Differential operators on polyhedral unstructured meshes

Goal

Let us consider a scalar function $\phi : \mathbb{R}^3 \to \mathbb{R}$, and a mesh composed by N polyhedral cells $\{c_i\}_{1,\dots,N}$. We assume to know the value of ϕ on each cell. We denote by ϕ_i the value of ϕ on the i^{th} cell. Similarly, we denote by $(\partial_x \phi)_i$ the value of the x derivative of ϕ on the i^{th} cell. The goal is to construct a matrix $D^{(x)}$ which calculates the x derivative:

$$(\partial_x \phi)_i = \sum_j D^{(x)}_{ij} \phi_j \tag{1}$$

and similarly for the y and z derivatives.

Concept

The method is based on the Green-Gauss theorem (see Sec. III.A of Ref. [1]). The average gradient of ϕ over one cell is:

$$(\overline{\boldsymbol{\nabla}\phi})_i = \frac{1}{V_i} \int_{c_i} dV \, \boldsymbol{\nabla}\phi = \frac{1}{V_i} \oint_{\partial c_i} dA \, \phi \, \hat{\boldsymbol{n}} \tag{2}$$

where V_i denotes the volume of a cell, ∂c_i the external surface, and $\hat{\boldsymbol{n}}$ the unit vector normal to the surface at a given point. For a polyhedral cell we have:

$$(\overline{\boldsymbol{\nabla}\phi})_i \to \frac{1}{V_i} \sum_f \overline{\phi}_f \hat{\boldsymbol{n}}_f A_f \tag{3}$$

where the index f runs over the external faces of the i^{th} cell, $\hat{\boldsymbol{n}}_f$ denotes the unit vector normal to the f^{th} face, A_f its area, and $\overline{\phi}_f$ is the average value of ϕ over the face. It is thus necessary to evaluate the face average $\overline{\phi}_f$. As pointed out in Ref. [1], several alternative methods exist, the simplest being averaging the two values assumed by ϕ over the the two cells i and i' that share the face f (see Sec. III.A.1 of Ref. [1]).

Implementation

The set of all the normal vectors to the faces is denoted by:

$$\{\hat{\boldsymbol{n}}_f\} \tag{4}$$

We introduce the matrix B having number of rows equal to the total number of faces, and number of columns equal to the total number of cells. The entry B_{fj} is equal to $+1$ if the face f belongs to the cell j and the normal is direct outwards, is equal to -1 if the face f belongs to the cell j and the normal is direct inwards, and is equal to 0 otherwise (i.e. if the face f does not belong to the cell j). By letting the index f run over *all* the faces (instead of only those belonging to the i^{th} cell), we can modify Eq. 3:

$$(\overline{\boldsymbol{\nabla}\phi})_i = \frac{1}{V_i} \sum_f B_{fi} \overline{\phi}_f \hat{\boldsymbol{n}}_f A_f \tag{5}$$

As mentioned, we can calculate $\overline{\phi}_f$ by averaging the value of ϕ over the two cells adjacent to the face f:

$$\overline{\phi}_f = \frac{1}{\sum_h |B_{fh}|} \sum_j |B_{fj}| \phi_j \tag{6}$$

The quantity $\sum_h |B_{fh}|$ corresponds to the number of cells sharing the face f, (i.e. 2 is the face is shared between two cells, and 1 if the face is on the boundary). Plugging Eq. 6 into Eq. 5 we get:

$$(\overline{\boldsymbol{\nabla}\phi})_i = \frac{1}{V_i} \sum_f B_{fi} \hat{\boldsymbol{n}}_f A_f \frac{1}{\sum_h |B_{fh}|} \sum_j |B_{fj}| \phi_j = \sum_j \boldsymbol{D}_{ij} \phi_j \tag{7}$$

with

$$\boldsymbol{D}_{ij} = \frac{1}{V_i} \sum_f B_{fi} \hat{\boldsymbol{n}}_f A_f \frac{1}{\sum_h |B_{fh}|} |B_{fj}| \tag{8}$$

The matrix $D^{(x)}$ is obtained from $\boldsymbol{D}$ by taking the scalar product with the unit vector $\hat{\boldsymbol{e}}_x$, and similarly for the y and z components of the gradient.

References

[1] E. Sozer, C. Brehm, and C.C. Kiris, *Gradient Calculation Methods on Arbitrary Polyhedral Unstructured Meshes for Cell-Centered CFD Solvers*, 52nd Aerospace Sciences Meeting (2014).