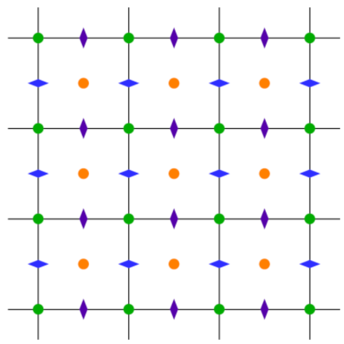
Discrete Operators and Implementation

These operators act on data located in different spaces, as indicated on the control volume document. Let the following notation $D_{F-C} = D : F \to C$ signify that the operator D operates on data that live on F and stores the result on C.

Order of accuracy

All of the below operators should be of 2nd order. The difference formulae do not look like a collocated 2nd order difference formula because of the staggered grid. This section shows how these seemingly 1st order accurate differences are in fact 2nd order.



1st derivative of data living on c, for ∇p $(c \to F)$

We may approximate the pressure at the cell center location j about the face $j + 1/2$. We may write this as a Taylor expansion as

$$p_{j+k} = p_j + (hk)p_j^{'} + \frac{1}{2!}(hk)^2 p_j^{''} + O(h^3) \qquad (for\ k > 0)$$

Similarly, we may approximate

$$p_{j-k} = p_j + (-hk)p_j^{'} + \frac{1}{2!}(-hk)^2 p_j^{''} + O(h^3) \qquad (for\ k < 1)$$

Subtracting these results together we have

$$p_{j+k} - p_{j-k} = 0 + 2hkp_j^{'} + O(h^3)$$

Or

$$p_j^{'} = \frac{p_{j+k} - p_{j-k}}{2hk} + O(h^2)$$

Assuming the face is half-way between the cell centers, we have $k = \frac{1}{2}$ which yields

$$p_j^{'} = \frac{p_{j+1/2} - p_{j-1/2}}{h} + O(h^2)$$

Note that ${p_j}'$ lives on the face corresponding to q_j, and the two pressures on the RHS correspond to the finite difference formula

$$p_j^{'} = \frac{p_j - p_{j-1}}{h} + O(h^2)$$

The second order accurate first derivative.

1st derivative of data living on F, for $\nabla \cdot q$ $(F \rightarrow C)$

We may approximate the velocity at the cell face location j about the node $j + 1/2$ and $j - 1/2$. We may write this as a Taylor expansion as

$$q_j = q_{j+k} + (-hk)q_{j+k}^{'} + \frac{1}{2!}(-hk)^2 q_{j+k}^{''} + O(h^3) \qquad (for\ k > 0)$$

Similarly, we may approximate

$$q_{j+1} = q_{j+k} + (hk)q_{j+k}^{'} + \frac{1}{2!}(hk)^2 q_{j+k}^{''} + O(h^3) \qquad (for\ k < 1)$$

Subtracting these results together we have

$$q_j - q_{j+1} = 0 - 2hkq_{j+k}^{'} + O(h^3)$$

Or

$$q_{j+k}^{'} = \frac{q_{j+1} - q_j}{2hk} + O(h^2)$$

Assuming the face is half-way between the cell centers, we have $k = \frac{1}{2}$ which yields

$$q_{j+1/2}^{'} = \frac{q_{j+1} - q_j}{h} + O(h^2)$$

The second order accurate first derivative. Note that $q_{j+1/2}^{'}$ lives on the cell center.

2nd derivative of data living on F, for $L_{F\rightarrow F}q$

The 2nd derivative of data living on F is the same as an ordinary collocated grid, however, the boundaries must be modified accordingly. See the last section for details.

2nd derivative of data living on C, for $L_{C\rightarrow C}p$

The 2nd derivative of data living on C is the same as an ordinary collocated grid.

Operators and Spaces

Divergence

$$D_{F\rightarrow c} = D : F \rightarrow C$$

$$(Dq)_{ijk} = \frac{(q_{x,i+1,j,k} - q_{x,i,j,k})}{\Delta x} + \frac{(q_{y,i,j+1,k} - q_{x,i,j,k})}{\Delta y} + \frac{(q_{x,i,j,k+1} - q_{x,i,j,k})}{\Delta z}$$

Where $q \in F$ and $Dq \in C$. This is the analog of $\nabla \cdot u$.

Cell centered Gradient

$$G_{c-F} = G : C \to F$$

$$(Gp)_{x,i,j,k} = \frac{(p_{i,j,k} - p_{i-1,j,k})}{\Delta x}$$
$$(Gp)_{y,i,j,k} = \frac{p_{i,j,k} - p_{i,j-1,k}}{\Delta y}$$
$$(Gp)_{z,i,j,k} = \frac{p_{i,j,k} - p_{i,j,k-1}}{\Delta z}$$

Where $q \in C$ and $Gq \in F$. This is the analog of ∇p.

edgeCurl (nodeCurl in 2D)

$$C_{\varepsilon\to F} = C_\varepsilon : \varepsilon \to F$$

$$(C_\varepsilon\psi)_{x,i,j,k} = (\psi_{i,j+1,k} - \psi_{i,j,k})$$
$$(C_\varepsilon\psi)_{y,i,j,k} = -(\psi_{i+1,j,k} - \psi_{i,j,k})$$
$$(C_\varepsilon\psi)_{z,i,j,k} = (\psi_{i,j,k} - \psi_{i,j,k})$$

$$(C_\varepsilon\psi)_{x,i,j,k} = \frac{(\psi_{z,i,j+1,k} - \psi_{z,i,j,k})}{\Delta y} - \frac{(\psi_{y,i,j,k+1} - \psi_{y,i,j,k})}{\Delta z}$$
$$(C_\varepsilon\psi)_{y,i,j,k} = -\left[\frac{(\psi_{z,i+1,j,k} - \psi_{z,i,j,k})}{\Delta x} - \frac{(\psi_{x,i,j,k+1} - \psi_{x,i,j,k})}{\Delta z}\right]$$
$$(C_\varepsilon\psi)_{z,i,j,k} = \frac{(\psi_{y,i+1,j,k} - \psi_{y,i,j,k})}{\Delta x} - \frac{(\psi_{x,i,j+1,k} - \psi_{x,i,j,k})}{\Delta y}$$

Where $\psi \in \varepsilon$ and $C_\varepsilon\psi \in F$. This is the discrete analog of $u = \nabla \times \psi$.

faceCurl (edgeCurl in 2D)

$$C_{F\to\varepsilon} = C_F : F \to \varepsilon$$

$$(C_F q)_{x,i,j,k} = \frac{(q_{z,i,j+1,k} - q_{z,i,j,k})}{\Delta y} - \frac{(q_{y,i,j,k+1} - q_{y,i,j,k})}{\Delta z}$$
$$(C_F q)_{y,i,j,k} = -\left[\frac{(q_{z,i+1,j,k} - q_{z,i,j,k})}{\Delta x} - \frac{(q_{x,i,j,k+1} - q_{x,i,j,k})}{\Delta z}\right]$$
$$(C_F q)_{z,i,j,k} = \frac{(q_{y,i+1,j,k} - q_{y,i,j,k})}{\Delta x} - \frac{(q_{x,i,j+1,k} - q_{x,i,j,k})}{\Delta y}$$

Where $q \in F$ and $C_F q \in \varepsilon$. This is the discrete analog of $\omega = \nabla \times u$.

edgeLaplacian (nodeLaplacian in 2D)

$$L_{\varepsilon\to\varepsilon} = L_\varepsilon : \varepsilon \to \varepsilon$$

$$L_\varepsilon = -C_F C_\varepsilon$$

Where $\omega \in \varepsilon$ and $L_\varepsilon\omega \in \varepsilon$. This is the discrete analog of $\nabla^2 f = -\nabla \times \nabla \times f$.

Cell-centered Laplacian

$$L_{c\to c} = L_c : C \to C$$

$$L_c p = DGp$$

Where $p \in C$ and $L_c p \in C$. This is the discrete analog of $\nabla^2 f = -\nabla \cdot \nabla f$.

Averages

edgeAverage

$$EA$$

faceAverage

$$FA_i = \frac{1}{4}(q_j)$$

Implementation details of boundary derivatives

The implementation details have been written in terms on normal and tangential components of the operator and vector field quantities. For example,

$$L_{Fn} q_t = \frac{\partial^2 q_t}{\partial n^2}$$

These two derivatives must be calculated using a modified stencil near the boundary since the data that live tangent wrt the boundary do not intersect with the boundary. These modified stencils can be computed by using Taylor expansions on and near the boundary.

Modified boundary stencils for first order derivatives of face-based data

Normal derivatives

Interior (CD2)

$$\left(\frac{\partial q_n}{\partial n}\right)_i = \frac{q_{n,i+1} - q_{n,i-1}}{2dn}$$

Start Boundary (Ordinary upwind)

$$\left(\frac{\partial q_n}{\partial n}\right)_{i,1} = \frac{-q_{n,i+2} + 4q_{n,i+1} - 3q_{n,i}}{2dn}$$

End Boundary (Ordinary downwind)

$$\left(\frac{\partial q_n}{\partial n}\right)_{i,N} = \frac{3q_{n,i} - 4q_{n,i-1} + q_{n,i-2}}{2dn}$$

Tangential derivatives

Interior (CD2)

$$\left(\frac{\partial q_n}{\partial n}\right)_i = \frac{q_{n,i+1} - q_{n,i-1}}{2dn}$$

Start Boundary (modified stencil)

$$\left(\frac{\partial q_t}{\partial n}\right)_{i,1} = \frac{\underbrace{-\frac{4}{3} q_{t\,i,1}}_{BC} + q_{t\,i,2} + \frac{1}{3} q_{t\,i,3}}{dn}$$

End Boundary (modified stencil)

$$\left(\frac{\partial q_t}{\partial n}\right)_{i,N} = \frac{\underbrace{\frac{4}{3} q_{t\,i,N}}_{BC} - \ q_{t\,i,N-1} - \frac{1}{3} q_{t\,i,N-2}}{dn}$$

Modified boundary stencils for second order derivatives of face-based data

Normal derivatives

Interior (CD2)

$$(L_{Fn} q_n)_i = \left(\frac{\partial^2 q_n}{\partial n^2}\right)_i = \frac{q_{n,i+1} + q_{n,i-1} - 2q_{n,i}}{dn^2}$$

Start Boundary (Ordinary upwind)

End Boundary (Ordinary downwind)

Tangential derivatives

Interior (CD2)

$$(L_{Fn} q_t)_i = \left(\frac{\partial^2 q_t}{\partial n^2}\right)_i = \frac{q_{t,i+1} + q_{t,i-1} - 2q_{t,i}}{dn^2}$$

Start Boundary (modified stencil)

$$(L_{Fn} q_t)_{i,3} = \frac{\frac{4}{3} q_{t,3} - 4q_{t,2} + \underbrace{\frac{8}{3} q_{t,1/2}}_{BC}}{\Delta n^2}$$

End Boundary (modified stencil)

$$(L_{Fn} q_t)_{i,N-1} = \frac{\underbrace{\frac{8}{3} q_{t,i,N-1/2}}_{BC} - 4q_{t,i,N-1} + \frac{4}{3} q_{t,i,N-2}}{\Delta n^2}$$