Spiral-Spectral Fluid Simulation (Supplementary Material)

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1 CODIMENSIONAL SPHERICAL BASIS FUNCTIONS

We now show that the polar approach from the main document generalizes to codimensional (surface-based) flow on a sphere.

1.1 Generating Principal Spherical Functions

The spherical divergence-free condition is

$$\nabla \cdot \mathbf{s} = \frac{1}{r^2 \sin(\theta)} \left[\sin(\theta) \frac{\partial r^2 \mathbf{s}_r}{\partial r} + r \frac{\partial \mathbf{s}_\theta \sin(\theta)}{\partial \theta} + r \frac{\partial \mathbf{s}_\phi}{\partial \phi} \right]. \quad (1)$$

By constraining the domain to the surface of a unit sphere, this simplifies to:

$$\frac{\partial \mathbf{s}_\theta}{\partial \theta} \sin(\theta) + \mathbf{s}_\theta \cos(\theta) + \frac{\partial \mathbf{s}_\phi}{\partial \phi} = 0. \quad (2)$$

Applying principle 2, we specify that $\mathbf{s}_\theta = T_\theta(i_1\theta)P_\theta(i_2\phi)$. Solving for the unknown $\mathbf{s}_\phi = T_\phi(\theta)P_\phi(\phi)$ yields:

$$T_\phi(\theta) = -\frac{\partial T_\theta(i_1\theta)}{\partial \theta} \sin(\theta) - T_\theta(i_1\theta)\cos(\theta) \quad (3)$$

$$P_\phi(\phi) = \int P_\theta(i_2\phi) + L(\theta). \quad (4)$$

We will next present boundary conditions for the surface of a sphere before generating explicit expressions for the principal functions.

1.2 Codimensional Boundary Conditions

Similar to the polar case, a periodic boundary condition is needed: $\Phi(\theta, \phi) = \Phi(\theta, \phi + 2\pi)$. Unlike the polar case, we now have *two* singularities, one at the north ($\theta = 0$) and another at the south ($\theta = \pi$) pole. Another consistency condition can be derived from the velocity transformation between spherical and Cartesian coordinates:

$$\begin{bmatrix} \mathbf{u}_x \\ \mathbf{u}_y \\ \mathbf{u}_z \end{bmatrix} = \begin{bmatrix} \sin(\theta)\cos(\phi) & \cos(\theta)\cos(\phi) & -\sin(\phi) \\ \sin(\theta)\sin(\phi) & \cos(\theta)\sin(\phi) & \cos(\phi) \\ \cos(\theta) & -\sin(\theta) & 0 \end{bmatrix} \begin{bmatrix} 0 \\ \mathbf{u}_\theta \\ \mathbf{u}_\phi \end{bmatrix}. \quad (5)$$

By solving $\frac{\partial \mathbf{u}_x}{\partial \phi} = 0$ and $\frac{\partial \mathbf{u}_y}{\partial \phi} = 0$ at two poles, we obtain the consistency conditions [Hill and Henderson 2016]:

$$\frac{\partial \mathbf{u}_\phi}{\partial \phi} = -\mathbf{u}_\theta \qquad \frac{\partial \mathbf{u}_\theta}{\partial \phi} = \mathbf{u}_\phi \qquad \theta = 0, \quad (6)$$

$$\frac{\partial \mathbf{u}_\phi}{\partial \phi} = \mathbf{u}_\theta \qquad \frac{\partial \mathbf{u}_\theta}{\partial \phi} = -\mathbf{u}_\phi \qquad \theta = \pi, \quad (7)$$

where $\mathbf{u}$ are a vector field on the surface. These boundary conditions are similar to Eqn. 18 in the main paper, and suggest an $i_2 = 1$ constraint in the ϕ direction for any enrichment functions. We will now use these boundary conditions to generate explicit basis functions.

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1.3 The Codimensional Basis Functions

Principal Basis Functions: Our first principal basis function $\mathbf{\Phi}^0_*$ is obtained by applying principle 1 and setting $P_\theta = \sin(i_2\phi)$:

$$\begin{cases} \mathbf{\Phi}^0_\theta & = \sin(i_1\theta)\cos(i_2\phi),\ i_1 > 0,\ i_2 > 0, \\ \mathbf{\Phi}^0_\phi & = -\frac{1}{i_2}\left(\cos(\theta)\sin(i_1\theta) + i_1\sin(\theta)\cos(i_1\theta)\right)\sin(i_2\phi). \end{cases} \quad (8)$$

Our second vector function $\mathbf{\Phi}^1_*$ is obtained using $P_\theta = \cos(i_2\phi)$:

$$\begin{cases} \mathbf{\Phi}^1_\theta & = \sin(i_1\theta)\sin(i_2\phi),\ i_1 > 0,\ i_2 > 0, \\ \mathbf{\Phi}^1_\phi & = \frac{1}{i_2}\left(\cos(\theta)\sin(i_1\theta) + i_1\sin(\theta)\cos(i_1\theta)\right)\cos(i_2\phi). \end{cases} \quad (9)$$

The periodic boundary condition along ϕ is satisfied by setting $i_2 \in \mathbb{Z}^+$, and $i_1 \in \mathbb{Z}^+$ satisfies Eqns. 6 and 7 as the functions become zero at both poles. We next derive two enrichment basis functions to resolve non-zero velocities at the poles.

Enrichment Basis Functions: Similar to the polar case, we obtain two enrichment functions by setting $T_\theta(i_1\theta) = \cos(i_1\theta)$ and $i_2 = 1$:

$$\begin{cases} \mathbf{\Phi}^2_\theta & = \cos(i_1\theta)\cos(\phi) \\ \mathbf{\Phi}^2_\phi & = \left(-\cos(\theta)\cos(i_1\theta) + i_1\sin(\theta)\sin(i_1\theta)\right)\sin(\phi), \end{cases} \quad (10)$$

$$\begin{cases} \mathbf{\Phi}^3_\theta & = \cos(i_1\theta)\sin(\phi) \\ \mathbf{\Phi}^3_\phi & = \left(\cos(\theta)\cos(i_1\theta) - i_1\sin(\theta)\sin(i_1\theta)\right)\cos(\phi). \end{cases} \quad (11)$$

Following the polar case, $\mathbf{\Phi}^2_*$ evaluates to $\mathbf{\Phi}^2_\theta = \cos(\phi)$ and $\mathbf{\Phi}^2_\phi = -\sin(\phi)$ at the north pole ($\theta = 0$), which corresponds to the x-translation of $\mathbf{u}_x = 1, \mathbf{u}_y = 0, \mathbf{u}_z = 0$. Correspondingly, $\mathbf{\Phi}^3_*$ evaluates to a y-translation of $\mathbf{u}_x = 0, \mathbf{u}_y = 1, \mathbf{u}_z = 0$. A third z-translation is not relevant in this case, as we are capturing surface-based flow, and the z-axis points out of the surface. Thus, $\mathbf{\Phi}^2_*$ and $\mathbf{\Phi}^3_*$ are sufficient to represent non-zero velocities at the poles.

The last enrichment function similarly samples $L(\theta)$ from Eqn. 4, to represent a rigid-rotation-like circulation flow along the surface:

$$\mathbf{\Phi}^4_\theta = 0 \qquad \mathbf{\Phi}^4_\phi = \sin(i_1\theta). \quad (12)$$

These basis functions $\{\mathbf{\Phi}^0_*, \mathbf{\Phi}^1_*, \mathbf{\Phi}^2_*, \mathbf{\Phi}^3_*, \mathbf{\Phi}^4_*\}$ are now sufficient for spiral-spectral simulations on the surface of a sphere.

2 VOLUMETRIC CYLINDRICAL BASIS

We now generalize the polar approach to a volumetric cylinder.

2.1 Cylindrical Divergence Operator

A Cartesian point $\mathbf{p}$ is parameterized in cylindrical coordinates as:

$$\mathbf{p}_x = r\cos(\theta) \qquad \mathbf{p}_y = r\sin(\theta) \qquad \mathbf{p}_\zeta = b\zeta, \tag{13}$$

where $r \in [0,1]$, $\theta \in [0, 2\pi)$, $\zeta \in [0,1]$, and b denotes height of the cylinder. The divergence operator in cylindrical coordinates is:

$$\nabla \cdot \mathbf{s} = \frac{1}{r}(r\frac{\partial \mathbf{s}_r}{\partial r} + \mathbf{s}_r + \frac{\partial \mathbf{s}_\theta}{\partial \theta}) + \frac{1}{b}\frac{\partial \mathbf{s}_\zeta}{\partial \zeta}. \tag{14}$$

2.2 Generate Cylindrical Basis Functions

Using principle 2, we assume the separate forms,

$$\mathbf{s}_r = A_r(r)A_\theta(\theta)B(\zeta) \quad \mathbf{s}_\theta = C_r(r)C_\theta(\theta)D(\zeta) \quad \mathbf{s}_\zeta = E_r(r)E_\theta(\theta)F(\zeta),$$

which yields:

$$b\left[A_r(r)A_\theta(\theta)B(\zeta) + r\frac{\partial A_r(r)}{\partial r}A_\theta(\theta)B(\zeta) + C_r(r)\frac{\partial C_\theta(\theta)}{\partial \theta}D(\zeta)\right] + rE_rE_\theta\frac{\partial F(\zeta)}{\partial \zeta} = 0. \tag{15}$$

Components along ζ can be solved by setting $B(\zeta) = D(\zeta) = \frac{\partial F(\zeta)}{\partial \zeta}$, which leads to:

$$b\left(A_rA_\theta + \frac{\partial C_\theta}{\partial \theta}C_r\right) + r\left(b\frac{\partial A_r}{\partial r}A_\theta + E_rE_\theta\right) = 0. \tag{16}$$

Components along θ can be solved by setting $A_\theta = \frac{\partial C_\theta}{\partial \theta} = E_\theta$, which simplifies the divergence-free condition to:

$$b\,(A_r + C_r) + r\left(b\frac{\partial A_r}{\partial r} + E_r\right) = 0. \tag{17}$$

Assuming that each addend separately sums to zero yields the terms:

$$C_r = -A_r \qquad E_r = -b\frac{\partial A_r}{\partial r}, \tag{18}$$

and the general solution follows:

$$\begin{cases} \mathbf{s}_r &= -A_r\frac{\partial C_\theta}{\partial \theta}\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{s}_\theta &= A_rC_\theta\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{s}_\zeta &= b\frac{\partial A_r}{\partial r}\frac{\partial C_\theta}{\partial \theta}F(\zeta) \end{cases}. \tag{19}$$

2.3 Setting Boundary Conditions

Similar to the polar case, a periodic boundary condition is needed: $\mathbf{\Phi}(\theta) = \mathbf{\Phi}(\theta + 2\pi)$. The consistency requirements can be derived by transforming a cylindrical velocity to a Cartesian velocity:

$$\begin{bmatrix}\mathbf{u}_x \\ \mathbf{u}_y \\ \mathbf{u}_z\end{bmatrix} = \begin{bmatrix}\cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}\mathbf{u}_r \\ \mathbf{u}_\theta \\ \mathbf{u}_\zeta\end{bmatrix}. \tag{20}$$

At the centerline, consistency requirements can be derived by requiring the Cartesian velocity $\mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z$ be constant which respect to θ, which results in:

$$\frac{\partial \mathbf{u}_r}{\partial \theta} = \mathbf{u}_\theta \qquad \frac{\partial \mathbf{u}_\theta}{\partial \theta} = -\mathbf{u}_r \qquad \frac{\partial \mathbf{u}_\zeta}{\partial \theta} = 0 \qquad \text{at } r = 0. \tag{21}$$

2.4 Principal Basis Functions

Next, we will generate principal basis functions with Eqn. 19. The boundary condition in Eqn. 21 can be satisfied by choosing $A_r = \sin(\frac{\pi}{2}r)\sin(i_1\pi r)$. This results in two sets of principal basis functions:

$$\begin{cases} \mathbf{\Phi}_r^0 &= -i_2\sin(\frac{\pi}{2}r)\sin(i_1\pi r)\cos(i_2\theta)\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{\Phi}_\theta^0 &= \sin(\frac{\pi}{2}r)\sin(i_1\pi r)\sin(i_2\theta)\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{\Phi}_\zeta^0 &= i_2L(r)\cos(i_2\theta)bF(\zeta) \end{cases}, \tag{22}$$

where the scalar function $L(r)$ denotes

$$L(r) = \left(\frac{\pi}{2}\cos(\omega)\sin(i_1\pi r) + i_1\pi\sin(\omega)\cos(i_1\pi r)\right), \tag{23}$$

and $\omega = \frac{\pi r}{2}$, whereas the second set is:

$$\begin{cases} \mathbf{\Phi}_r^1 &= i_2\sin(\frac{\pi}{2}r)\sin(i_1\pi r)\sin(i_2\theta)\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{\Phi}_\theta^1 &= \sin(\frac{\pi}{2}r)\sin(i_1\pi r)\cos(i_2\theta)\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{\Phi}_\zeta^1 &= -i_2L(r)\sin(i_2\theta)bF(\zeta) \end{cases}. \tag{24}$$

The function $F(\zeta)$ is determined by the boundary condition at $\zeta = 0$ and $\zeta = 1$, similar to Laplacian basis functions in Cui et al. [2018]. There are four combinations:

$\zeta = 0$	$\zeta = 1$	$F(\zeta)$
Dirichlet	Dirichlet	$\sin(i_3\pi\zeta), i_3 \in \mathbb{Z}^+$
Dirichlet	Neumann	$\sin(i_3\pi\zeta), i_3 \in \mathbb{Z}^+ - 0.5$
Neumann	Neumann	$\cos(i_3\pi\zeta), i_3 \in \mathbb{Z}^+$
Neumann	Dirichlet	$\cos(i_3\pi\zeta), i_3 \in \mathbb{Z}^+ - 0.5$

For the principal basis functions, the periodic boundary is satisfied by setting $i_2 \in \mathbb{Z}^+$. Dirichlet boundaries at $r = 0$ can be attained by setting $i_1 \in \mathbb{Z}^+$, and Neumann can be attained with $i_1 \in (\mathbb{Z}^+ - 1/2)$.

2.5 Enrichment Basis Functions

The first two enrichment basis functions are obtained with $A_r = \cos(i_1\pi r)$, which directly extend the enrichment basis functions in polar coordinates:

$$\begin{cases} \mathbf{\Phi}_r^2 = \cos(i_1\pi r)\cos(\theta)\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{\Phi}_\theta^2 = -\cos(i_1\pi r)\sin(\theta)\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{\Phi}_\zeta^2 = i_1\pi\sin(i_1\pi r)\cos(\theta)bF(\zeta) \end{cases} \tag{25}$$

$$\begin{cases} \mathbf{\Phi}_r^3 = \cos(i_1\pi r)\sin(\theta)\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{\Phi}_\theta^3 = \cos(i_1\pi r)\cos(\theta)\frac{\partial F(\zeta)}{\partial \zeta} \\ \mathbf{\Phi}_\zeta^3 = i_1\pi\sin(i_1\pi r)\sin(\theta)bF(\zeta) \end{cases}. \tag{26}$$

Checking the center for $\mathbf{\Phi}^2$,

$$\mathbf{\Phi}_*^2(r=0) = \frac{\partial F(\zeta)}{\partial \zeta}\begin{bmatrix}\cos(\theta) & -\sin(\theta) & 0\end{bmatrix}^T, \tag{27}$$

satisfies the boundary condition in 21. Checking the center again for $\mathbf{\Phi}_*^3$

$$\mathbf{\Phi}_*^3(r=0) = \frac{\partial F(\zeta)}{\partial \zeta}\begin{bmatrix}\sin(\theta) & \cos(\theta) & 0\end{bmatrix}^T, \tag{28}$$

also satisfies the boundary condition. Neumann boundaries at $r = 0$ can be attained by setting $i_1 \in \mathbb{Z}$, and Dirichlet can be attained with $i_1 \in (\mathbb{Z}^+ - 1/2)$.

Next, an extra set of enrichment basis functions is needed for z direction. In this case, the boundary condition in Eqn. 21 along ζ implies $E_\theta = 1$ in Eqn. 15. The solution $C_\theta = \theta$ does not satisfy the periodic boundary condition, so for this basis function, we let $\mathbf{s}_\theta = 0$. This simplifies the divergence free constraint to:

$$A_r + r\frac{\partial A_r}{\partial r} + rE_r = 0. \tag{29}$$

Assigning $A_r = r\cos(i_1\pi r)$, we obtain:

$$\begin{cases} \Phi_r^4 &= r\cos(i_1\pi r)F'(\zeta) \\ \Phi_\theta^4 &= 0 \\ \Phi_\zeta^4 &= (-2\cos(i_1\pi r) + i_1\pi r\sin(i_1\pi r))\, bF(\zeta), \end{cases}. \tag{30}$$

Checking the center for Φ_*^4:

$$\Phi_*^4(r=0) = -2F(\zeta)\begin{bmatrix}0 & 0 & 1\end{bmatrix}, \tag{31}$$

satisfies the smoothness boundary condition in Eqn. 21. The Dirichlet boundary condition at $r = 1$ is obtained with $i_1 \in \mathbb{Z}^+ - 0.5$. When Neumann boundary condition at $r = 1$ is desired, The r appearing in Φ_r^4 prevents the velocity derivative from going to zero. To address this issue, the following version can be used instead:

$$\begin{cases} \Phi_r^{4N} &= rM(r)\frac{\partial F(\zeta)}{\partial \zeta} \\ \Phi_\theta^{4N} &= 0 \\ \Phi_\zeta^{4N} &= \left[-2M(r) + \pi r\left(i_1\sin(i_1\pi r) + i_1^*\cos(i_1^*\pi r)\right)\right] bF(\zeta), \end{cases}$$

where the scalar function $M(r)$ denotes:

$$M(r) = \cos(i_1\pi r) - \sin(i_1^*\pi r), \tag{32}$$

and $i_1^* = i_1 + 1/2$. By assigning $i_1 \in \mathbb{Z}$, Neumann boundary can be attained.

Finally, to capture circular flows along the z axis, we add the last enrichment basis:

$$\begin{cases} \Phi_r^5 &= \Phi_\zeta^5 = 0 \\ \Phi_\theta^5 &= \sin(i_1\pi r)\cos(i_3\pi\zeta) \end{cases}. \tag{33}$$

The final volumetric cylindrical basis is the union $\{\Phi_*^0, \Phi_*^1, \ldots, \Phi_*^5\}$.

3 VOLUMETRIC TOROIDAL BASIS

We now generalize to a volumetric torus.

3.1 Toroidal Divergence Operator

A Cartesian point $\mathbf{p}$ is parameterized in toroidal coordinates as

$$\mathbf{p}_x = (r\sin(\theta) + a)\cos(\phi) \qquad \mathbf{p}_y = (r\sin(\theta) + a)\sin(\phi) \tag{34}$$

$$\mathbf{p}_z = r\cos(\theta), \tag{35}$$

where $a > 1$ denotes the major radius of the torus, and $r \in [0, 1]$, $\theta \in [0, 2\pi)$, and $\phi \in [0, 2\pi)$. This results a torus with inner radius $a - 1$ and outer radius $a + 1$. The coordinate parameterization is visualized in Fig. 1. The inverse of the toroidal coordinate is:

$$r = \sqrt{a^2 + x^2 + y^2 - 2a\sqrt{x^2 + y^2} + z^2} \tag{36}$$

$$\theta = \arccos\left(\frac{z}{r}\right) \qquad \phi = \operatorname{atan2}(y, x) \tag{37}$$

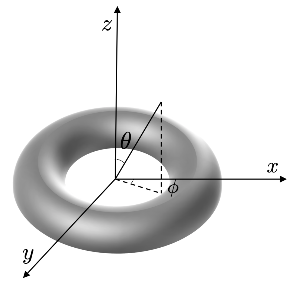

Fig. 1. 3D toroidal coordinates.

The sign of θ is determined by its z value. If $x^2 + y^2 \geq a^2$, then $\theta \in [0, \pi]$. If $x^2 + y^2 \leq a^2$, then $\theta \in [\pi, 2\pi)$. The arctangent is computed with the `atan2` function in C++.

The divergence-free constraint in toroidal coordinates is:

$$\nabla \cdot \mathbf{s} = (\nabla_s + a\nabla_p) \cdot \mathbf{s} = 0 \tag{38}$$

$$\nabla_s \cdot \mathbf{s} = \sin(\theta)\frac{\partial}{\partial r}(r^2\mathbf{s}_r) + r\frac{\partial}{\partial\theta}(\mathbf{s}_\theta\sin(\theta)) + r\frac{\partial \mathbf{s}_\phi}{\partial\phi} \tag{39}$$

$$\nabla_p \cdot \mathbf{s} = \frac{\partial}{\partial r}(r\mathbf{s}_r) + \frac{\partial \mathbf{s}_\theta}{\partial\theta}. \tag{40}$$

The operators ∇_s, ∇_p correspond to the divergence operator in spherical and polar coordinates.

3.2 Generating Toroidal Basis Functions

The toroidal coordinate is a rotation of polar coordinates around the z-axis. Observing this, we take basis functions in polar coordinates, rotate them along ϕ, and make them divergence-free. For example, we first assign $\mathbf{s}_r$ and $\mathbf{s}_\theta$ with the first principal basis functions in polar coordinates:

$$\begin{cases} \mathbf{s}_r &= i_2\sin(i_1\pi r)\cos(i_2\theta) \\ \mathbf{s}_\theta &= -(\sin(i_1\pi r) + \pi i_1 r\cos(i_1\pi r))\sin(i_2\theta) \\ \mathbf{s}_\phi &= 0 \end{cases}. \tag{41}$$

We can weigh the above function along ϕ with a sine function, which results in:

$$\begin{cases} \mathbf{s}_r &= i_2\sin(i_1\pi r)\cos(i_2\theta)\sin(i_3\phi) \\ \mathbf{s}_\theta &= -(\sin(i_1\pi r) + \pi i_1 r\cos(i_1\pi r))\sin(i_2\theta)\sin(i_3\phi) \\ \mathbf{s}_\phi &= 0 \end{cases}. \tag{42}$$

Obviously, the basis function is divergence-free under ∇_p: $\nabla_p\mathbf{s} = 0$. This simplifies the divergence-free constraint in Eqn. 38 into:

$$\nabla_s \cdot \mathbf{s} = 0. \tag{43}$$

In this equation, two components $\mathbf{s}_r$ and $\mathbf{s}_\theta$ are already specified as in Eqn. 42. The remaining component $\mathbf{s}_\phi$ is solved by requiring the divergence ∇_s to be zero, i.e.,

$$\frac{\partial \mathbf{s}_\phi}{\partial\phi} = -\frac{1}{r}\sin(\theta)\frac{\partial}{\partial r}(r^2\mathbf{s}_r) - \frac{\partial}{\partial\theta}(\mathbf{s}_\theta\sin(\theta)). \tag{44}$$

This will result in a set of divergence-free basis functions in toroidal coordinates. The geometry factor a is decoupled, which leads to basis functions that are invariant in a.

3.3 Setting Boundary Conditions

In toroidal coordinates, the periodic boundary condition extends to both θ and ϕ directions: $\mathbf{\Phi}(\theta) = \mathbf{\Phi}(\theta + 2\pi)$ and $\mathbf{\Phi}(\phi) = \mathbf{\Phi}(\phi + 2\pi)$. Similar to polar coordinates, the toroidal coordinates contain singularities along the centerline ($r = 0$), where the parameter θ maps to a single physical point. The boundary condition can be expressed as:

$$\frac{\partial \mathbf{u}_r}{\partial \theta} = \mathbf{u}_\theta \qquad \frac{\partial \mathbf{u}_\theta}{\partial \theta} = -\mathbf{u}_r \qquad \text{at } r = 0. \tag{45}$$

The velocity transform between Cartesian and toroidal is:

$$\begin{bmatrix} \mathbf{u}_x \\ \mathbf{u}_y \\ \mathbf{u}_z \end{bmatrix} = \begin{bmatrix} \sin(\theta)\cos(\phi) & \cos(\theta)\cos(\phi) & -\sin(\phi) \\ \sin(\theta)\sin(\phi) & \cos(\theta)\sin(\phi) & \cos(\phi) \\ \cos(\theta) & -\sin(\theta) & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}_r \\ \mathbf{u}_\theta \\ \mathbf{u}_\phi \end{bmatrix}. \tag{46}$$

3.4 Principal Basis Functions

Principal basis functions can be generated by assigning $\mathbf{s}_r$, $\mathbf{s}_\theta$ in Eqn. 44 with two principal basis functions from polar coordinates and solving for $\mathbf{s}_\phi$. The function along ϕ can be either $\sin(i_3\phi)$ or $\cos(i_3\phi)$. This results in four sets of principal basis functions:

$$\begin{cases} \mathbf{\Phi}^0_r = & i_2 i_3 \sin(i_1\pi r)\cos(i_2\theta)\sin(i_3\phi) \\ \mathbf{\Phi}^0_\theta = & -i_3 L(r)\sin(i_2\theta)\sin(i_3\phi) \\ \mathbf{\Phi}^0_\phi = & -(-i_2\sin(i_1\pi r)\sin(\theta)\cos(i_2\theta) + \\ & L(r)\cos(\theta)\sin(i_2\theta))\cos(i_3\phi), \end{cases} \tag{47}$$

$$\begin{cases} \mathbf{\Phi}^1_r = & i_2 i_3 \sin(i_1\pi r)\cos(i_2\theta)\cos(i_3\phi) \\ \mathbf{\Phi}^1_\theta = & -i_3 L(r)\sin(i_2\theta)\cos(i_3\phi) \\ \mathbf{\Phi}^1_\phi = & (-i_2\sin(i_1\pi r)\sin(\theta)\cos(i_2\theta) + \\ & L(r)\cos(\theta)\sin(i_2\theta))\sin(i_3\phi), \end{cases} \tag{48}$$

$$\begin{cases} \mathbf{\Phi}^2_r = & i_2 i_3 \sin(i_1\pi r)\sin(i_2\theta)\sin(i_3\phi) \\ \mathbf{\Phi}^2_\theta = & i_3 L(r)\cos(i_2\theta)\sin(i_3\phi) \\ \mathbf{\Phi}^2_\phi = & (i_2\sin(i_1\pi r)\sin(\theta)\sin(i_2\theta) + \\ & L(r)\cos(\theta)\cos(i_2\theta))\cos(i_3\phi), \end{cases} \tag{49}$$

$$\begin{cases} \mathbf{\Phi}^3_r = & i_2 i_3 \sin(i_1\pi r)\sin(i_2\theta)\cos(i_3\phi) \\ \mathbf{\Phi}^3_\theta = & i_3 L(r)\cos(i_2\theta)\cos(i_3\phi) \\ \mathbf{\Phi}^3_\phi = & -(i_2\sin(i_1\pi r)\sin(\theta)\sin(i_2\theta) + \\ & L(r)\cos(\theta)\cos(i_2\theta))\sin(i_3\phi). \end{cases} \tag{50}$$

where $L(r)$ denotes:

$$L(r) = \sin(i_1\pi r) + i_1\pi r\cos(i_1\pi r). \tag{51}$$

These functions are zero at $r = 0$, and the boundary conditions in Eqn. 45 are satisfied. In all the previous cases, periodic boundary conditions along θ and ϕ are satisfied by requiring $i_2, i_3 \in \mathbb{Z}^+$. Dirichlet boundary conditions at $r = 1$ can be attained with $i_1 \in \mathbb{Z}^+$. Neumann can be attained with $i_1 \in \mathbb{Z}^+ - 1/2$.

3.5 Enrichment Basis Functions

The enrichment basis functions can be derived by assigning $\mathbf{s}_r$, $\mathbf{s}_\theta$ in Eqn. 44 with two enrichment basis functions in polar coordinates. We obtain four enrichment basis functions. The first two sets are:

$$\begin{cases} \mathbf{\Phi}^4_r & = i_3\cos(i_1\pi r)\sin(\theta)\sin(i_3\phi) \\ \mathbf{\Phi}^4_\theta & = i_3\left(\cos(i_1\pi r) - i_1\pi r\sin(i_1\pi r)\right)\cos(\theta)\sin(i_3\phi) \\ \mathbf{\Phi}^4_\phi & = \left(\cos(i_1\pi r) - i_1\pi r\cos^2(\theta)\sin(i_1\pi r)\right)\cos(i_3\phi), \end{cases} \tag{52}$$

$$\begin{cases} \mathbf{\Phi}^5_r & = i_3\cos(i_1\pi r)\sin(\theta)\cos(i_3\phi) \\ \mathbf{\Phi}^5_\theta & = i_3\left(\cos(i_1\pi r) - i_1\pi r\sin(i_1\pi r)\right)\cos(\theta)\cos(i_3\phi) \\ \mathbf{\Phi}^5_\phi & = -\left(\cos(i_1\pi r) - i_1\pi r\cos^2(\theta)\sin(i_1\pi r)\right)\sin(i_3\phi). \end{cases} \tag{53}$$

Checking the center to verify the consistency boundary condition,

$$\mathbf{\Phi}^4_*(r=0) = \begin{bmatrix} i_3\sin(\theta)\sin(i_3\phi) \\ i_3\cos(\theta)\sin(i_3\phi) \\ \cos(i_3\phi) \end{bmatrix} \quad \mathbf{\Phi}^5_*(r=0) = \begin{bmatrix} i_3\sin(\theta)\cos(i_3\phi) \\ i_3\cos(\theta)\cos(i_3\phi) \\ -\sin(i_3\phi) \end{bmatrix} \tag{54}$$

both satisfy the boundary condition in Eqn. 45. At $r = 0$, the basis functions $\mathbf{\Phi}^4_*$ align with the second row of the velocity transformation matrix in Eqn. 46 when $i_3 = 1$, and thus represent a constant flow along y-axis. Basis functions $\mathbf{\Phi}^5_*$ align with the first row, and are able to represent a constant flow along the x-axis.

The next two sets are:

$$\begin{cases} \mathbf{\Phi}^6_r & = i_3\cos(i_1\pi r)\cos(\theta)\sin(i_3\phi) \\ \mathbf{\Phi}^6_\theta & = i_3\left(i_1\pi r\sin(i_1\pi r) - \cos(i_1\pi r)\right)\sin(\theta)\sin(i_3\phi) \\ \mathbf{\Phi}^6_\phi & = i_1\pi r\sin(i_1\pi r)\sin(\theta)\cos(\theta)\cos(i_3\phi) \end{cases} \tag{55}$$

$$\begin{cases} \mathbf{\Phi}^7_r & = i_3\cos(i_1\pi r)\cos(\theta)\cos(i_3\phi) \\ \mathbf{\Phi}^7_\theta & = i_3\left(i_1\pi r\sin(i_1\pi r) - \cos(i_1\pi r)\right)\sin(\theta)\cos(i_3\phi) \\ \mathbf{\Phi}^7_\phi & = -i_1\pi r\sin(i_1\pi r)\sin(\theta)\cos(\theta)\sin(i_3\phi) \end{cases} \tag{56}$$

Checking the center yields

$$\mathbf{\Phi}^6_*(r=0) = \sin(i_3\phi)\begin{bmatrix}\cos(\theta) & -\sin(\theta) & 0\end{bmatrix}^T, \tag{57}$$

$$\mathbf{\Phi}^7_*(r=0) = \cos(i_3\phi)\begin{bmatrix}\cos(\theta) & -\sin(\theta) & 0\end{bmatrix}^T, \tag{58}$$

where both $\mathbf{\Phi}^6_*$, $\mathbf{\Phi}^7_*$ align with the last column of the transform. Thus, they are able to represent constant flow along the z-axis.

Finally, rotating the circular basis in polar coordinates is not necessary, because $\mathbf{\Phi}^2_*$ with $i_2 = 0$ already captures that mode. The last two circular enrichment modes are:

$$\begin{cases} \mathbf{\Phi}^8_r & = \mathbf{\Phi}^8_\theta = 0 \\ \mathbf{\Phi}^8_\phi & = \cos(i_1\pi r)\sin(i_2\theta), \end{cases} \tag{59}$$

$$\begin{cases} \mathbf{\Phi}^9_r & = \mathbf{\Phi}^9_\theta = 0 \\ \mathbf{\Phi}^9_\phi & = \cos(i_1\pi r)\cos(i_2\theta), \end{cases} \tag{60}$$

which represents circular motions along the z-axis. The final volumetric toroidal basis is the union $\{\mathbf{\Phi}^0_*, \mathbf{\Phi}^1_*, \ldots, \mathbf{\Phi}^9_*\}$.

4 CODIMENSIONAL TOROIDAL BASIS

In this case, the divergence-free constraint (Eqn. 38) simplifies to:

$$\nabla \cdot \mathbf{s} = a\frac{\partial \mathbf{s}_\theta}{\partial \theta} + \frac{\partial}{\partial \theta}(\mathbf{s}_\theta \sin(\theta)) + \frac{\partial \mathbf{s}_\phi}{\partial \phi} = 0. \tag{61}$$

Compared to the codimensional sphere case, the extra term is $a\frac{\partial \mathbf{f}_\theta}{\partial \theta}$. Therefore, we assign $\mathbf{s}_\theta$ with the θ component of the codimensional spherical basis functions and solve for $\mathbf{s}_\phi$. There are no coordinate singularities on the surface of a torus, and only periodic boundary conditions along both θ and ϕ are needed.

4.1 Principal Basis Functions

Four sets of principal basis functions are obtained by assigning either sine or cosine functions along θ and ϕ directions.

$$\begin{cases} \mathbf{\Phi}^0_\theta &= i_2 \sin(i_1\theta)\cos(i_2\phi) \\ \mathbf{\Phi}^0_\phi &= -\left(i_1\cos(i_1\theta)(a+\sin(\theta)) + \cos(\theta)\sin(i_1\theta)\right)\sin(i_2\phi) \end{cases} \tag{62}$$

$$\begin{cases} \mathbf{\Phi}^1_\theta &= i_2 \sin(i_1\theta)\sin(i_2\phi) \\ \mathbf{\Phi}^1_\phi &= \left(i_1\cos(i_1\theta)(a+\sin(\theta)) + \cos(\theta)\sin(i_1\theta)\right)\cos(i_2\phi) \end{cases} \tag{63}$$

$$\begin{cases} \mathbf{\Phi}^2_\theta &= i_2 \cos(i_1\theta)\sin(i_2\phi) \\ \mathbf{\Phi}^2_\phi &= \left(\cos(\theta)\cos(i_1\theta) - i_1(a+\sin(\theta))\sin(i_1\theta)\right)\cos(i_2\phi) \end{cases} \tag{64}$$

$$\begin{cases} \mathbf{\Phi}^3_\theta &= i_2 \cos(i_1\theta)\cos(i_2\phi) \\ \mathbf{\Phi}^3_\phi &= -\left(\cos(\theta)\cos(i_1\theta) - i_1(a+\sin(\theta))\sin(i_1\theta)\right)\sin(i_2\phi) \end{cases} \tag{65}$$

The periodic boundary condition along ϕ is satisfied by assigning $i_2 \in \mathbb{Z}^+$. The periodic boundary condition along θ is satisfied with $i_1 \in \mathbb{Z}^+$ for $\mathbf{\Phi}^0_*, \mathbf{\Phi}^1_*$ and $i_1 \in \mathbb{Z}$ for $\mathbf{\Phi}^2_*, \mathbf{\Phi}^3_*$.

4.2 Enrichment Basis Functions

Similar to the volumetric toroidal basis functions, two circulation enrichment functions are added:

$$\begin{cases} \mathbf{\Phi}^4_\theta &= 0 \\ \mathbf{\Phi}^4_\phi &= \cos(i_1\theta) \end{cases} \tag{66}$$

$$\begin{cases} \mathbf{\Phi}^5_\theta &= 0 \\ \mathbf{\Phi}^5_\phi &= \sin(i_1\theta) \end{cases}. \tag{67}$$

The final codimensional toroidal basis is the union $\{\mathbf{\Phi}^0_*, \mathbf{\Phi}^1_*, \ldots, \mathbf{\Phi}^5_*\}$.

5 VOLUMETRIC SPHEROIDAL BASIS

In this section, we extend the spherical basis functions to prolate and oblate spheroids, where stretching and compressing the sphere along the z-axis respectively results in the prolate and oblate cases. Examples are shown in Fig. 2.

A point $\mathbf{p}$ is parameterized in prolate coordinates as:

$$\mathbf{p}_x = br\sin(\theta)\cos(\phi) \quad \mathbf{p}_y = br\sin(\theta)\sin(\phi) \quad \mathbf{p}_z = a\rho\cos(\theta),$$

where $\rho = \sqrt{1+c^2r^2}$. Oblate coordinates are:

$$\mathbf{p}_x = a\rho\sin(\theta)\cos(\phi) \quad \mathbf{p}_y = a\rho\sin(\theta)\sin(\phi) \quad \mathbf{p}_z = br\cos(\theta).$$

Similar to elliptical coordinates, we use b to denote the minor axis of the spheroid, and which is then folded into the constants $a = \sqrt{1-b^2}$ and $c = b/a$. Both coordinate systems converge to spherical coordinates when $b \to 1$.

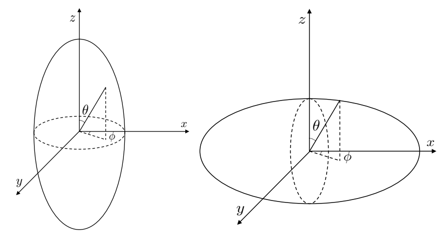

Fig. 2. Left: Prolate spheroidal coordinates. Right: Oblate coordinates

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5.1 Prolate Basis Functions

First, we will derive the basis functions in prolate coordinates. The divergence operator in prolate coordinates is:

$$\nabla \cdot \mathbf{s} = \frac{1}{h_r h_\theta h_\phi}\left[\frac{\partial}{\partial r}\left(h_\theta h_\phi \mathbf{s}_r\right) + \frac{\partial}{\partial \theta}\left(h_r h_\phi \mathbf{s}_\theta\right) + \frac{\partial}{\partial \phi}\left(h_r h_\theta \mathbf{s}_\phi\right)\right] \tag{68}$$

By inserting the scale factors:

$$h_r = ac\frac{h}{\rho} \quad h_\theta = ah \quad h_\phi = acr\sin(\theta) \quad h = \sqrt{c^2r^2 + \sin^2(\theta)},$$

the divergence-free constraint becomes:

$$\left(\sin(\theta)\frac{\partial}{\partial r}(hr\mathbf{s}_r) + r\frac{\partial}{\partial \theta}\left(\frac{\sin(\theta)ch}{\rho}\mathbf{s}_\theta\right) + \frac{h^2}{\rho}\frac{\partial \mathbf{s}_\phi}{\partial \phi}\right) = 0. \tag{69}$$

Compare this to the spherical coordinates case:

$$\left(\sin(\theta)\frac{\partial}{\partial r}\left(r^2\mathbf{u}_r\right) + r\frac{\partial}{\partial \theta}(\sin(\theta)\mathbf{u}_\theta) + r\frac{\partial \mathbf{u}_\phi}{\partial \phi}\right) = 0. \tag{70}$$

Given a divergence-free basis $\mathbf{\Phi}$ in spherical coordinates, it can be converted to prolate spheroidal basis functions $\mathbf{\Psi}$ as follows:

$$\mathbf{\Psi}_r = \frac{cr}{h}\mathbf{\Phi}_r \qquad \mathbf{\Psi}_\theta = \frac{\rho}{h}\mathbf{\Phi}_\theta \qquad \mathbf{\Psi}_\phi = \frac{cr\rho}{h^2}\mathbf{\Phi}_\phi. \tag{71}$$

By inserting $\mathbf{\Psi}_*$ into Eqn. 69, we reduced the divergence-free constraint to the spherical case (Eqn.70), which should be zero because $\mathbf{\Phi}_*$ is divergence-free in spherical coordinates. Similar to the elliptical basis functions, two enrichment basis functions need attention.

The velocity transformation between Cartesian coordinates and prolate coordinates is:

$$\begin{bmatrix}\mathbf{u}_x \\ \mathbf{u}_y \\ \mathbf{u}_z\end{bmatrix} = \frac{1}{h}\begin{bmatrix}\rho\sin(\theta)\cos(\phi) & cr\cos(\theta)\cos(\phi) & -h\sin(\phi) \\ \rho\sin(\theta)\sin(\phi) & cr\cos(\theta)\sin(\phi) & h\cos(\phi) \\ cr\cos(\theta) & -\rho\sin(\theta) & 0\end{bmatrix}\begin{bmatrix}\mathbf{u}_r \\ \mathbf{u}_\theta \\ \mathbf{u}_\phi\end{bmatrix} \tag{72}$$

The factors in Eqn. 71 do not align with the first and second rows of the transform. Therefore, the enrichment modes $\mathbf{\Psi}^7_*$ and $\mathbf{\Psi}^8_*$ should be redesigned as the following:

$$\begin{cases} \mathbf{\Psi}^7_r = & \frac{\rho}{h}\cos(i_1\pi r)\sin(\theta)\sin(\phi) \\ \mathbf{\Psi}^7_\theta = & \frac{cr}{h}(-i_1\pi r\sin(i_1\pi r) + \cos(i_1\pi r))\cos(\theta)\sin(\phi) \\ \mathbf{\Psi}^7_\phi = & \frac{1}{h^2}\left(\cos(i_1\pi r)(1+c^2r^2-\cos^2(\theta)) - \right. \\ & \left. i_1\pi r\sin(i_1\pi r)(c^2r^2\cos^2(\theta)+\sin^2(\theta))\right)\cos(\phi) \end{cases}. \tag{73}$$

Checking $i_1 = 0$, the basis function evaluates to:

$$\mathbf{\Psi}^7_* = \frac{1}{h}\left[\rho\sin(\theta)\sin(\phi) \quad cr\cos(\theta)\sin(\phi) \quad h\cos(\phi)\right]^T, \tag{74}$$

which aligns with the second row of Eqn. 72. Thus, it is able to represent translation along the y-axis, similar to $\mathbf{\Phi}_*^7$ in spherical coordinates. The next enrichment basis function is

$$\begin{cases} \mathbf{\Psi}_r^8 = & \frac{\rho}{h}\cos(i_1\pi r)\sin(\theta)\cos(\phi) \\ \mathbf{\Psi}_\theta^8 = & \frac{cr}{h}(-i_1\pi r\sin(i_1\pi r)+\cos(i_1\pi r))\cos(\theta)\cos(\phi) \\ \mathbf{\Psi}_\phi^8 = & \frac{1}{h^2}[-\cos(i_1\pi r)(1+c^2r^2-\cos^2(\theta))+ \\ & i_1\pi r\sin(i_1\pi r)(c^2r^2\cos^2(\theta)+\sin^2(\theta))]\sin(\phi) \end{cases}. \quad (75)$$

Checking $i_1 = 0$, the basis function evaluates to:

$$\mathbf{\Psi}_*^8 = \frac{1}{h}\left[\rho\sin(\theta)\cos(\phi) \quad cr\cos(\theta)\cos(\phi) \quad -h\sin(\phi)\right]^T \quad (76)$$

which aligns with the first row of Eqn. 72. Thus, it is able to represent the x-translation similar to $\mathbf{\Phi}_*^8$ in spherical coordinates.

5.2 Oblate Basis Functions

Next, we proceed with oblate coordinates. The divergence-free constraint can be expressed by inserting the scale factors

$$h_c = \sqrt{c^2r^2+\cos^2(\theta)} \quad h_r = ac\frac{h_c}{\rho} \quad h_\theta = ah_c \quad h_\phi = a\rho\sin(\theta),$$

into Eqn. 68:

$$\left(\sin(\theta)\frac{\partial}{\partial r}\left(\frac{h_c}{c}\rho\mathbf{s}_r\right)+\frac{\partial}{\partial\theta}\left(h_c\sin(\theta)\mathbf{s}_\theta\right)+\frac{\partial}{\partial\phi}\left(\frac{h_c^2}{\rho}\mathbf{s}_\phi\right)\right)=0. \quad (77)$$

The spherical basis functions $\mathbf{\Phi}$ can be converted to oblate basis $\mathbf{\Psi}$ functions as follows:

$$\mathbf{\Psi}_r = \frac{c^2r^2}{h_c\rho}\mathbf{\Phi}_r \qquad \mathbf{\Psi}_\theta = \frac{cr}{h_c}\mathbf{\Phi}_\theta \qquad \mathbf{\Psi}_\phi = \frac{cr\rho}{h_c^2}\mathbf{\Phi}_\phi. \quad (78)$$

For oblate basis functions, three enrichment basis functions need attention. The velocity transform between Cartesian and oblate coordinates is:

$$\begin{bmatrix}\mathbf{u}_x\\ \mathbf{u}_y\\ \mathbf{u}_z\end{bmatrix} = \frac{1}{h_c}\begin{bmatrix} cr\sin(\theta)\cos(\phi) & \rho\cos(\theta)\cos(\phi) & -h_c\sin(\phi) \\ cr\sin(\theta)\sin(\phi) & \rho\cos(\theta)\sin(\phi) & h_c\cos(\phi) \\ \rho\cos(\theta) & -cr\sin(\theta) & 0 \end{bmatrix}\begin{bmatrix}\mathbf{u}_r\\ \mathbf{u}_\theta\\ \mathbf{u}_\phi\end{bmatrix}. \quad (79)$$

The conversion in Eqn. 78 does not align with any rows of Eqn. 79. We begin with $\mathbf{\Psi}_*^6$:

$$\begin{cases} \mathbf{\Psi}_r^6 & = \frac{\rho}{h_c}\cos(i_1\pi r)\cos(\theta) \\ \mathbf{\Psi}_\theta^6 & = \frac{1}{h_c}(-cr\cos(i_1\pi r)+\frac{i_1\pi}{2c}\rho^2\sin(i_1\pi r))\sin(\theta) \\ \mathbf{\Psi}_\phi^6 & = 0 \end{cases}. \quad (80)$$

Checking $i_1 = 0$, the basis function evaluates to

$$\mathbf{\Psi}_*^6 = \frac{1}{h_c}\left[\rho\cos(\theta) \quad -cr\sin(\theta) \quad 0\right]^T, \quad (81)$$

which aligns with the last row of Eqn. 79. Thus, it represents translation along z-axis, similar to $\mathbf{\Phi}_*^6$ in spherical coordinates. Next, $\mathbf{\Phi}_*^7$ becomes

$$\begin{cases} \mathbf{\Psi}_r^7 = & \frac{cr}{h_c}\cos(i_1\pi r)\sin(\theta)\sin(\phi) \\ \mathbf{\Psi}_\theta^7 = & \frac{\rho}{h_c}(-i_1\pi r\sin(i_1\pi r)+\cos(i_1\pi r))\cos(\theta)\sin(\phi) \\ \mathbf{\Psi}_\phi^7 = & \frac{1}{h_c^2}(\cos(i_1\pi r)h_c^2 - i_1\pi r\rho^2\cos^2(\theta)\sin(i_1\pi r))\cos(\phi) \end{cases}. \quad (82)$$

Checking $i_1 = 0$, the basis function evaluates to:

$$\mathbf{\Psi}_*^7 = \frac{1}{h_c}\left[cr\sin(\theta)\sin(\phi) \quad \rho\cos(\theta)\sin(\phi) \quad h_c\cos(\phi)\right]^T. \quad (83)$$

This is the second row of Eqn. 79, and represents y-translation similar to $\mathbf{\Phi}_*^7$ in spherical coordinates. Finally:

$$\begin{cases} \mathbf{\Psi}_r^8 = & \frac{cr}{h}\cos(i_1\pi r)\sin(\theta)\cos(\phi) \\ \mathbf{\Psi}_\theta^8 = & \frac{\rho}{h}(-i_1\pi r\sin(i_1\pi r)+\cos(i_1\pi r))\cos(\theta)\cos(\phi) \\ \mathbf{\Psi}_\phi^8 = & \frac{1}{h_c^2}(-\cos(i_1\pi r)h_c^2 + i_1\pi r\rho^2\cos^2(\theta)\sin(i_1\pi r))\sin(\phi) \end{cases}. \quad (84)$$

Checking $i_1 = 0$, the basis function evaluates to,

$$\mathbf{\Psi}_*^8 = \frac{1}{h_c}\left[cr\sin(\theta)\cos(\phi) \quad \rho\cos(\theta)\cos(\phi) \quad -h_c\sin(\phi)\right]^T, \quad (85)$$

which is the first row of Eqn. 79, and represents x-translation similar to $\mathbf{\Phi}_*^8$ in spherical coordinates.

5.3 Computation of Dot Products and Advection Tensors

The scale factors appearing in spheroid basis functions prevent analytical integrations along θ and r. For example, integrations of the following functions are needed to compute both dot products and the advection tensor:

$$\begin{cases} G_{ss}(r,\theta) & = h^p\rho^q r^l\sin(k_1\pi r)\sin(k_2\theta) \\ G_{sc}(r,\theta) & = h^p\rho^q r^l\sin(k_1\pi r)\cos(k_2\theta) \\ G_{cs}(r,\theta) & = h^p\rho^q r^l\cos(k_1\pi r)\sin(k_2\theta) \\ G_{cc}(r,\theta) & = h^p\rho^q r^l\cos(k_1\pi r)\cos(k_2\theta), \end{cases} \quad (86)$$

where p, q and l are integers powers, i.e., $p = -2$ for h^{-2}, $q = 2$ for ρ^2 and $l = -1$ for r^{-1}. Constants k_1 and k_2 are integer wavenumbers. When $p < 0$ or p is odd, the integration is no longer separable along r and θ, and have to be integrated numerically. In our implementation, we evaluate some combinations of p, q, l analytically, e.g., when both $p, q > 0$ are even. For other combinations, we numerically compute a lookup table containing integer wavenumbers k_1 and k_2, and then query it when computing the integrations.

6 CODIMENSIONAL SPHEROIDAL BASIS

The codimensional spherical basis can be extended to codimensional spheroidal basis. The extension to prolate is:

$$\mathbf{\Psi}_\theta = \frac{1}{b}\mathbf{\Phi}_\theta \qquad \mathbf{\Psi}_\phi = \frac{1}{ah}\mathbf{\Phi}_\phi. \quad (87)$$

The extension to oblate is:

$$\mathbf{\Psi}_\theta = \frac{1}{a\rho}\mathbf{\Phi}_\theta \qquad \mathbf{\Psi}_\phi = \frac{1}{ah_c}\mathbf{\Phi}_\phi. \quad (88)$$

These factors are used to convert all codimensional spherical basis functions to codimensional spheroids.

7 COMPLETENESS OF SPHERICAL SURFACE BASIS

To demonstrate the completeness of our basis functions, i.e. their ability to represent arbitrary vector fields, we will show that we can represent vector spherical harmonics, which is known to be complete [Hill 1954] using our functions. We will shown that any vector from the span of vector spherical harmonics have a non-zero projection into our basis functions.

7.1 Preliminaries

We will start with the scalar spherical harmonics,

$$Y_l^m(\theta, \phi) = \alpha_l^m P_l^m(\cos(\theta)) e^{im\phi}, \tag{89}$$

where $i = \sqrt{-1}$, $\alpha_l^m = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}$, $l \in \mathbb{N}$, $-l \le m \le l$. We use P_l^m to denote the associated Legendre polynomials. A closed form formula of P_l^m is given in Korn and Korn [2000]:

$$\begin{aligned} P_l^m(\cos(\theta)) &= \sin^m(\theta) \sum_{k=m}^{l} a_{klm} \cos(\theta)^{k-m} \\ a_{klm} &= (-1)^m 2^l \frac{k!}{(k-m)!} \binom{l}{k} \binom{\frac{l+1-1}{2}}{k}. \end{aligned} \tag{90}$$

The derivative of the above equation is:

$$\begin{aligned} \frac{P_l^m(\cos(\theta))}{\partial\theta} =& m \sin^{m-1}(\theta) \cos(\theta) \sum_{k=m}^{l} a_{klm} \cos(\theta)^{k-m} - \\ & \sin^m(\theta) \sum_{k=m}^{l} (k-m) a_{klm} \cos(\theta)^{k-m-1} \sin(\theta). \end{aligned} \tag{91}$$

We will also make use of the following formulas from Korn and Korn [2000]:

$$\sin(n\theta) = \sum_{k \in \text{odd}} (-1)^{\frac{k-1}{2}} \binom{n}{k} \cos^{n-k}(\theta) \sin^k(\theta) \tag{92}$$

$$\cos(n\theta) = \sum_{k \in \text{even}} (-1)^{\frac{k}{2}} \binom{n}{k} \cos^{n-k}(\theta) \sin^k(\theta). \tag{93}$$

7.2 Vector Spherical Harmonics

We will compare our basis functions on a sphere with the divergence-free vector spherical harmonics from Hill [1954]:

$$\begin{cases} \chi_\theta = \frac{-mY_l^m}{\sqrt{(l(l+1))}\sin(\theta)} \\ \chi_\phi = \frac{-i}{\sqrt{(l(l+1))}} \frac{\partial Y_l^m}{\partial\theta} \end{cases} \tag{94}$$

These vector spherical harmonics are both complete, and eigenfunctions of the Laplacian operator on the surface of a sphere [Barrera et al. 1985]. For brevity, we ignore the $\frac{-1}{\sqrt{(l(l+1))}}$ constant in both components of χ. Inserting the definition of Y_l^m into Eqn. 94 yields

$$\begin{cases} \chi_\theta = m \frac{P_l^m(\cos(\theta))}{\sin(\theta)} e^{im\phi} \\ \chi_\phi = i \frac{\partial P_l^m(\cos(\theta))}{\partial\theta} e^{im\phi}. \end{cases} \tag{95}$$

We will focus on the imaginary part of the above equation,

$$\begin{cases} \Im(\chi_\theta) = m \frac{P_l^m(\cos(\theta))}{\sin(\theta)} \sin(m\phi) \\ \Im(\chi_\phi) = \frac{\partial P_l^m(\cos(\theta))}{\partial\theta} \cos(m\phi), \end{cases} \tag{96}$$

because the real part of χ is the same function with sine and cosine swapped along ϕ. Once the imaginary case is established, the real case follows. Additionally, since $P_l^{-m}(x) = (-1)^m (l-m)!/(l+m)! P_l^m(x)$ [Korn and Korn 2000], it is sufficient to focus on the cases where $m \ge 0$.

To show the completeness of our basis $\{\Phi^0, \Phi^1, \Phi^2, \Phi^3, \Phi^4\}$, we must prove that for any vector in the span of $\chi(m, l)$, there exists a function Φ, that has a non-zero projection onto that vector. This will be shown by expanding both χ and Φ into polynomials with respect to $\cos(\theta)$, and by showing that they span the same polynomial space of $\cos(\theta)$. This will be proven by showing that the transformation matrix between the span of χ and Φ is non-singular.

The proof will cover different enrichment function cases, since each case has a slightly different polynomial form. We will begin with the easiest case of $\chi(0, l)$, and show that its span has a non-zero projection onto Φ^4.

7.3 The $\chi(0, l)$ Case

We first examine the $m = 0$ case, where the vector spherical harmonics become (for readability, we have dropped the $\Im$ operator):

$$\chi_\theta(0, l) = 0 \qquad \chi_\phi(0, l) = \frac{\partial P_l^0(\cos(\theta))}{\partial\theta} \tag{97}$$

This corresponds to our enrichment modes Φ^4 on the sphere. The first two modes are

$$\chi_\theta(0, 1) = 0 \qquad \chi_\phi(0, 1) = -\sin(\theta) \tag{98}$$

$$\chi_\theta(0, 2) = 0 \qquad \chi_\phi(0, 2) = -\frac{3}{2}\sin(2\theta), \tag{99}$$

which aligns exactly with Φ^4 with $i_1 = 1, i_1 = 2$. We then need to prove that for any $\chi(0, l), l \in \mathbb{Z}^+$, there exists $i_1 \in \mathbb{Z}^+$, such that Φ^4 has a non-zero projection onto $\chi(0, l)$. To establish this, we first insert $m = 0$ into Eqn. 91,

$$\chi_\theta(0, l) = \frac{P_l^0(\cos(\theta))}{\partial\theta} = -\sin(\theta) \sum_{k=0}^{l} k a_{kl0} \cos(\theta)^{k-1}, \tag{100}$$

and then expand Φ^4 using Eqn. 93 to obtain:

$$\Phi_\phi^4(i_1) = \sin(i_1\theta) = \sum_{k \in \text{odd}} (-1)^{\frac{k-1}{2}} \binom{i_1}{k} \cos^{i_1-k}(\theta) \sin^k(\theta). \tag{101}$$

The $\chi_\theta(0, l)$ term is of order l, e.g., $\sin(\theta)\cos(\theta)^{l-1}$, while the expansion of $\Phi_\phi^4(i_1) = \sin(i_1\theta)$ is of order i_1, e.g., $\cos^{i_1-1}(\theta)\sin(\theta)$. Because χ is complete, Φ^4 can be expanded by $\chi(0, l)$ into the following form:

$$\Phi_\phi^4(i_1) = c_{i_1}\chi(0, i_1) + \sum_{l}^{i_1-1} c_l \chi(0, l). \tag{102}$$

Linear combinations of the $\chi(0, l)$ terms with order less than i_1 ($l < i_1$) are not able to represent $\Phi_\phi^4(i_1) = \sin(i_1\theta)$, which is of order i_1. Thus, for any Φ^4 with wavenumber i_1, there exists $l = i_1$, such that Φ^4 has non-zero projection onto $\chi(0, l)$. This means c_{i_1} is non-zero. Therefore, the transformation matrix between span of Φ^4, and $\chi(0, l)$ must be a lower-triangular matrix with a non-zero diagonal $1, 1, c_3, \ldots, c_i$. Thus, the transformation matrix between the linear spaces of χ and Φ is invertible, and the two spaces must share the same span. In the following cases, the proof is similar, and we will only show the diagonal entries c_{i_1} of the transformation matrix are non-zero.

7.4 The $\chi(1,l)$ Case

Next, we will prove for any $\chi(1,l), l \in \mathbb{Z}^+$, there exists $i_1 \in \mathbb{N}$, such that Φ^3 have non-zero projections onto $\chi(1,l)$. We will focus on Φ^3 because when $m = 1$, the imaginary part of χ corresponds to enrichment basis functions Φ^3. Two examples of $\chi(1,l)$ are given:

$$\chi_\theta(1,1) = -\sin(\phi) \qquad \chi_\phi(1,1) = -\cos(\theta)\cos(\phi) \tag{103}$$

$$\chi_\theta(1,2) = -3\cos(\theta)\sin(\phi) \qquad \chi_\phi(1,2) = -3\cos(2\theta)\cos(\phi) \tag{104}$$

which exactly align with Φ^3 when $i_1 = 0, i_1 = 1$. Next, $\chi(1,l)$ can be expanded as:

$$\begin{cases} \chi_\theta(1,l) = & \sum_{k=1}^{l} a_{kl1}\cos(\theta)^{k-1}\sin(\phi) \\ \chi_\phi(1,l) = & (\cos(\theta)\sum_{k=1}^{l} a_{kl1}\cos(\theta)^{k-1} - \\ & \sin(\theta)\sum_{k=1}^{l}(k-1)a_{kl1}\cos(\theta)^{k-2}\sin(\theta))\cos(\phi) \end{cases} \tag{105}$$

The highest order terms are:

$$\begin{cases} \chi_\theta(1,l) &= \cos(\theta)^{l-1}\sin(\phi) \\ \chi_\phi(1,l) &= (\cos(\theta)\cos(\theta)^{l-1} - (l-1)\cos(\theta)^{l-2}\sin^2(\theta))\cos(\phi) \end{cases} \tag{106}$$

The enrichment basis function Φ^3 is:

$$\begin{cases} \Phi^3_\theta &= \cos(i_1\theta)\sin(\phi) \\ \Phi^3_\phi &= (\cos(\theta)\cos(i_1\theta) - i_1\sin(\theta)\sin(i_1\theta))\cos(\phi) \end{cases} \tag{107}$$

Following Eqn. 93, Φ^3_θ is an order i_1 polynomial along θ, and Φ^3_ϕ is an order $i_1 + 1$ polynomial along θ. By expanding Φ^3 with $\chi(1,l)$, we have:

$$\Phi^3(i_1) = c_{i_1+1}\chi(1, i_1+1) + \sum_{l=1}^{i_1+1} c_l\chi(1,l). \tag{108}$$

Thus, for any $\chi(1,l), l \in \mathbb{Z}^+$, there exists $i_1 = l-1$ such that Φ^3 have a non-zero projection onto $\chi(1,l)$, which will resolve the highest order terms. This means the diagonal entries c_{i_1+1} of the transformation matrix are non-zero, and the transformation matrix is invertible.

7.5 The $\chi(m,l)$ Case Where $m > 1$

Lastly, we will prove that for any $\chi(m,l)$ where $m > 1$, there exists Φ^1 that have non-zero projection onto χ. We will focus on Φ^1, because it aligns with the imaginary component of χ. The projection of the imaginary part of $\chi(m,l)$ onto $\Phi^1(i_1,i_2)$ (Eqn. 9 multipled by i_2) is:

$$\begin{cases} \chi_\theta = m\frac{P_l^m(\cos(\theta))}{\sin(\theta)}\sin(m\phi) \\ \chi_\phi = \frac{\partial P_l^m(\cos(\theta))}{\partial\theta}\cos(m\phi), \end{cases} \tag{109}$$

$$\begin{cases} \Phi^1_\theta &= i_2\sin(i_1\theta)\sin(i_2\phi) \\ \Phi^1_\phi &= (\cos(\theta)\sin(i_1\theta) + i_1\sin(\theta)\cos(i_1\theta))\cos(i_2\phi) \end{cases} \tag{110}$$

$$\begin{aligned} \langle\chi(m,l), \Phi^1(i_1,i_2)\rangle = &\int_\theta f(\theta)d\theta\int_{\phi=0}^{2\pi}\sin(m\phi)\sin(i_2\phi)d\phi + \\ &\int_\theta f(\theta)d\theta\int_{\phi=0}^{2\pi}\cos(m\phi)\cos(i_2\phi)d\phi \end{aligned} \tag{111}$$

The dot product is non-zero if and only if $i_2 = m$, because $\int_{\phi=0}^{2\pi}\sin(m\phi)\sin(i_2\phi)d\phi = \pi\delta_{i_2,m}$, and $\int_{\phi=0}^{2\pi}\cos(m\phi)\cos(i_2\phi)d\phi = \pi\delta_{i_2,m}$. Therefore for any spherical harmonics $\chi(m,l)$, only selecting $i_2 = m$ for Φ^1 could possibly results in a non-zero projection onto the spherical harmonics.

$$\begin{cases} \Phi^1_\theta &= m\sin(i_1\theta)\sin(m\phi) \\ \Phi^1_\phi &= (\cos(\theta)\sin(i_1\theta) + i_1\sin(\theta)\cos(i_1\theta))\cos(m\phi) \end{cases} \tag{112}$$

The highest order terms appearing in $\chi(m,l)$ are

$$\begin{cases} \chi_\theta(m,l) = & m\sin^{m-1}(\theta)\cos(\theta)^{l-m}\sin(m\phi) \\ \chi_\phi(m,l) = & (m\sin^{m-1}(\theta)\cos(\theta)^{l-m+1} - \\ & (l-m)\sin^{m+1}(\theta)\cos(\theta)^{l-m-1})\cos(m\phi), \end{cases} \tag{113}$$

which are respectively of order $l-1$ and l. By expanding $\Phi^1(i_1,m)$ with $\chi(m,l)$, we have:

$$\Phi^1(i_1,m) = c_{i_1+1}\chi(m, i_1+1) + \sum_{l=1}^{i_1+1} c_l\chi(m,l). \tag{114}$$

Again Φ^1_θ is an order i_1 polynomial along θ, while Φ^1_ϕ is an order $i_1 + 1$ polynomial along θ Thus, for any $\chi(m,l)$, there exists $i_1 = l-1, i_2 = m$, where Φ^1 has a non-zero projection onto χ, which resolves the highest order terms in Φ^1. This means the diagonal entries c_{i_1+1} of the transformation matrix are non-zero, and the transformation matrix is invertible.

In conclusion, we have shown the span of vector spherical harmonics shares the same span as our basis functions. Thus, our surface basis functions $\{\Phi^0, \Phi^1, \Phi^2, \Phi^3, \Phi^4\}$ are complete.

8 THE MODIFIED CONJUGATE GRADIENT SOLVER

The equation we want to solve is:

$$\left(\mathbf{I} - \frac{\Delta t}{2}\mathbf{C}\right)\mathbf{w}^{t+1} = \frac{\Delta t}{2}\mathbf{C}\mathbf{w}^t + \mathbf{w}^t + \mathbf{f}. \tag{115}$$

Applying the normal equations and $\mathbf{C}^T = -\mathbf{C}$, we obtain:

$$\left(\mathbf{I} + \frac{\Delta t^2}{4}\mathbf{C}^T\mathbf{C}\right)\mathbf{w}^{t+1} = \Delta t\mathbf{C}\mathbf{w}^t + \frac{\Delta t^2}{4}\mathbf{C}\mathbf{C}\mathbf{w}^t + \mathbf{w}^t. \tag{116}$$

The following algorithm describes the modified CG solver to solve Eqn. 116.

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