Notes on computing reference space–to–physical–space Jacobian on the sphere in GeoFLOW

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We present miscellaneous notes about GeoFLOW discretization.

I. INTEGRATION AND JACOBIAN MATRIX

We define the tensor product basis function in an embedded space at reference location (ξ, η, ζ) as:

$$\Psi_{I(i,j)}(\xi, \eta, \zeta) = h_i(\xi) h_j(\eta) \delta(1 - \zeta), \tag{1}$$

where ζ represents a reference coordinate pointing 'outward' from the center of the 'embedding' coordinates (e.g., center of the sphere), and $I(i,j)$ represents a tensor product index combining the 1d indices i, and j that label the 1d shape functions.

In order to compute spatial derivatives in Cartesian coordinates, $x^i = (x, y, z)$, we must compute the Jacobian matrix of the transformation from reference space to Cartesian space:

$$J_{ij} = \frac{\partial x^i}{\partial \xi^j} = \begin{pmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \zeta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \zeta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \zeta} \end{pmatrix} \tag{2}$$

For embedded or other complex geometries, for which we have no analytic relation between reference space and physical space, we assume that we can expand the Cartesian coordinates just like any other square-integrable (Sobolev space) function in terms of the shape functions:

$$x^j = \sum_{I(i,j)} \hat{x}_I^j \Psi_I, \tag{3}$$

where $\hat{x}_I^j$ is value of the Cartesian coordinate, x^j, at node location $I(i,j)$. Then evaluating the derivatives in Eq. 2 presents no difficulty. We note that from Eq. 2 that

$$J_{i3} = -h_i(\xi) h_j(\eta) \frac{\delta(1 - \zeta)}{1 - \zeta}, \tag{4}$$

using the well-known expression for the derivative of $\delta(x)$. Even though these components are ill-defined at $\zeta = 1$, we use them formally to show why the expansion Eq. 1 is appropriate, even though the distribution, $\delta(1 - \zeta)$ cannot be encoded directly.

To compute the spatial derivative of function, f, at a reference interval node location, we evaluate

$$\frac{df}{dx^j} = \sum_{k=1}^{2} \frac{d\xi^k}{dx^j} \frac{df}{d\xi^k}, \tag{5}$$

where it is assumed that f is square integrable, and may therefore be expanded in terms of the basis functions, Ψ_I, as in Eq. 3. Thus, we require the inverse of the Jacobian matrix, Eq. 2. We examine this now. From the components, J_{ij} of Eq. 2, we can immediately write the inverse as

$$J_{ij}^{-1} = \frac{\partial \xi^i}{\partial x^j} = \frac{1}{|J|} \begin{pmatrix} J_{22}J_{33} - J_{23}J_{23} & J_{32}J_{13} - J_{12}J_{33} & J_{12}J_{23} - J_{22}J_{13} \\ J_{31}J_{23} - J_{21}J_{33} & J_{11}J_{33} - J_{31}J_{13} & J_{21}J_{13} - J_{11}J_{23} \\ J_{21}J_{32} - J_{32}J_{22} & J_{31}J_{12} - J_{11}J_{32} & J_{11}J_{22} - J_{21}J_{12} \end{pmatrix} = \begin{pmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} & \frac{\partial \xi}{\partial z} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} & \frac{\partial \eta}{\partial z} \\ \frac{\partial \zeta}{\partial x} & \frac{\partial \zeta}{\partial y} & \frac{\partial \zeta}{\partial z} \end{pmatrix}. \tag{6}$$

The determinant $|J|$ is given by

$$|J| = J_{11}(J_{22}J_{33} - J_{32}J_{23}) - J_{12}(J_{21}J_{33} - J_{31}J_{23}) + J_{13}(J_{21}J_{32} - J_{31}J_{22}). \tag{7}$$

We can now note that in Eq. 7, each term contains a factor $J_{i3} \sim \frac{\delta(1-\zeta)}{1-\zeta}$, and in Eq. 6, each term in the first two rows contains the same factor, so these factors cancel. But in the last row of Eq. 6, there is no such factor, so at $\zeta = 1$, this row in J_{ij}^{-1} is 0. This means that, when computing the derivative, Eq. 5, we do not need to add in the final reference interval derivative with respect to ζ, which is why the sum in Eq. 5 only goes over [1,2], reflecting reference derivatives only in the two required reference directions.

The significance of this can be seen in the following. If instead of expansion Eq. 1 we chose

$$\Psi_{I(i,j)}(\xi, \eta, \zeta) = h_i(\xi)h_j(\eta)\zeta, \tag{8}$$

as in [1], then the final row of Eq. 6 would, in general, be non-zero, and the sum in Eq. 5 would include an additional term

$$\frac{d\zeta}{dx^j}\frac{df}{d\zeta}.$$

which is non-zero. So, if f is a constant in Eq. 5, the first two summands would evaluate to 0, since the derivative matrices, $d\Psi_I/d\xi$ and $d\Psi_I/d\eta$ acting on a constant would give 0, but the final term, $d\Psi_I/d\zeta$, would not. Hence, it is unclear how, for example, the advection operator, $\mathbf{A}_{ijk}$, in Eq. (6) and written out explicitly below Eq. (13) of [1] can be zero when acting on a constant, as it must.

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[1] F. X. Giraldo, "A spectral element shallow water model on spherical geodesic grids," International Journal for Numerical Methods in Fluids. **35**, 869–901 (2001).