Poisson Equation - Operator Approach

James C. Sutherland

The Poisson equation is given as

$$\nabla^2 \phi = \gamma(\mathbf{x}, t).$$

The discrete representation of this is $\mathsf{L}\phi = \gamma$ or n equations

$$\sum_{j=1}^{n} \mathsf{L}_{ij} \phi_j = \gamma_i. \tag{1}$$

Let us consider a staggered scheme where ϕ is stored at cell centroids with n_g ghost cells on ϕ. We solve (1) on the interior of the domain. We define $\mathsf{S} = \mathsf{DG}$, where D and G are the discrete divergence and gradient operators, respectively. Note that both D and G have ghost cell information embedded in them and, thus, S has all ghost information retained. L has no ghost information, and is thus a subset of S. We place a restriction on these operators (D, G, and R - the interpolant operator) at physical boundaries: they must have precisely one nonzero ghost cell coefficient. This implies that at physical boundaries the stencils may not be symmetric. The reason for this restriction is that boundary condition implementation can become problematic for more than one ghost point on a boundary. Note that for second order FV schemes this is a moot point, since the stencils have a half-width of one.

Let ϕ_{BC} represent the boundary value at the surface. This can be expressed in terms of the boundary operator as

$$\phi_{BC} = \mathsf{B}_{kg} \phi_g + \sum_{j_{\text{interior}}} \mathsf{B}_{kj} \phi_j, \tag{2}$$

where B is an appropriate boundary operator which includes ghost cell coefficients, ϕ_g is the ghost value, and B_{kg} is the stencil coefficient on the ghost cell. For Dirichlet conditions, we choose B as the interpolant operator ($\mathsf{B} = \mathsf{R}$) while for Neumann conditions we choose B as the gradient operator, ($\mathsf{B} = \mathsf{G}$). If we have operators for the x, y, and z directions and a unit normal $\mathbf{n} = n_x \vec{i} + n_y \vec{j} + n_z \vec{k}$ then $\mathsf{B} = n_x \mathsf{B}_x + n_y \mathsf{B}_y + n_z \mathsf{B}_z$. We need to solve for the ghost value, ϕ_g, in terms of ϕ_{BC}, $\mathsf{B}_{kj_{\text{interior}}}$, and $\phi_{j_{\text{interior}}}$. We can use the columns of B to solve for ϕ_g,

$$\phi_g = \frac{1}{\mathsf{B}_{kg}} \left(\phi_{BC} - \sum_{j_{\text{interior}}} \mathsf{B}_{kj} \phi_j \right). \tag{3}$$

The i^{th} row in S is now modified using the information contained in (3) to eliminate the coefficients on the ghost values by augmenting those in the interior. This is done by writing

$$\begin{aligned} \sum_{j=1}^{n} \mathsf{S}_{ij} \phi_j &= \gamma_i, \\ \mathsf{S}_{ig} \phi_g + \sum_{j_{interior}} \mathsf{S}_{ij} \phi_j &= \gamma_i. \end{aligned}$$

Substituting (3) we find

$$\begin{aligned} \frac{\mathsf{S}_{ig}}{\mathsf{B}_{kg}} \phi_{BC} + \sum_{j_{interior}} \left(\mathsf{S}_{ij} - \frac{\mathsf{B}_{kj}}{\mathsf{B}_{kg}} \right) \phi_j &= \gamma_i, \\ \sum_{j_{interior}} \left(\mathsf{S}_{ij} - \mathsf{S}_{ig} \frac{\mathsf{B}_{kj}}{\mathsf{B}_{kg}} \right) \phi_j &= \gamma_i - \frac{\mathsf{S}_{ig}}{\mathsf{B}_{kg}} \phi_{BC}. \end{aligned}$$

Therefore, L can be written as

$$\mathsf{L}_{ij} = \mathsf{S}_{ij} - \mathsf{S}_{ig}\frac{\mathsf{B}_{kj}}{\mathsf{B}_{kg}} \quad \forall \text{ interior } j, \tag{4}$$

and γ_i is augmented on the interior as

$$\gamma_i = \gamma_i - \mathsf{S}_{ig}\frac{\phi_{BC}}{\mathsf{B}_{kg}}. \tag{5}$$

Example - One Dimensional FV Uniform Mesh, 2^{nd} Order

Consider a one-dimensional, staggered, uniform mesh that we wish to discretize with second order accuracy. The elements of the divergence and gradient operators are given by

$$\mathsf{D}_{ij} = \frac{1}{\Delta x}\begin{cases} -1 & j = i - \frac{1}{2} \\ 1 & j = i + \frac{1}{2} \end{cases} \qquad i = 1 \ldots n+1.$$

and

$$\mathsf{G}_{ij} = \tfrac{1}{\Delta x}\begin{cases} -1 & j = i - \frac{1}{2} \\ 1 & j = i + \frac{1}{2} \end{cases} \qquad \tfrac{1}{2} \le i \le n - \tfrac{1}{2},$$

respectively so that D is $(n \times n+1)$ while G is $(n+1 \times n)$. Application of G to a cell-centered field results in a field shifted by $\frac{\Delta x}{2}$, and D is applied to a staggered field to produce a cell-centered field. There are no modifications to G or D required at boundaries. We have components of $\mathsf{S} = \mathsf{DG}$ defined as

$$\mathsf{S}_{ij} = \frac{1}{\Delta x^2}\begin{cases} 1 & j = i-1 \\ -2 & j = i \\ 1 & j = i+1 \end{cases} \qquad 1 \le i \le n,$$

where the interior cells are numbered $1 \ldots n$.

Dirichlet Conditions. At the left boundary $(k = 1/2)$, Dirichlet conditions are given by the interpolant operator, whose coefficients for second-order interpolation are

$$R_{ij} = \begin{cases} 1/2 & j = i - \frac{1}{2} \\ 1/2 & j = i + \frac{1}{2} \end{cases} \qquad \tfrac{1}{2} \le i \le n - \tfrac{1}{2}.$$

Therefore, at $i = 1/2$ we obtain (from (3))

$$\phi_{BC} = \tfrac{1}{2}\phi_0 + \tfrac{1}{2}\phi_1 \quad \Rightarrow \quad \phi_0 = 2\phi_{BC} - \phi_1.$$

Therefore, from (4), the nonzero entries of L_{1j} are

$$\mathsf{L}_{1j} = \frac{1}{\Delta x^2}\begin{cases} -3 & j = 1 \\ 1 & j = 2 \end{cases},$$

and from (5), γ_1 is augmented by $-\frac{2\phi_{bc}}{\Delta x^2}$. The equation for the first cell is thus

$$\gamma_1 - \frac{2\phi_{bc}}{\Delta x^2} = \frac{-3\phi_1 + \phi_2}{\Delta x^2}.$$

Boundary conditions would still need to be applied on L_{nj} following the same procedure for $i = n$.

Neumann Conditions. At the left boundary ($i=1/2$), Neumann conditions are given by the gradient operator, whose coefficients for second-order derivatives are

$$\mathsf{G}_{ij} = \frac{1}{\Delta x}\begin{cases} -1 & j = i - \frac{1}{2} \\ 1 & j = i + \frac{1}{2} \end{cases} \qquad \tfrac{1}{2} \leq i \leq n - \tfrac{1}{2}.$$

At $i=1/2$ we obtain (from (3))

$$\phi_{BC} = \frac{-\phi_0 + \phi_1}{\Delta x} \quad \Rightarrow \quad \phi_0 = \phi_1 - \Delta x \phi_{BC}.$$

From(4), the nonzero entries of L_{1j} are

$$\mathsf{L}_{1j} = \frac{1}{\Delta x^2}\begin{cases} -1 & j = 1 \\ 1 & j = 2 \end{cases},$$

and from (5), γ_1 is augmented by $\phi_{BC}/\Delta x$. The equation for the first cell is thus

$$\gamma_1 + \frac{\phi_{BC}}{\Delta x} = \frac{-\phi_1 + \phi_2}{\Delta x^2}.$$

Boundary conditions would still need to be applied on L_{nj} following the same procedure for $i = n$.

Example - Higher Order FV Uniform mesh

Consider a one-dimensional, finite-volume, uniform mesh that we wish to discretize with fourth-order accuracy. We have components of $\mathsf{S} = \mathsf{DG}$ defined as

$$\mathsf{S}_{ij} = \frac{1}{\Delta x^2}\begin{cases} -1/12 & j = i-2 \\ 4/3 & j = i-1 \\ -5/12 & j = i \\ 4/3 & j = i+1 \\ -1/12 & j = i+2 \end{cases} \qquad 2 \leq i \leq n-1,$$

while at $n = 1$ we have

$$\mathsf{S}_{1j} = \frac{1}{\Delta x^2}\begin{cases} 11/12 & j = 0 \\ -5/3 & j = 1 \\ 1/2 & j = 2 \\ 1/3 & j = 3 \\ -1/12 & j = 4 \end{cases}.$$

Dirichlet Condition. The fourth-order boundary point stencil for the interpolant operator is given as

$$\mathsf{B}_{\frac{1}{2}j} = \mathsf{R}_{\frac{1}{2}j} = \begin{cases} 5/16 & j = 0 \\ 15/16 & j = 1 \\ -5/16 & j = 2 \\ 1/16 & j = 3 \end{cases},$$

Therefore, at $i=1/2$ we obtain (from (3))

$$\phi_{BC} = \tfrac{5}{16}\phi_0 + \tfrac{15}{16}\phi_1 - \tfrac{5}{16}\phi_2 + \tfrac{1}{16}\phi_3 \quad \Rightarrow \quad \phi_0 = \tfrac{16}{5}\phi_{BC} - 3\phi_1 + \phi_2 - \tfrac{1}{5}\phi_3.$$

Therefore, from (4), the nonzero entries of L_{1j} are

$$\mathsf{L}_{1j} = \frac{1}{\Delta x^2}\begin{cases} -14/3 & j = 1 \\ 3/2 & j = 2 \\ 2/15 & j = 3 \\ -1/12 & j = 4 \end{cases},$$

and from (5), γ_1 is augmented by $-\frac{16\phi_{bc}}{5\Delta x^2}$. The equation for the first cell is thus

$$\gamma_1 - \frac{16\phi_{bc}}{5\Delta x^2} = \frac{-\frac{14}{3}\phi_1 - \frac{3}{2}\phi_2 + \frac{2}{15}\phi_3 - \frac{1}{12}\phi_4}{\Delta x^2}.$$

Neumann Conditions. At the left boundary ($i = 1/2$), Neumann conditions are given by the gradient operator, whose coefficients for fourth-order derivatives at $i = \frac{1}{2}$ are

$$\mathsf{B}_{\frac{1}{2}j} = \mathsf{G}_{\frac{1}{2}j} = \frac{1}{\Delta x} \begin{cases} 1/24 & j = 0 \\ -9/8 & j = 1 \\ 9/8 & j = 2 \\ -1/24 & j = 3 \end{cases} .$$

At $i = 1/2$ we obtain (from (3))

$$\phi_{BC} = \frac{\frac{1}{24}\phi_0 - \frac{9}{8}\phi_1 + \frac{9}{8}\phi_2 - \frac{1}{24}\phi_3}{\Delta x} \quad \Rightarrow \quad \phi_0 = 24\Delta x \phi_{BC} + \frac{9}{8}\phi_1 - \frac{9}{8}\phi_2 + \frac{1}{24}\phi_3.$$

From(4), the nonzero entries of L_{1j} are

$$\mathsf{L}_{1j} = \frac{1}{\Delta x^2} \begin{cases} 335/12 & j = 1 \\ -53/2 & j = 2 \\ -2/3 & j = 3 \\ -1/12 & j = 4 \end{cases} .$$

and from (5), γ_1 is augmented by $24\phi_{BC}/\Delta x$. The equation for the first cell is thus

$$\gamma_1 + \frac{24\phi_{BC}}{\Delta x} = \frac{\frac{335}{12}\phi_1 - \frac{53}{2}\phi_2 - \frac{2}{3}\phi_3 - \frac{1}{12}\phi_4}{\Delta x^2}.$$