1 Spatial Discretization (Galerkin Methods)

1.1 Background

- Assume a differential equation of the type:

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0$$

- There are two classes of spatial discretization methods:

  - 1. Finite Difference Methods: discretize in differential form

$$\frac{\partial u_i}{\partial t} + \frac{f^n_{i+1} - f^n_{i-1}}{2\Delta x} = 0$$

where the differencing stencil are constructed via Taylor series expansions. For example, the derivative $\frac{\partial f}{\partial x}$ is approximated as follows:

$$f_{i+1} = f_i + \Delta x \frac{\partial f_i}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 f_i}{\partial x^2} + O(\Delta x^3)$$

and

$$f_{i-1} = f_i - \Delta x \frac{\partial f_i}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 f_i}{\partial x^2} - O(\Delta x^3)$$

which, subtracting, gives

$$f_{i+1} - f_{i-1} = 2\Delta x \frac{\partial f_i}{\partial x} + O(\Delta x^3)$$

which then gives:

$$\frac{f_{i+1} - f_{i-1}}{2\Delta x} = \frac{\partial f_i}{\partial x} + O(\Delta x^2)$$

If a higher order approximation is desired we then require information from additional grid points. For example:

$$f_{i+1} = f_i + \Delta x \frac{\partial f_i}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 f_i}{\partial x^2} + \frac{\Delta x^3}{6}\frac{\partial^3 f_i}{\partial x^3} + O(\Delta x^4),$$

$$f_{i-1} = f_i - \Delta x \frac{\partial f_i}{\partial x} + \frac{\Delta x^2}{2}\frac{\partial^2 f_i}{\partial x^2} - \frac{\Delta x^3}{6}\frac{\partial^3 f_i}{\partial x^3} + O(\Delta x^4),$$

and

$$f_{i+2} = f_i + 2\Delta x \frac{\partial f_i}{\partial x} + \frac{(2\Delta x)^2}{2}\frac{\partial^2 f_i}{\partial x^2} + \frac{(2\Delta x)^3}{6}\frac{\partial^3 f_i}{\partial x^3} + O(\Delta x^4)$$

2. Galerkin Methods - discretize in integral form

$$\int_\Omega \psi \left(\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} \right) d\Omega = 0$$

where

$$u(x) = \sum_{i=0}^{N} u_i \psi_i(x) \quad \text{and} \quad f(x) = \sum_{i=0}^{N} f_i \psi_i(x)$$

and $\psi$are basis functions.
To construct a higher order approximation we merely change the basis functions.

2 Introduction to Galerkin Methods

- For all Galerkin methods the idea is to solve any differential operator

$$L(u) = 0$$

by approximating u as a polynomial expansion

$$u(x) = \sum_{i=0}^{N} a_i \psi_i(x) \tag{1}$$

where ψ are the polynomials (basis functions) and a are the expansion coefficients.

  - The statement of the problem is as follows: find $u \in H^1$ such that

$$\int_\Omega L(u)\psi \; d\Omega = 0 \qquad \forall\, \psi \in H^1.$$

- Thus we seek a set of basis functions ψ and coefficients a such that the inner product of the basis functions to the differential operator is orthogonal

$$(L(u), \psi) = 0$$

where the inner product is defined in the Hilbert space (of square integrable functions)

$$\int_\Omega L(u)\psi \; d\Omega = 0.$$

- Depending on what we pick for a and ψ will determine which spatial discretization method we are using. The following definition is required.

Definition 1 *A Hilbert space is an inner product space, with inner product defined as*

$$(u, v) = \int_\Omega uv \; d\Omega$$

which is complete. In other words, there exists a set of linearly independent vectors (v) in which any point in the space can be expanded in terms of these linearly independent vectors. A complete set of linearly independent vectors forms a basis.

- Sturm-Liouville Operator

$$\frac{d}{dx}\left(p(x)\frac{d\phi}{dx}\right) + \lambda\sigma(x)\phi = 0$$

contains the largest class of operators contained in most differential equations. The eigenfunctions and corresponding eigenvectors of this operator form a complete basis in the space where the operator is defined. This means that as $N \to \infty$ the interpolation error goes to zero converging exponentially. Thus if we were to solve semi-analytically a differential equation containing any portion of this operator, we would expand the coefficients in terms of such functions (e.g., eigenfunction expansions and separation of variables).

  - 1D Periodic BC: for the domain $x \in [0, 2\pi]$ the eigenfunctions are the Fourier series.

- 1D Non-Periodic BC: for the domain $x \in [-1, +1]$ the eigenfunctions are the Legendre polynomials.
- 2D Quadrilateral: for the domain $(x, y) \in [-1, +1]$ the eigenfunctions are the tensor product of Legendre polynomials.
- 2D Triangle: for the domain comprised of a triangle, the eigenfunctions are the Proriol-Koornwinder-Dubiner (PKD) polynomials - which represent a warped tensor product of Jacobi polynomials.

2.1 Spectral Transform Method (Spherical Harmonics)

Remark 1 *Spectral models (spherical harmonics) use Fourier series in the latitude circles ($\lambda \in [0, 2\pi]$) and Legendre polynomials in the longitude semi-circles ($\theta \in [-\frac{\pi}{2}, +\frac{\pi}{2}] \Longleftrightarrow [-1, +1]$).*

- spectral transform methods: use modal expansions such as

$$u(\xi) = \sum_{m=0}^{N} \widetilde{u}_m L_m(\xi)$$

  where $\widetilde{u}_m, L_m$ represent the amplitude and frequency of the mth mode

2.2 Finite/Spectral Element Method

Remark 2 *In contrast finite/spectral element methods remap the global domain into pieces with domains $[-1, +1]$ where the Legendre polynomials are the natural basis.*

- Finite/Spectral Element Methods: use either modal or nodal expansions
- Nodal expansions are

$$u(\xi) = \sum_{n=0}^{N} u_n \psi_n(\xi)$$

  where u_n, ψ_n are the values and cardinal functions at the nth node

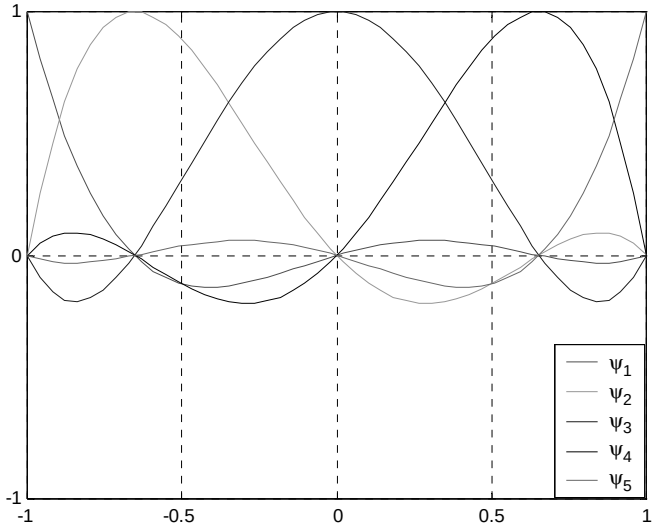


Figure 1: $N = 4$ cardinal functions.

Remark 3 *A cardinal function is a Lagrange polynomial with the characteristic of a Kronecker delta function δ_{ij}. Simply put, a cardinal function is 1 at its gridpoint and zero at all other gridpoints. However, between grid points the function will oscillate and will be an Nth order polynomial. Here is an example of 4th order cardinal functions.*

- Modal expansions: we can map any modal expansion

$$u(\xi) = \sum_{m=0}^{N} \widetilde{u}_m L_m(\xi)$$

  to the nodal expansion

$$u(\xi) = \sum_{n=0}^{N} u_n \psi_n(\xi)$$

  via the Legendre transform thus these two expansions are equivalent

- H-type (FEM): use low order basis functions (N) but many elements

- P-type (SEM): uses high order basis functions (N) but few elements
  - $N = 1$ yields the finite element method
  - $N \to \infty$ yields the spectral transform method

2.3 Numerical Integration

2.3.1 Introduction

- Because Galerkin methods use the integral form of the equations we then need to evaluate integrals
- It is far more general to perform the integration numerically since then we can use any order polynomial without having to worry about exact integration

2.3.2 Efficiency

- For an integral of the type

$$\int_{-1}^{+1} \psi_i(\xi)\psi_j(\xi)\, d\xi = \sum_{q=0}^{Q} w_q \psi_i(\xi_q)\psi_j(\xi_q)$$

  we know that $Q = \frac{cN}{2} + 1$ for exact integration where $c = 4$ for the atmospheric hydrostatic primitive equations (for $N = 8$ we need $Q = 19$!).
- For $i, j = 0..., N$ this results in a $(N + 1) \times (N + 1)$ matrix
- Instead, we use $Q = N$ which results in

$$\int_{-1}^{+1} \psi_i(\xi)\psi_j(\xi)\, d\xi = w_i \delta_{ij}$$

  where

$$\delta_{ij} = \begin{cases} 1 & \text{for} \quad i = j \\ 0 & \text{for} \quad i \neq j \end{cases}$$

- This now yields an $(N + 1)$ vector (diagonal matrix)

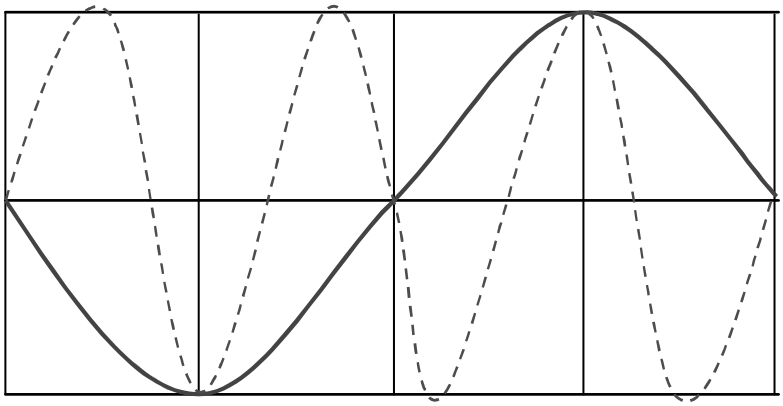


Figure 2: Aliasing Error: When the grid is not sufficiently resolved, high frequency waves may be interpretted as low frequency waves by the numerical scheme. This is known as aliasing errors.

2.3.3 Accuracy

- Is $Q = N$ accurate?
- For $N \geq 4$ using $Q = N$ versus $Q = \frac{cN+1}{2}$ makes absolutely no difference in terms of accuracy - both yield exponential convergence (Giraldo 1998).
- For $N < 4$ it does make a big difference
- Typically we use $N \in [8, 16]$

2.4 Filters

2.4.1 Aliasing Error

- All high order methods suffer from aliasing errors Note that the high frequency wave (red dashed line) is interpreted by the grid and the scheme as the thick (blue) line. Low order methods do not suffer as severely from aliasing errors because they are too diffusive and thereby either damp out or ignore the high frequency waves altogether. In essence, low order schemes have implicit filters. However, these low

order filters are not scale selective and thus can damp out most of the waves including those containing pertinent information. Therefore, high order methods need to filter these high frequency waves before they *pollute* the solution.

2.4.2 Diffusion Operators

- Gridpoint models use diffusion operators

$$\nabla^F u$$

  as filters where F corresponds to the order of the filter operator

- Usually $F = 4$ is used (COAMPS, NOGAPS, ans WRF)

- Unfortunately this is not very scale selective - that is, any wave higher than 4th order will be wiped out.

2.4.3 Spectral Filters

- A better approach is to use spectral-type filters

- We map the nodal expansion

$$u(\xi) = \sum_{n=0}^{N} u_n \psi_n(\xi)$$

  into the modal expansion

$$u(\xi) = \sum_{m=0}^{N} \widetilde{u}_m L_m(\xi)$$

  where $\widetilde{u}$, L are Legendre coefficients and Legendre functions

- In nodal space the basis functions ψ_n are simply high order approximations which yield the physical values

- In modal space the basis functions L_m are the wave/frequency modes (and $\widetilde{u}$ are their amplitudes)

- We can then map from nodal to modal space via the Legendre transform (see Equation 36 in the notes on page 33)

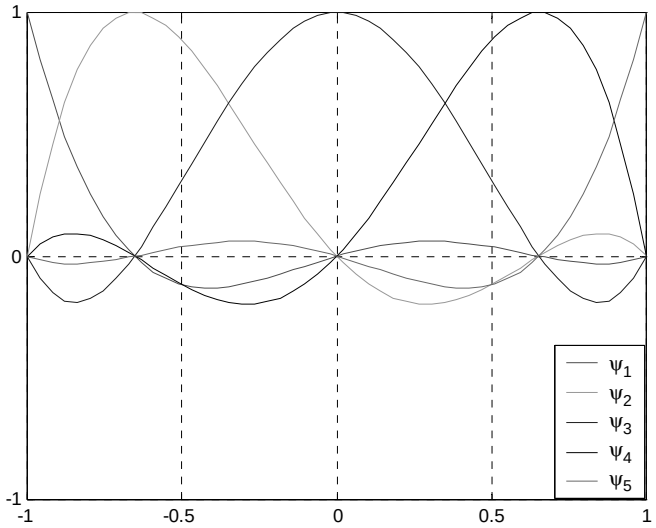


Figure 3: A nodal expansion for $N = 4$.

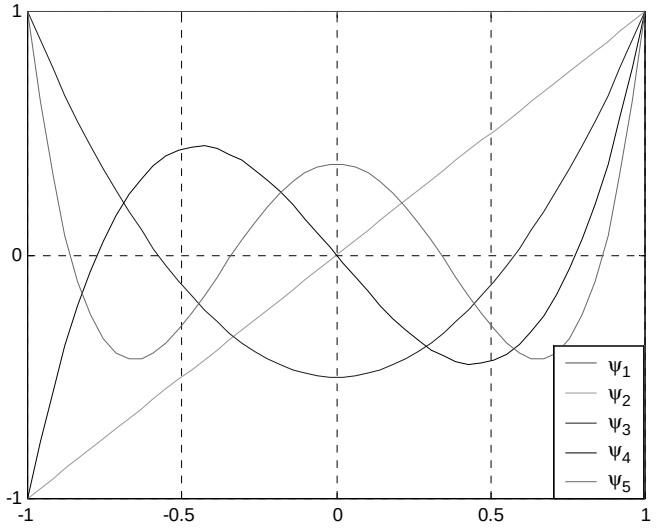


Figure 4: A modal expansion for $N = 4$.

- In this fashion we can construct a general filter equivalent to

$$\nabla^F u$$

  without having to compute derivatives

- We typically use $F = 12$ which is far more scale selective than $F = 4$

2.5 Application of Finite/Spectral Element Method

2.5.1 1D Wave Equation

- Conservation Law

$$\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = 0 \quad \text{where} \quad f = au$$

- Weak integral form

$$\int_\Omega \psi_i \left(\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} \right) d\Omega = 0$$

- Approximation $N = 1$ gives

$$u(x,t) = \sum_{j=0}^{1} u_j(t)\psi_j(x) \quad \text{and} \quad f(x,t) = \sum_{j=0}^{1} f_j(t)\psi_j(x)$$

- Substituting these expansions gives

$$\int_\Omega \psi_i \psi_j \, d\Omega \frac{\partial u_j}{\partial t} + \int_\Omega \psi_i \frac{\partial \psi_j}{\partial x} \, d\Omega f_j = 0$$

- Matrix form

$$M_{ij} \frac{\partial u_j}{\partial t} + A_{ij} f_j = 0$$

  where

$$M_{ij} = \int_\Omega \psi_i \psi_j \, d\Omega \quad \text{and} \quad A_{ij} = \int_\Omega \psi_i \frac{\partial \psi_j}{\partial x} \, d\Omega, \text{ for } i, j = 0, .., 1$$

Basis Functions

- For 2 grid points per element (linear) let

$$u = \begin{cases} u_0 & \text{for} \quad x = x_0 \\ u_1 & \text{for} \quad x = x_1 \end{cases} .$$

- Mapping from physical space $x \in [x_0, x_1]$ to computational space $\xi \in [-1, +1]$ yields

$$x = \begin{cases} x_0 & \text{for} \quad \xi_0 = -1 \\ x_1 & \text{for} \quad \xi_1 = +1 \end{cases}$$

- Therefore we seek ψ such that

$$\xi = \psi_0(\xi)\xi_0 + \psi_1(\xi)\xi_1 \quad \text{and} \quad 1 = \psi_0(\xi) + \psi_1(\xi)$$

  and inverting this system yields the basis functions

$$\psi_0(\xi) = \frac{1}{2}(1 - \xi) \quad \text{and} \quad \psi_1(\xi) = \frac{1}{2}(1 + \xi)$$

  which can be written as

$$\psi_i(\xi) = \frac{1}{2}(1 + \xi_i\xi)$$

- More generally we can write

$$\psi_i(\xi) = \prod_{\substack{j=0, \\ j \neq i}}^{N} \left(\frac{\xi - \xi_j}{\xi_i - \xi_j} \right)$$

  which is the definition of a Lagrange polynomial.

- From

$$x = \sum_{j=0}^{1} x_j \psi_j(x) = \frac{1}{2}(1 - \xi)x_0 + \frac{1}{2}(1 + \xi)x_1$$

  we get the Jacobian of this transformation as

$$dx = \frac{\Delta x}{2} d\xi$$

Mass Matrix

- From physical $x \in [x_0, x_1]$ to computational space $\xi \in [-1, +1]$ we get

$$M_{ij} = \int_{x_0}^{x_1} \psi_i(x)\psi_j(x)\,dx \; = \int_{-1}^{+1} \psi_i(\xi)\psi_j(\xi)\frac{\Delta x}{2}d\xi$$

- In matrix form

$$M_{ij} = \frac{\Delta x}{2}\int_{-1}^{+1} \begin{pmatrix} \psi_1\psi_1 & \psi_1\psi_2 \\ \psi_2\psi_1 & \psi_2\psi_2 \end{pmatrix} d\xi$$

- Substituting ψ

$$M_{ij} = \frac{\Delta x}{2}\int_{-1}^{+1} \begin{pmatrix} \frac{1}{2}(1-\xi)\frac{1}{2}(1-\xi) & \frac{1}{2}(1-\xi)\frac{1}{2}(1+\xi) \\ \frac{1}{2}(1+\xi)\frac{1}{2}(1-\xi) & \frac{1}{2}(1+\xi)\frac{1}{2}(1+\xi) \end{pmatrix} d\xi$$

- Integrating analytically

$$M_{ij} = \frac{\Delta x}{6}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

- Integrating numerically ($Q = \frac{1}{2}cN + 1$ where $c = 2$) gives $Q = 2$

$$M_{ij} = \frac{\Delta x}{2}\sum_{q=0}^{2} w_q\psi_i(\xi_q)\psi_j(\xi_q)$$

where

$$w_{0,1,2} = \frac{1}{3}, \frac{4}{3}, \frac{1}{3}$$

are the Gauss-Lobatto quadrature weights and

$$\xi_{0,1,2} = -1, 0, +1$$

are the Gauss-Lobatto quadrature points gives

$$M_{ij} = \frac{\Delta x}{6}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

- Integrating numerically ($Q = N$)

$$M_{ij} = \frac{\Delta x}{2} \sum_{q=0}^{1} w_q \psi_i(\xi_q) \psi_j(\xi_q)$$

where

$$w_{0,1} = 1, 1$$

and

$$\xi_{0,1} = -1, +1$$

gives

$$M_{ij} = \frac{\Delta x}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

which is diagonal

Advection Matrix

- In computational space we get

$$A_{ij} = \int_{x_0}^{x_1} \psi_i(x) \frac{\partial \psi_j}{\partial x}(x)\, dx = \int_{-1}^{+1} \psi_i(\xi) \frac{\partial \psi_j}{\partial \xi}(\xi) \frac{\partial \xi}{\partial x} \frac{\Delta x}{2} d\xi$$

where

$$\frac{\partial \psi_j}{\partial x}(x) = \frac{\partial \psi_j}{\partial \xi}(\xi) \frac{\partial \xi}{\partial x}$$

and

$$\frac{\partial \psi_j}{\partial \xi}(\xi) = \frac{1}{2} \xi_j \quad \text{and} \quad \frac{\partial \xi}{\partial x} = \frac{2}{\Delta x}$$

- Substituting ψ

$$A_{ij} = \frac{2}{\Delta x} \frac{\Delta x}{2} \int_{-1}^{+1} \begin{pmatrix} \frac{1}{2}(1-\xi)\frac{1}{2}(-1) & \frac{1}{2}(1-\xi)\frac{1}{2}(+1) \\ \frac{1}{2}(1+\xi)\frac{1}{2}(-1) & \frac{1}{2}(1+\xi)\frac{1}{2}(+1) \end{pmatrix} d\xi$$

- Integrating

$$A_{ij} = \frac{1}{4} \begin{pmatrix} -\xi + \frac{1}{2}\xi^2 & \xi - \frac{1}{2}\xi^2 \\ -\xi - \frac{1}{2}\xi^2 & \xi + \frac{1}{2}\xi^2 \end{pmatrix} \Bigg|_{-1}^{+1}$$

- Evaluating

$$A_{ij} = \frac{1}{2} \begin{pmatrix} -1 & +1 \\ -1 & +1 \end{pmatrix}$$

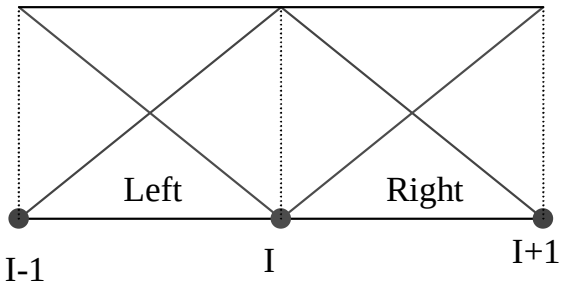


Figure 5: SEM: Contribution to the gridpoint i from the left $(i-1, i)$ and right $(i, i+1)$ elements.

Resulting Element Equations

- Resulting equation which must be satisfied within each element

$$\frac{\Delta x}{6}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} \frac{\partial u_0}{\partial t} \\ \frac{\partial u_1}{\partial t} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} -1 & +1 \\ -1 & +1 \end{pmatrix}\begin{pmatrix} f_0 \\ f_1 \end{pmatrix} = 0$$

  where the subscript 0 and 1 denote the element's grid points

Element Contribution to Grid Point "i"

Left Element

- Left element equation is

$$\frac{\Delta x}{6}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} \frac{\partial u_{i-1}}{\partial t} \\ \frac{\partial u_i}{\partial t} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} -1 & +1 \\ -1 & +1 \end{pmatrix}\begin{pmatrix} f_{i-1} \\ f_i \end{pmatrix} = 0$$

- Contribution to gridpoint i is

$$\frac{\Delta x}{6}\left[\frac{\partial u_{i-1}}{\partial t} + 2\frac{\partial u_i}{\partial t}\right] + \frac{1}{2}\left[-f_{i-1} + f_i\right] = 0$$

Right Element

- Right element equation is

$$\frac{\Delta x}{6}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} \frac{\partial u_i}{\partial t} \\ \frac{\partial u_{i+1}}{\partial t} \end{pmatrix} + \frac{1}{2}\begin{pmatrix} -1 & +1 \\ -1 & +1 \end{pmatrix}\begin{pmatrix} f_i \\ f_{i+1} \end{pmatrix} = 0$$

- Contribution to i is

$$\frac{\Delta x}{6}\left[2\frac{\partial u_i}{\partial t} + \frac{\partial u_{i+1}}{\partial t}\right] + \frac{1}{2}\left[-f_i + f_{i+1}\right] = 0$$

Total Contribution

- Summing up Left and Right element contributions to i gives

$$\frac{\Delta x}{6}\left[\frac{\partial u_{i-1}}{\partial t} + 4\frac{\partial u_i}{\partial t} + \frac{\partial u_{i+1}}{\partial t}\right] + \frac{1}{2}\left[-f_{i-1} + f_i - f_i + f_{i+1}\right] = 0$$

  and simplifying

$$\frac{1}{6}\left[\frac{\partial u_{i-1}}{\partial t} + 4\frac{\partial u_i}{\partial t} + \frac{\partial u_{i+1}}{\partial t}\right] + \frac{f_{i+1} - f_{i-1}}{2\Delta x} = 0$$

- Diagonalizing the mass matrix gives

$$\frac{\partial u_i}{\partial t} + \frac{f_{i+1} - f_{i-1}}{2\Delta x} = 0.$$

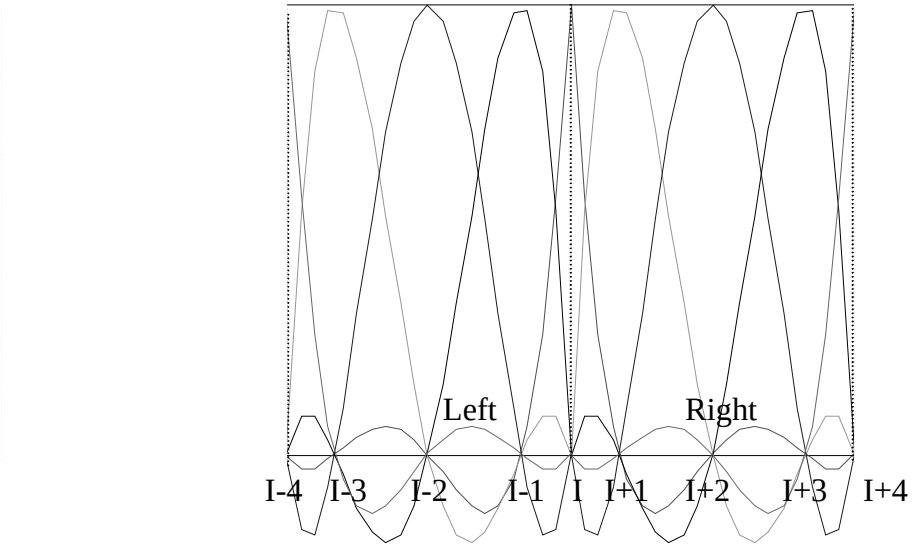
  which is the same difference equation we get for centered (2nd order) finite differences. Note that this can be written as

$$\frac{\partial u_i}{\partial t} + \sum_{k=i-1}^{i+1} \frac{\alpha_k f_k}{\Delta x} = 0.$$

  In general for finite/spectral elements with Nth order polynomials we get $N + 1$ accuracy.

Remark 4 *While the FEM/SEM is very much local in nature (since the solution is constructed in an element-by-element procedure) each element then contributes a portion of its solution to global gridpoints. This is the only interprocessor communication required by the FEM/SEM.*

High Order Approximation Note that if we were to use a high order element such as $N = 4$ then the elements would like like



Element contribution for $N = 4$

and the difference equation would be

$$\frac{\partial u_i}{\partial t} + \sum_{k=i-4}^{i+4} \frac{\alpha_k f_k}{\Delta x} = 0$$

assuming $Q = N$.

2.5.2 Shallow Water Equations on the Sphere

Let us now turn to the discretization of the shallow water equations.

Governing Equations The spherical shallow water equations in Cartesian advection form are

$$\frac{\partial}{\partial t}\begin{pmatrix}\varphi\\u\\v\\w\end{pmatrix}+u\frac{\partial}{\partial x}\begin{pmatrix}\varphi\\u\\v\\w\end{pmatrix}+v\frac{\partial}{\partial y}\begin{pmatrix}\varphi\\u\\v\\w\end{pmatrix}+w\frac{\partial}{\partial z}\begin{pmatrix}\varphi\\u\\v\\w\end{pmatrix}=\begin{pmatrix}-\varphi\boldsymbol{\nabla}\cdot\mathbf{u}\\-\frac{\partial(\varphi+\varphi_s)}{\partial x}-\frac{f}{a}(yw-zv)+\mu x\\-\frac{\partial(\varphi+\varphi_s)}{\partial y}-\frac{f}{a}(zu-xw)+\mu y\\-\frac{\partial(\varphi+\varphi_s)}{\partial z}-\frac{f}{a}(xv-yu)+\mu z\end{pmatrix}. \tag{2}$$

These equations can be written more compactly in vector form as

$$\frac{\partial\boldsymbol{\varphi}}{\partial t}+\mathbf{u}\cdot\boldsymbol{\nabla}\boldsymbol{\varphi}=\mathbf{S}(\boldsymbol{\varphi})$$

where

$$\boldsymbol{\varphi}=\begin{pmatrix}\varphi\\u\\v\\w\end{pmatrix},\quad \mathbf{u}=\begin{pmatrix}u\\v\\w\end{pmatrix},\quad \mathbf{S}(\boldsymbol{\varphi})=\mathbf{F}_D+\mathbf{F}_P+\mathbf{F}_R+\mathbf{F}_C\ ,$$

$$\mathbf{F}_D=-\varphi\boldsymbol{\nabla}\cdot\mathbf{u},\quad \mathbf{F}_P=-\boldsymbol{\nabla}\left(\varphi+\varphi_s\right),\quad \mathbf{F}_R=-\frac{f}{a}(\mathbf{x}\times\mathbf{u}),\quad \mathbf{F}_C=\mu\mathbf{x},$$

and

$$f=\frac{2\Omega z}{a}$$

where Ω and a are the rotation of the earth and its radius, respectively. In the above relations $\mathbf{F}_D$ is the force due to the divergence of velocity, $\mathbf{F}_P$ is the force due to pressure, $\mathbf{F}_R$ is the force due to the rotation (Coriolis) of the earth, and $\mathbf{F}_C$ is the force required to constrain the fluid particles to remain on the surface of the sphere, and μ is a Lagrange multiplier used to satisfy this condition.

Remark 5 *Since we have chosen to use Cartesian coordinates then we have introduced an additional momentum equation. But since flow on a sphere is not really 3D then we need to constrain the fluid particles to remain on the sphere since they now have 3 spatial degrees of freedom.*

Let's see how we can use the SEM to discretize these equations.

Spatial Discretization Beginning with the compact form we can define a Galerkin formulation by taking the weak form

$$\int_\Omega \psi \left[\frac{\partial \boldsymbol{\varphi}}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \boldsymbol{\varphi} - \mathbf{S}(\boldsymbol{\varphi}) \right] \, d\Omega = 0$$

to arrive at

$$\int_\Omega \psi \frac{\partial \boldsymbol{\varphi}}{\partial t} d\Omega = - \int_\Omega \psi \left(\mathbf{u} \cdot \boldsymbol{\nabla} \boldsymbol{\varphi} \right) \, d\Omega + \int_\Omega \psi \, \mathbf{S}(\boldsymbol{\varphi}) \, d\Omega.$$

By letting the functions $\boldsymbol{\varphi}$ be approximated as

$$\boldsymbol{\varphi} = \sum_{j=1}^{N_P} \psi_j \, \boldsymbol{\varphi}_j$$

where $N_P = P^2$ represents the total number of collocation points within each element, we can then write relations for the integrals above. This yields the following integral equation

$$\int_\Omega \psi_i \psi_j d\Omega \frac{\partial \boldsymbol{\varphi}_j}{\partial t} = - \left(\int_\Omega \psi_i \boldsymbol{\nabla} \psi_j \psi_k d\Omega \right) \cdot \mathbf{u}_k \boldsymbol{\varphi}_j \; + \int_\Omega \psi_i \, \mathbf{S}(\psi_j \boldsymbol{\varphi}_j) \, d\Omega$$

which can be written in the matrix form

$$M_{ij} \frac{\partial \boldsymbol{\varphi}_j}{\partial t} = - \left(\mathbf{A}_{ijk} \cdot \mathbf{u}_k \right) \boldsymbol{\varphi}_j + S_i(\boldsymbol{\varphi}) \tag{3}$$

where it is understood that $i, j, k = 1, ..., N_P$. The mass matrix M_{ij} is of dimension N_P^2, the advection matrix $\mathbf{A}_{ijk}$ is N_P^3, and the forcing vector S_i is N_P.

Element Matrices Substituting the forces $S(\boldsymbol{\varphi})$ from the right hand side of (2) into (3) allows us to write all of the element matrices as follows

$$M_{ij} = \int_\Omega \psi_i \psi_j d\Omega,$$

$$\mathbf{A}_{ijk} = \int_\Omega \psi_i \boldsymbol{\nabla} \psi_j \psi_k d\Omega,$$

and

$$S_i(\boldsymbol{\varphi}) = \begin{pmatrix} -\mathbf{D}_{ijk} \cdot \mathbf{u}_k \varphi_j \\ -P_{ij}^x \left(\varphi + \varphi_s\right)_j - R_{ij}^y w_j + R_{ij}^z v_j \\ -P_{ij}^y \left(\varphi + \varphi_s\right)_j - R_{ij}^z u_j + R_{ij}^x w_j \\ -P_{ij}^z \left(\varphi + \varphi_s\right)_j - R_{ij}^x v_j + R_{ij}^y u_j \end{pmatrix}$$

where

$$\mathbf{D}_{ijk} = \int_\Omega \psi_i \psi_j \boldsymbol{\nabla} \psi_k d\Omega,$$

$$P_{ij}^x = \int_\Omega \psi_i \frac{\partial \psi_j}{\partial x} d\Omega, \quad P_{ij}^y = \int_\Omega \psi_i \frac{\partial \psi_j}{\partial y} d\Omega, \quad P_{ij}^z = \int_\Omega \psi_i \frac{\partial \psi_j}{\partial z} d\Omega$$

and

$$R_{ij}^{\mathbf{x}} = \int_\Omega \psi_i \psi_j \left(\sum_{k=1}^{N_P} \psi_k f_k \right) \left(\sum_{l=1}^{N_P} \psi_l \frac{\mathbf{x}_l}{a} \right) d\Omega.$$

The matrices M, $\mathbf{A}$, $\mathbf{D}$, $P^{\mathbf{x}}$, and $R^{\mathbf{x}}$ represent the mass, advection, divergence, pressure, and rotation matrices, respectively. All of these matrices are independent of the conservation variables $\boldsymbol{\varphi}$ and only need to be computed once because they remain constant throughout the integration. The Lagrange multiplier μ has not been included in the force vector $S_i(\boldsymbol{\varphi})$. This term is actually computed at the discrete level and only after each time integration has been completed.

Lagrange Multiplier Constraint Once the solution has been obtained at the new time step, we need to constrain the fluid particles to remain on the surface of the sphere. We then have for the momentum equations

$$\mathbf{u}_c^{n+1} = \mathbf{u}_u^{n+1} + \mu \mathbf{x}$$

where the subscripts c and u denote the constrained and unconstrained values. Taking the scalar product of $\mathbf{r}$, where $\mathbf{r}$ is the coordinate vector of each grid point, gives

$$\mathbf{x} \cdot \mathbf{u}_c^{n+1} = \mathbf{x} \cdot \mathbf{u}_u^{n+1} + \mu a^2. \tag{4}$$

For a fluid particle to remain on the surface of the sphere, the velocity field must be orthogonal to the coordinate (radial) vector of its grid point. In other words,

$$\mathbf{u} \cdot \mathbf{x} = 0.$$

This means that the left hand side term in (4) vanishes, and after rearranging, yields

$$\mu = -\frac{\mathbf{x} \cdot \mathbf{u}_u^{n+1}}{a^2}.$$

Remark 6 *The procedure for calculating the constraining term can be viewed as a projection method very much related to fractional-step methods (see Perot [?][?] and Chang [?] for details on fractional step methods).*

High Order Basis Function on a Sphere In this section we discuss how to construct high order basis functions on any curved surface (e.g., a sphere). Note that we have written the equations completely in 3D Cartesian space. Therefore our Cartesian basis functions will also be 3D and thus will look like volume integrals. However, since flow constrained to the sphere must only involve area integrals we then seek to construct basis functions that essentially split the sphere into 2 directions: the horizontal (i.e. on the sphere) and the normal to the sphere (i.e. the vertical/radial coordinate). In other words rather than seeking functions in the physical 3D Cartesian space of the type $\psi(x, y, z)$ instead we seek functions in the local computational space

$$\psi_i(\xi, \eta, \varsigma) = \zeta \widehat{\psi}_i(\xi, \eta)$$

where the functions $\widehat{\psi}_i(\xi, \eta)$ are 2D functions and ζ denotes the local coordinate which is normal to the sphere (radial component).

Remark 7 *By using this mapping we do not have to come up with our very own ad hoc curved basis functions in 3D Cartesian space. Instead, we can use any 2D basis function and the global physical to local computational mapping will now take care of the curvature of the sphere.*

This mapping is shown graphically in figure 6.The statement of this mapping is: find the nonsingular mapping $\mathbf{x} = \mathbf{\Psi}(\boldsymbol{\xi})$ which connects the physical coordinates $\mathbf{x} = (x, y, z)$ defined on Ω with a reference coordinate system $\boldsymbol{\xi} = (\xi, \eta, \zeta)$. From the chain rule

$$d\mathbf{x} = \frac{\partial \mathbf{x}}{\partial \xi} d\xi + \frac{\partial \mathbf{x}}{\partial \eta} d\eta + \frac{\partial \mathbf{x}}{\partial \zeta} d\zeta$$

we get the system

$$\begin{pmatrix} dx \\ dy \\ dz \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \zeta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \zeta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \zeta} \end{pmatrix} \begin{pmatrix} d\xi \\ d\eta \\ d\zeta \end{pmatrix}$$

where

$$J = \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \zeta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \zeta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \zeta} \end{pmatrix} \tag{5}$$

is the Jacobian of this transformation. Alternatively, we can write the derivatives of $\boldsymbol{\xi}(x, y, z)$ to get

$$\begin{pmatrix} d\xi \\ d\eta \\ d\zeta \end{pmatrix} = \begin{pmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial z} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} & \frac{\partial \eta}{\partial z} \\ \frac{\partial \zeta}{\partial x} & \frac{\partial \zeta}{\partial y} & \frac{\partial \zeta}{\partial z} \end{pmatrix} \begin{pmatrix} dx \\ dy \\ dz \end{pmatrix}$$

where

$$J^{-1} = \begin{pmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial z} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} & \frac{\partial \eta}{\partial z} \\ \frac{\partial \zeta}{\partial x} & \frac{\partial \zeta}{\partial y} & \frac{\partial \zeta}{\partial z} \end{pmatrix}$$

is the inverse Jacobian of the transformation. Again, using the chain rule, we can write the derivatives in the global space in terms of the local surface element space as

$$\frac{\partial}{\partial \mathbf{x}} = \frac{\partial \xi}{\partial \mathbf{x}} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial \mathbf{x}} \frac{\partial}{\partial \eta} + \frac{\partial \zeta}{\partial \mathbf{x}} \frac{\partial}{\partial \zeta}.$$

Expanding, we see that the derivatives are in fact given by

$$\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} = J^{-1} \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \\ \frac{\partial}{\partial \zeta} \end{pmatrix}$$

where the inverse Jacobian matrix is

$$J^{-1} = \frac{1}{|J|} \begin{pmatrix} \frac{1}{\zeta}\left(\frac{\partial y}{\partial \eta} z - y \frac{\partial z}{\partial \eta}\right) & \frac{1}{\zeta}\left(x \frac{\partial z}{\partial \eta} - \frac{\partial x}{\partial \eta} z\right) & \frac{1}{\zeta}\left(\frac{\partial x}{\partial \eta} y - x \frac{\partial y}{\partial \eta}\right) \\ \frac{1}{\zeta}\left(y \frac{\partial z}{\partial \xi} - \frac{\partial y}{\partial \xi} z\right) & \frac{1}{\zeta}\left(\frac{\partial x}{\partial \xi} z - x \frac{\partial z}{\partial \xi}\right) & \frac{1}{\zeta}\left(x \frac{\partial y}{\partial \xi} - \frac{\partial x}{\partial \xi} y\right) \\ \left(\frac{\partial y}{\partial \xi}\frac{\partial z}{\partial \eta} - \frac{\partial y}{\partial \eta}\frac{\partial z}{\partial \xi}\right) & \left(\frac{\partial x}{\partial \eta}\frac{\partial z}{\partial \xi} - \frac{\partial x}{\partial \xi}\frac{\partial z}{\partial \eta}\right) & \left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}\right) \end{pmatrix} \tag{6}$$

after inverting (5). The determinant of the Jacobian matrix (5) can be written in the following form

$$|J| = \frac{\partial \mathbf{x}}{\partial \zeta} \cdot \mathbf{G}$$

where

$$\mathbf{G} = \frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta} \tag{7}$$

and $|\mathbf{G}|$ denotes the magnitude of the normal vector of the surface element $\widehat{\Omega}$ in local space. In other words, it represent a ratio of areas from the physical space to the local computational space. From the chain rule we can compute derivatives as

$$\frac{\partial \psi}{\partial \mathbf{x}}(\xi,\eta,\zeta) = \zeta \frac{\partial \widehat{\psi}}{\partial \xi}(\xi,\eta)\frac{\partial \xi}{\partial \mathbf{x}} + \zeta \frac{\partial \widehat{\psi}}{\partial \eta}(\xi,\eta)\frac{\partial \eta}{\partial \mathbf{x}} + \widehat{\psi}(\xi,\eta)\frac{\partial \zeta}{\partial \mathbf{x}}$$

and every operator can now be written in this new computational space.

Remark 8 *The nice thing about this method is that if we want to use different element shapes (i.e. quadrilaterals or triangles) or different basis functions (i.e. modal or nodal, high or low order, continuous or discontinuous) we only need to change the functions $\widehat{\psi}(\xi,\eta)$ and nothing else!*

This novel approach to solving partial differential equations on the sphere or any other curved manifold was introduced in Giraldo [**?**] (awarded the Alan Berman Research Prize).

Derivatives Recall that any variable within an element is approximated by the basis functions as

$$\boldsymbol{\varphi} = \sum_{i=1}^{N_P} \psi_i \boldsymbol{\varphi}_i = \sum_{i=1}^{N_P} \zeta \widehat{\psi}_i \boldsymbol{\varphi}_i$$

where

$$\psi_i(\xi,\eta,\zeta) = \zeta \widehat{\psi}_i(\xi,\eta). \tag{8}$$

Using the chain rule, the derivative of $\boldsymbol{\varphi}$ in the x direction can be approximated by

$$\frac{\partial \boldsymbol{\varphi}}{\partial x} = \sum_{i=1}^{N_P} \left(\frac{\partial \psi_i}{\partial \xi}\frac{\partial \xi}{\partial x} + \frac{\partial \psi_i}{\partial \eta}\frac{\partial \eta}{\partial x} + \frac{\partial \psi_i}{\partial \zeta}\frac{\partial \zeta}{\partial x} \right) \boldsymbol{\varphi}_i \qquad \forall\, \mathbf{x} \in \Omega$$

where Ω is the particular element we are integrating. Substituting for ψ_i from (8) yields

$$\frac{\partial \boldsymbol{\varphi}}{\partial x} = \sum_{i=1}^{N_P} \left(\zeta \frac{\partial \widehat{\psi}_i}{\partial \xi} \frac{\partial \xi}{\partial x} + \zeta \frac{\partial \widehat{\psi}_i}{\partial \eta} \frac{\partial \eta}{\partial x} + \widehat{\psi}_i \frac{\partial \zeta}{\partial x} \right) \boldsymbol{\varphi}_i.$$

Similarly, one can obtain the y derivative

$$\frac{\partial \boldsymbol{\varphi}}{\partial y} = \sum_{i=1}^{N_P} \left(\zeta \frac{\partial \widehat{\psi}_i}{\partial \xi} \frac{\partial \xi}{\partial y} + \zeta \frac{\partial \widehat{\psi}_i}{\partial \eta} \frac{\partial \eta}{\partial y} + \widehat{\psi}_i \frac{\partial \zeta}{\partial y} \right) \boldsymbol{\varphi}_i$$

as well as the z derivative

$$\frac{\partial \boldsymbol{\varphi}}{\partial z} = \sum_{i=1}^{N_P} \left(\zeta \frac{\partial \widehat{\psi}_i}{\partial \xi} \frac{\partial \xi}{\partial z} + \zeta \frac{\partial \widehat{\psi}_i}{\partial \eta} \frac{\partial \eta}{\partial z} + \widehat{\psi}_i \frac{\partial \zeta}{\partial z} \right) \boldsymbol{\varphi}_i$$

where the metric terms such as $\frac{\partial \xi}{\partial x}$ come from the inverse Jacobian

$$\begin{aligned} J^{-1} &= \begin{pmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial z} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} & \frac{\partial \eta}{\partial z} \\ \frac{\partial \zeta}{\partial x} & \frac{\partial \zeta}{\partial y} & \frac{\partial \zeta}{\partial z} \end{pmatrix} \\ &= \frac{1}{|J|} \begin{pmatrix} \frac{1}{\zeta}\left(\frac{\partial y}{\partial \eta} z - y \frac{\partial z}{\partial \eta}\right) & \frac{1}{\zeta}\left(x \frac{\partial z}{\partial \eta} - \frac{\partial x}{\partial \eta} z\right) & \frac{1}{\zeta}\left(\frac{\partial x}{\partial \eta} y - x \frac{\partial y}{\partial \eta}\right) \\ \frac{1}{\zeta}\left(y \frac{\partial z}{\partial \xi} - \frac{\partial y}{\partial \xi} z\right) & \frac{1}{\zeta}\left(\frac{\partial x}{\partial \xi} z - x \frac{\partial z}{\partial \xi}\right) & \frac{1}{\zeta}\left(x \frac{\partial y}{\partial \xi} - \frac{\partial x}{\partial \xi} y\right) \\ \left(\frac{\partial y}{\partial \xi}\frac{\partial z}{\partial \eta} - \frac{\partial y}{\partial \eta}\frac{\partial z}{\partial \xi}\right) & \left(\frac{\partial x}{\partial \eta}\frac{\partial z}{\partial \xi} - \frac{\partial x}{\partial \xi}\frac{\partial z}{\partial \eta}\right) & \left(\frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}\right) \end{pmatrix}. \end{aligned}$$

Integration The mass, advection, pressure and rotation matrices become

$$M_{ij} = \int_\Omega \psi_i \psi_j d\Omega = \sum_{q=1}^{N_Q} w_q \zeta^2 \left| \mathbf{G}\left(\xi_q, \eta_q\right) \right| \widehat{\psi}_i\left(\xi_q, \eta_q\right) \widehat{\psi}_j\left(\xi_q, \eta_q\right),$$

$$A^{\mathbf{x}}_{ijk} = \int_\Omega \psi_i \boldsymbol{\nabla} \psi_j \psi_k d\Omega, = \sum_{q=1}^{N_Q} w_q \zeta^2 \left| \mathbf{G}\left(\xi_q, \eta_q\right) \right| \widehat{\psi}_i\left(\xi_q, \eta_q\right) \left(\zeta \frac{\partial \widehat{\psi}_j}{\partial \xi} \frac{\partial \xi}{\partial \mathbf{x}} + \zeta \frac{\partial \widehat{\psi}_j}{\partial \eta} \frac{\partial \eta}{\partial \mathbf{x}} + \widehat{\psi}_j \frac{\partial \zeta}{\partial \mathbf{x}} \right) \widehat{\psi}_k\left(\xi_q\right.$$

$$D^{\mathbf{x}}_{ijk} = \int_\Omega \psi_i \psi_j \boldsymbol{\nabla} \psi_k d\Omega = \sum_{q=1}^{N_Q} w_q \zeta^2 \left| \mathbf{G}\left(\xi_q, \eta_q\right) \right| \widehat{\psi}_i\left(\xi_q, \eta_q\right) \widehat{\psi}_j\left(\xi_q, \eta_q\right) \left(\zeta \frac{\partial \widehat{\psi}_k}{\partial \xi} \frac{\partial \xi}{\partial \mathbf{x}} + \zeta \frac{\partial \widehat{\psi}_k}{\partial \eta} \frac{\partial \eta}{\partial \mathbf{x}} + \widehat{\psi}_k \right.$$

$$P_{ij}^{\mathbf{x}} = \int_{\Omega} \psi_i \frac{\partial \psi_j}{\partial \mathbf{x}} d\Omega = \sum_{q=1}^{N_Q} w_q \zeta \left|\mathbf{G}\left(\xi_q, \eta_q\right)\right| \widehat{\psi}_i\left(\xi_q, \eta_q\right) \left(\zeta \frac{\partial \widehat{\psi}_j}{\partial \xi} \frac{\partial \xi}{\partial \mathbf{x}} + \zeta \frac{\partial \widehat{\psi}_j}{\partial \eta} \frac{\partial \eta}{\partial \mathbf{x}} + \widehat{\psi}_j \frac{\partial \zeta}{\partial \mathbf{x}} \right),$$

$$\begin{aligned} R_{ij}^{\mathbf{x}} &= \int_{\Omega} \psi_i \psi_j \left(\sum_{k=1}^{N_P} \psi_k f_k \right) \left(\sum_{l=1}^{N_P} \psi_l \frac{\mathbf{x}_l}{a} \right) d\Omega \\ &= \sum_{q=1}^{N_Q} w_q \zeta^4 \left|\mathbf{G}\left(\xi_q, \eta_q\right)\right| \widehat{\psi}_i\left(\xi_q, \eta_q\right) \widehat{\psi}_j\left(\xi_q, \eta_q\right) \left(\sum_{k=1}^{N_P} \psi_k\left(\xi_q, \eta_q\right) f_k \right) \left(\sum_{l=1}^{N_P} \psi_l\left(\xi_q, \eta_q\right) \frac{\mathbf{x}_l}{a} \right) \end{aligned}$$

where

$$\mathbf{A}_{ijk} = A_{ijk}^x \mathbf{i} + A_{ijk}^y \mathbf{j} + A_{ijk}^z \mathbf{k} \quad \text{and} \quad \mathbf{D}_{ijk} = D_{ijk}^x \mathbf{i} + D_{ijk}^y \mathbf{j} + D_{ijk}^z \mathbf{k}$$

and $\mathbf{i}, \mathbf{j}, \mathbf{k}$ denote the Cartesian directional vectors. The value of ζ need not be of any concern because at the surface of the sphere it is defined by $\zeta = 1$. The integer N_Q represents the total number of LGL quadrature points required within each element. Therefore $N_Q = Q^2$. Recall that $\left|\mathbf{G}\left(\xi_q, \eta_q\right)\right|$ is the Jacobian of the surface area integral and is defined as

$$\left|\mathbf{G}\left(\xi_q, \eta_q\right)\right| = \left| \frac{\partial \mathbf{x}}{\partial \xi}\left(\xi_q, \eta_q\right) \times \frac{\partial \mathbf{x}}{\partial \eta}\left(\xi_q, \eta_q\right) \right|.$$

Final Form If we assume that $Q = P$ and use the same basis functions in both directions (ξ, η) then we can simplify the above relations significantly. For example our basis functions now become

$$\widehat{\psi}_i\left(\xi, \eta\right) = h_j(\xi) h_k(\eta)$$

where

$$h_j(\xi) = \prod_{\substack{l=1 \\ l \neq j}}^{P} \left(\frac{\xi - \xi_l}{\xi_j - \xi_l} \right) \quad \text{and} \quad h_k(\eta) = \prod_{\substack{l=1 \\ l \neq k}}^{P} \left(\frac{\eta - \eta_l}{\eta_k - \eta_l} \right).$$

By assuming both of these things and that $\zeta = 1$ on the surface of the sphere we can now write the above matrices as a tensor product of the 1D functions as such

$$M_{ij,kl} = w_i w_j \left|\mathbf{G}\left(\xi_i,\eta_j\right)\right| \delta_{ik}\delta_{jl},$$

$$A^{\mathbf{x}}_{ij,kl,mn} = w_i w_j \left|\mathbf{G}\left(\xi_i,\eta_j\right)\right| \left(\frac{dh_k}{d\xi}(\xi_i)\frac{\partial \xi_{i,j}}{\partial \mathbf{x}}\delta_{jl} + \frac{dh_l}{d\eta}(\eta_j)\frac{\partial \eta_{i,j}}{\partial \mathbf{x}}\delta_{ik} + \delta_{ik}\delta_{jl}\frac{\partial \zeta_{i,j}}{\partial \mathbf{x}}\right)\delta_{im}\delta_{jn},$$

$$D^{\mathbf{x}}_{ij,kl,mn} = w_i w_j \left|\mathbf{G}\left(\xi_i,\eta_j\right)\right| \left(\frac{dh_m}{d\xi}(\xi_i)\frac{\partial \xi_{i,j}}{\partial \mathbf{x}}\delta_{jn} + \frac{dh_n}{d\eta}(\eta_j)\frac{\partial \eta_{i,j}}{\partial \mathbf{x}}\delta_{im} + \delta_{im}\delta_{jn}\frac{\partial \zeta_{i,j}}{\partial \mathbf{x}}\right)\delta_{ik}\delta_{jl},$$

$$P^{\mathbf{x}}_{ij,kl} = w_i w_j \left|\mathbf{G}\left(\xi_i,\eta_j\right)\right| \left(\frac{dh_k}{d\xi}(\xi_i)\frac{\partial \xi_{i,j}}{\partial \mathbf{x}}\delta_{jl} + \frac{dh_l}{d\eta}(\eta_j)\frac{\partial \eta_{i,j}}{\partial \mathbf{x}}\delta_{ik} + \delta_{ik}\delta_{jl}\frac{\partial \zeta_{i,j}}{\partial \mathbf{x}}\right),$$

$$R^{\mathbf{x}}_{ij,kl} = w_i w_j \left|\mathbf{G}\left(\xi_i,\eta_j\right)\right| f_{ij}\frac{\mathbf{x}_{ij}}{a}\delta_{ik}\delta_{jl}$$

where $i,j,k,l,m,n = 1,...,P$ and δ is the Kronecker-delta function with the property

$$\delta_{ij} = \begin{cases} 1 & \text{for} \quad i = j \\ 0 & \text{for} \quad i \neq j \end{cases}.$$

Remark 9 *Each of these matrices are defined within an element only. However, because we have continuous basis functions then each element contributes a portion of its solution to the global gridpoints that are shared by neighboring elements; this element contribution to the global gridpoints is called a* ***global assembly****. Thus if we have N gridpoints in the entire grid then we would have a system of $N \times N$ to invert if we did not have diagonal mass matrices. However, for diagonal mass matrices we have N vector operations to perform in order to obtain our global solution.*

$$STOP$$

2.5.3 Atmospheric Equations

Let us now turn to the discretization of the atmospheric equations.

Governing Equations The atmospheric equations in Cartesian advection form are

$$\frac{\partial}{\partial t}\begin{pmatrix}\pi\\u\\v\\w\\\theta\end{pmatrix}+u\frac{\partial}{\partial x}\begin{pmatrix}\pi\\u\\v\\w\\\theta\end{pmatrix}+v\frac{\partial}{\partial y}\begin{pmatrix}\pi\\u\\v\\w\\\theta\end{pmatrix}+w\frac{\partial}{\partial z}\begin{pmatrix}\pi\\u\\v\\w\\\theta\end{pmatrix}+\dot{\sigma}\frac{\partial}{\partial\sigma}\begin{pmatrix}\pi\\u\\v\\w\\\theta\end{pmatrix}=$$
$$\begin{pmatrix}-\pi\left(\boldsymbol{\nabla}\cdot\mathbf{u}+\frac{\partial\dot{\sigma}}{\partial\sigma}\right)\\-\frac{\partial\varphi}{\partial x}-cp\theta\frac{\partial P}{\partial\pi}\frac{\partial\pi}{\partial x}-\frac{f}{a}(yw-zv)+\mu x\\-\frac{\partial\varphi}{\partial y}-cp\theta\frac{\partial P}{\partial\pi}\frac{\partial\pi}{\partial y}-\frac{f}{a}(zu-xw)+\mu y\\-\frac{\partial\varphi}{\partial z}-cp\theta\frac{\partial P}{\partial\pi}\frac{\partial\pi}{\partial z}-\frac{f}{a}(xv-yu)+\mu z\\0\end{pmatrix}$$

where the geopotential (equation of state) is

$$\frac{\partial\varphi}{\partial P}=-c_p\theta$$

where

$$P=\left(\frac{p}{p_o}\right)^{\kappa}.$$

These equations can be written more compactly in vector form as

$$\frac{\partial\pi}{\partial t}+\boldsymbol{\nabla}\cdot(\pi\mathbf{u})+\frac{\partial}{\partial\sigma}\left(\pi\dot{\boldsymbol{\sigma}}\right)=0$$

$$\frac{\partial\mathbf{u}}{\partial t}+\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u}+\dot{\boldsymbol{\sigma}}\frac{\partial\mathbf{u}}{\partial\sigma}=-\boldsymbol{\nabla}\varphi-c_p\theta\frac{\partial P}{\partial\pi}\boldsymbol{\nabla}\pi-\frac{f}{a}(\mathbf{x}\times\mathbf{u})$$

$$\frac{\partial\theta}{\partial t}+\mathbf{u}\cdot\boldsymbol{\nabla}\theta+\dot{\boldsymbol{\sigma}}\frac{\partial\theta}{\partial\sigma}=0$$

Vertical Integration To solve the atmospheric equations we split the spatial operators into vertical and horizontal components. Therefore for a given σ value (vertical level), we solve the horizontal operators. In the vertical, the equations are currently discretized using a conservative finite difference (finite volume-type) flux-form. This is the same vertical differencing currently used in NOGAPS.

Surface Pressure Beginning with the equation for surface pressure

$$\frac{\partial \pi}{\partial t} + \boldsymbol{\nabla} \cdot (\pi \mathbf{u}) + \frac{\partial}{\partial \sigma} (\pi \dot{\boldsymbol{\sigma}}) = 0$$

we then integrate from the top ($\sigma = 0$) to the bottom ($\sigma = 1$) of the atmosphere giving

$$\frac{\partial \pi}{\partial t} [\sigma]_{\sigma=0}^{\sigma=1} = - \int_0^1 \boldsymbol{\nabla} \cdot (\pi \mathbf{u}) \, d\sigma - [\pi \dot{\boldsymbol{\sigma}}]_{\sigma=0}^{\sigma=1} .$$

After applying no-flux boundaries at the top and bottom of the atmosphere we get

$$\begin{aligned} \frac{\partial \pi}{\partial t} &= - \int_0^1 \boldsymbol{\nabla} \cdot (\pi \mathbf{u}) \, d\sigma \\ &= - \sum_{l=1}^{N_{lev}} \boldsymbol{\nabla} \cdot (\pi \mathbf{u})_l \, \Delta \sigma_l \end{aligned}$$

which gives the surface pressure tendency as an integral of the divergence operator of the surface pressure transport in conservation form.

Vertical Velocity Once we know the surface pressure tendency, we can then determine the vertical velocity $\dot{\boldsymbol{\sigma}}$ at each vertical level by integrating the mass from the top of the atmosphere ($\sigma = 0$) to the desired vertical level k ($\sigma = \sigma_{k+1/2}$) thus giving

$$\begin{aligned} (\pi \dot{\boldsymbol{\sigma}})_{k+1/2} &= - \frac{\partial \pi}{\partial t} \sigma_{k+1/2} - \int_0^{\sigma_{k+1/2}} \boldsymbol{\nabla} \cdot (\pi \mathbf{u}) \, d\sigma \\ &= - \frac{\partial \pi}{\partial t} \sigma_{k+1/2} - \sum_{l=1}^{k} \boldsymbol{\nabla} \cdot (\pi \mathbf{u})_l \, \Delta \sigma_l . \end{aligned}$$

It should be stated that the vertical velocity $\dot{\boldsymbol{\sigma}}$ is computed at the half levels where the top and bottom of the atmosphere are at half levels.

Vertical Differencing The next step is to compute the vertically differenced terms $\dot{\boldsymbol{\sigma}}\frac{\partial}{\partial\sigma}$ in the momentum and energy equations. These terms are computed for any scalar f as follows

$$\left(\dot{\boldsymbol{\sigma}}\frac{\partial f}{\partial\sigma}\right)_k = \dot{\boldsymbol{\sigma}}_{k+1/2}\left(\frac{f_{k+1/2}-f_k}{\sigma_{k+1/2}-\sigma_{k-1/2}}\right) + \dot{\boldsymbol{\sigma}}_{k-1/2}\left(\frac{f_k-f_{k-1/2}}{\sigma_{k+1/2}-\sigma_{k-1/2}}\right)$$

where k denotes a full level and the $k \pm 1/2$ denotes the half levels of this staggered sigma coordinate system. The prognostic variables all reside at the full levels while the diagnostic variables at the half levels. Note that the top and bottom of the atmosphere reside at half levels. Thus we can discretize the terms $\dot{\boldsymbol{\sigma}}\frac{\partial \mathbf{u}_H}{\partial\sigma}$ and $\dot{\boldsymbol{\sigma}}\frac{\partial\theta}{\partial\sigma}$ in this manner. The pressure term $\frac{\partial P}{\partial\pi}$ is discretized as follows:

$$\frac{\partial P}{\partial\pi} = \frac{\partial P}{\partial p}\frac{\partial p}{\partial\pi} = \sigma\frac{\partial P}{\partial p}$$

because

$$\frac{\partial p}{\partial\pi} = \sigma.$$

Finally we discretize $\sigma\frac{\partial P}{\partial p}$ in a similar fashion as $\dot{\boldsymbol{\sigma}}\frac{\partial}{\partial\sigma}$ as follows

$$\left(\sigma\frac{\partial P}{\partial p}\right)_k = \sigma_{k+1/2}\left(\frac{P_{k+1/2}-P_k}{p_{k+1/2}-p_{k-1/2}}\right) + \sigma_{k-1/2}\left(\frac{P_k-P_{k-1/2}}{p_{k+1/2}-p_{k-1/2}}\right).$$

Momentum and Energy Equations The momentum and energy equations are discretized using the spectral element method exactly in the same manner that the shallow water equations were discretized. Since these equations are now a function of the vertical sigma coordinate, then the equations are discretized for every level k as follows

$$\frac{\partial\mathbf{u}}{\partial t} = -\mathbf{u}\cdot\boldsymbol{\nabla}\mathbf{u} - \left\{\dot{\boldsymbol{\sigma}}\frac{\partial\mathbf{u}}{\partial\sigma}\right\} - \boldsymbol{\nabla}\varphi - c_p\theta\left\{\frac{\partial P}{\partial\pi}\right\}\boldsymbol{\nabla}\pi - \frac{f}{a}(\mathbf{x}\times\mathbf{u})$$

$$\frac{\partial\theta}{\partial t} = -\mathbf{u}\cdot\boldsymbol{\nabla}\theta - \left\{\dot{\boldsymbol{\sigma}}\frac{\partial\theta}{\partial\sigma}\right\}$$

where the derivatives in $\{\}$ have already been discretized by the vertical differencing scheme.

Equation of State The only remaining value required is the geopotential variable φ. This term is obtained via the equation of state

$$\frac{\partial \varphi}{\partial P} = -c_p \theta$$

which is discretized in the following way

$$\varphi_k - \varphi_{k+1} = -c_p \theta_{k+1/2} \left(P_k - P_{k+1} \right)$$

where

$$\theta_{k+1/2} = \theta_k \frac{\left(P_{k-1/2} - P_k \right)}{\left(P_k - P_{k+1} \right)} + \theta_{k+1} \frac{\left(P_k - P_{k+1/2} \right)}{\left(P_k - P_{k+1} \right)}$$

and putting them together yields

$$\varphi_k - \varphi_{k+1} = c_p \theta_k \left(P_k - P_{k-1/2} \right) + c_p \theta_{k+1} \left(P_{k+1/2} - P_k \right) \tag{9}$$

Spatial Discretization

Surface Pressure Beginning with

$$\frac{\partial \pi}{\partial t} = - \sum_{l=1}^{N_{lev}} \boldsymbol{\nabla} \cdot \left(\pi \mathbf{u} \right)_l \, \Delta \sigma_l$$

we then take the weak integral form

$$\int_\Omega \psi \frac{\partial \pi}{\partial t} d\Omega = - \int_\Omega \psi \sum_{l=1}^{N_{lev}} \boldsymbol{\nabla} \cdot \left(\pi \mathbf{u} \right)_l \, \Delta \sigma_l d\Omega$$

and reordering gives

$$\int_\Omega \psi \frac{\partial \pi}{\partial t} d\Omega = - \sum_{l=1}^{N_{lev}} \left(\int_\Omega \psi \boldsymbol{\nabla} \cdot \left(\pi \mathbf{u} \right)_l \, d\Omega \right) \Delta \sigma_l$$

where

$$\pi = \sum_{j=1}^{N_P} \psi_j \pi_j \quad \text{and} \quad \mathbf{u} = \sum_{j=1}^{N_P} \psi_j \, \mathbf{u}_j$$

Momentum Beginning with

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \mathbf{u} + \dot{\boldsymbol{\sigma}} \frac{\partial \mathbf{u}}{\partial \sigma} = -\boldsymbol{\nabla} \varphi - c_p \theta \frac{\partial P}{\partial \pi} \boldsymbol{\nabla} \pi - \frac{f}{a} (\mathbf{x} \times \mathbf{u})$$

we get

$$\int_\Omega \psi \frac{\partial \mathbf{u}_k}{\partial t} d\Omega = -\int_\Omega \psi \left(\mathbf{u} \cdot \boldsymbol{\nabla} \mathbf{u} + \dot{\boldsymbol{\sigma}} \frac{\partial \mathbf{u}}{\partial \sigma} + \boldsymbol{\nabla} \varphi + c_p \theta \frac{\partial P}{\partial \pi} \boldsymbol{\nabla} \pi + \frac{f}{a} (\mathbf{x} \times \mathbf{u}) \right)_k d\Omega \quad \forall k \in [1, ..., N_{lev}]$$

Temperature The temperature equation

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \theta + \dot{\boldsymbol{\sigma}} \frac{\partial \theta}{\partial \sigma} = 0$$

is discretized by the spectral element method as follows

$$\int_\Omega \psi \frac{\partial \theta}{\partial t} d\Omega = -\int_\Omega \psi \left(\mathbf{u} \cdot \boldsymbol{\nabla} \theta + \dot{\boldsymbol{\sigma}} \frac{\partial \theta}{\partial \sigma} \right) d\Omega$$

where

$$\theta = \sum_{j=1}^{N_P} \psi_j \theta_j$$

Figure 6: Mapping from physical to computational space.