products of more than two functions will still have aliasing.

The spherical harmonics
When using spherical geometry (i.e. on the globe) it is natural to expand any dependent variable in terms of a truncated series of spherical harmonics which have the nice property of being eigenfunctions of the Laplacian in spherical geometry. Remember that when applying the semi-implicit approach for time stepping of the primitive equations we obtain a Helmholz equation. This approach simplifies solving this equation considerably. The spherical harmonics are,
$$\varphi(\lambda,\mu,t) = \sum_{m=-M}^{M} \left\{ \sum_{n=|m|}^{J} \varphi_n^m(t) Y_n^m(\lambda,\mu) \right\}$$
$\quad$ (24)
where λ is the longitude and $\mu = \sin(latitude)$. Again m is the zonal wave number, now n the total wavenumber and $n-|m|$ represents the effective meridional wave number. In (24) we can choose the truncation that we want.

(a) If *J=M* the truncation is described as <u>triangular</u> (a model with this truncation and *m=40* is

said to be a T40 model).

(b) For rhomboidal truncation $J=M+|m|$.

(If the circumference along a latitude around the globe is 20000 km (approximately at 60°N), T40 truncation means that there are 40 wavelengths around the globe at that latitude, i.e. the smallest wave length is 20000 km/40= 500km. If we assume that we need at least 4 gridlengths to resolve a wave, the effective resolution is 125 km.)

The reason for naming the truncations as triangular or rhomboidal respectively, becomes apparent when we plot a diagram of permissible values of *n* and *m* for fixed *M*; such diagrams for *M*=4 are shown in Fig. 1 below.
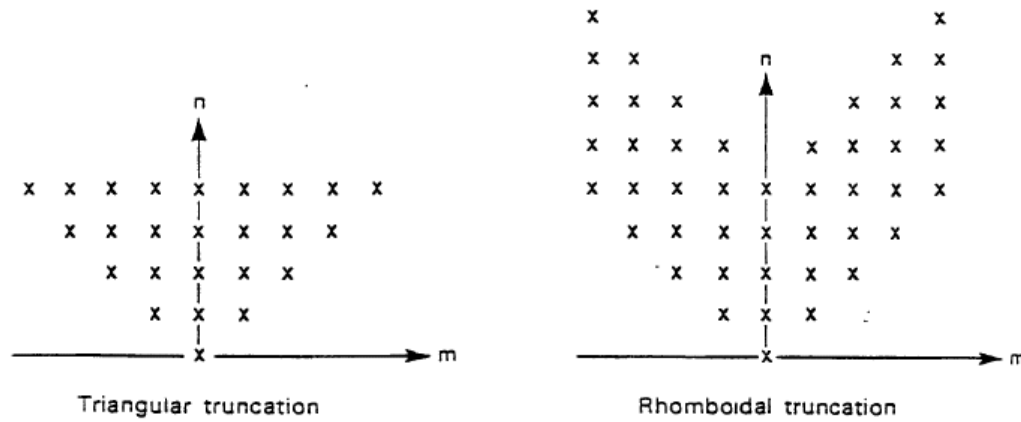

Fig. 1 Triangular truncation showing permissible values of m and n for the triangular and rhomboidal truncation for M=4.

The spherical harmonics have the nice property that

$$\nabla^2 Y_n^m = \frac{n(n+1)}{a^2} Y_m^m \qquad (25)$$

where is the Laplacian in spherical coordinates and is *a* the earth's radius. Another property is that $Y_m^m = P_m^m(\mu)e^{im\lambda}$ where P_m^m is the associated Legendre polynomial of degree *n* and order *m*.

The Legendre polynomials are orthogonal:

$$\frac{1}{2}\int_{-1}^{1} P_n^m(\mu)P_s^m(\mu)d\mu = \delta_{n,s}$$

The space derivatives can be computed analytically as:

$$\frac{\partial}{\partial \lambda} Y_m^m = im Y_m^m, \quad m \geq 0$$

and using the properties of the Legendre polynomial we have

$$(1 - \mu 2) \frac{\partial}{\partial \mu} Y_n^m = -n \varepsilon_{n+1}^m Y_{n+1}^m + (n+1) \varepsilon_n^m Y_{n-1}^m$$

$$\varepsilon_n^m = \left\{ \frac{n^2 - m^2}{4(n-1)} \right\}^{\frac{1}{2}}$$

For $m > 0$ we use the fact that $Y_m^{-m} = (Y_m^m)^*$ .With these relationships space derivatives can be calculated exactly leaving a set of ordinary differential equations for the time rate of change of the spherical harmonic coefficients φ_m^m .

Normally we have to deal with non-linear terms in which two spherical harmonics interact to produce a third. Unless the truncation is very severe the calculations are very time consuming. This problem can be overcome by the transform method introduced earlier.

 (a) Starting in spectral space, the spectral coefficients are used to calculate the dependent variables on a latitude–longitude grid (inverse spectral transform). For a regularly spaced longitude grid with at least *2M+1* points and a specially chosen latitude grid (the Gaussian latitudes which are almost regularly spaced), the transformation can be done exactly.

 (b) The non-linear dynamics and physical process terms of each prognostic equation are calculated in real space.

 (c) The non-linear terms are transformed back to the spectral domain (direct spectral transform).

In order to perform the spectral transforms it is convenient to introduce the Fourier coefficients

$$\varphi_n^m(t) = \frac{1}{4\pi} \int_0^{2\pi} \varphi(\lambda, \mu, t) e^{-im\lambda} d\lambda = \sum_{n=|m|}^{N} \varphi_n^m(t) P_n^m(\mu)$$

Scalarly multiplying (25) by each of the spherical harmonics and making use of the orthogonality properties of both the Fourier basis functions and the Legendre polynomials, we get

$$\varphi_n^m(t) = \frac{1}{4\pi} \int_0^1 \int_0^{2\pi} \varphi(\lambda, \mu, t) P_n^m(\mu) e^{-im\lambda} d\lambda d\mu$$

which is the direct spectral transform. This transform can be done by first performing the integral with respect to λ . This is a Fourier transform which will compute the Fourier coefficients. If the original function is given in a discrete set of longitude points, the transform is a discrete Fourier transform and, as discussed earlier it is exact if the longitude points are equally spaced and its number is at least 2M+1.

The integral with respect to the latitude can be performed from the Fourier coefficients by means of a Gaussian quadrature formula and it can be shown that this integral is exact if the latitudes at which the input data are given are taken at the points where

$$P_{N_G}^0 = 0$$

(these are called the Gaussian latitudes) with $N_G \geq (2M+1)/2$. Furthermore products of two functions can be computed alias-free if the number of Gaussian latitudes is $N_G \geq (3M+1)/2$. The Gaussian latitudes are not equally spaced as the points to compute the discrete Fourier transforms but they are nearly so and therefore this spacing is approximately the same as the longitudinal spacing.

The distribution of points allowing exact transforms is called the linear Gaussian grid and it has at least (2M+1) longitude points equally spaced at each of at least (2M+1)/2 Gaussian latitude rows. Products of two functions can be computed alias-free if we use a quadratic Gaussian grid which is made of at least (3M+1) equally spaced points in each of at least (3M+1)/2 Gaussian latitudes.

Finally it should be noted that only true scalars should be represented by a series of spherical harmonics: hence when spectral methods are used, the primitive equations are put in their vorticity and divergence form, rather than in their momentum (u and v) form.

Diffusion in spectral space
The linear diffusion equation in two dimensions for a variable A is

$$\partial_t A = K\nabla^2 A, \quad K > 0$$

Transforming to spectral space and making use of the property of the spherical harmonics we get

$$\partial_t A_n^m = -K\frac{n(n+1)}{a^2} A_n^m$$

As we know, applying the leapfrog time discretization we get two solutions, the physical solution which is unconditionally stable and a computational solution which is unconditionally unstable. If we apply a forward time-stepping scheme we get one solution which is conditionally stable. Finally if we apply a fully implicit (or backward) time-stepping scheme we get

$$A_n^m(t + \Delta t) = \frac{A_n^m(t)}{1 + \Delta t K n(n+1)/a^2}$$

which is a decoupled system of equations and the scheme is unconditionally stable.
There is no penalty for using an implicit time-stepping scheme because the basis functions are eigenfunctions of the equation operator. It is also straightforward to apply a superharmonic operator such as ∇^4, or even ∇^{2m} with any integer value of m. It suffices to substitute in the solution $n(n+1)/a^2$ by $(n(n+1)/a^2)^m$

Advantages and disadvantages

(a) Advantages.

(i) Space derivatives calculated exactly.

(ii) Non-linear quadratic terns calculated without aliasing (if computed in spectral space or using the quadratic grid).

(iii) For a given accuracy fewer degrees of freedom are required than in a grid-point model.

(iv) Easy to construct semi-implicit schemes since spherical harmonics are eigenfunctions of the

Helmholtz operator.

(v) On the sphere there is no pole problem.

(vi) Phase lag errors of mid-latitude synoptic disturbances are reduced.

(vii) The use of staggered grids is avoided.

(b) Disadvantages.

(i) The schemes appear complicated, though they are relatively easy to implement.

(ii) The calculation of the non-linear terms takes a long time unless the transform method is used.

(iii) Physical processes cannot be included unless the transform method is used.

(iv) As the horizontal resolution is refined, the number of arithmetic operations increases faster in spectral models than in grid-point models due to the Legendre transforms whose cost increases as N3.

(v) Spherical harmonics are not suitable for limited-area models.