High order finite volume operators in a cut cell context, part 1: system matrix conditioning for finite volume elliptic operators

D. Devendran [†] D. T. Graves *

August 14, 2023

Abstract

Devendran, et al. [4] present an algorithm that solves Poisson's equation to fourth-order accuracy using an EB grid. Generalizing somewhat the framework they present, we can define a family of elliptic operators. That algorithm is a special case of a family of finite volume elliptic operators. We present the formal process to generate these operators which includes inverting a system matrix. Overton-Katz, et al. [6], show that the system matrix can have solvability problems in the absence of boundary condition equations in the system matrix but Devendran uses boundary condition equations. We present data that shows these extra equations can improve the system matrix condition number. We also show that, for certain parameters of operator, this system matrix is still quite poorly conditioned.

1 Underlying mathematics

Embedded boundary (EB) grids are formed when one passes an surface through a Cartesian mesh. For sufficiently complex geometries, these methods are very attractive because grid generation is a solved problem even for moving grids [5]. In the current context, we form the cutting surface as the zero surface of a function of space $I(\mathbf{x})$, $\mathbf{x} \in R^D$. For smooth (I), moments can be generated to any accuracy [7].

Formally, the underlying description of space is given by rectangular control volumes on a Cartesian mesh $\Upsilon_{\mathbf{i}} = [(\mathbf{i} - \frac{1}{2}\mathbf{u})h, (\mathbf{i} + \frac{1}{2}\mathbf{u})h], \mathbf{i} \in \mathbf{Z}^D$, where D is the dimensionality of the problem, h is the mesh spacing, and \mathbf{u} is the vector whose entries are all one (note we use bold font $\mathbf{u} = (u_1, \dots, u_d, \dots, u_D)$ to indicate a vector quantity). Given an irregular domain Ω , we obtain control volumes $V_{\mathbf{i}} = \Upsilon_{\mathbf{i}} \cap \Omega$ and faces $A_{\mathbf{i},d\pm} = A_{\mathbf{i}\pm\frac{1}{2}\mathbf{e}_d}$ which are the intersection of the boundary of $\partial V_{\mathbf{i}}$ with the coordinate planes $\{\mathbf{x} : x_d = (i_d \pm \frac{1}{2})h\}$ (\mathbf{e}_d is the unit vector in the d direction). We also define $A_{B,\mathbf{i}}$ to be the intersection of the boundary of the irregular domain with the Cartesian control volume: $A_{B,\mathbf{i}} = \partial \Omega \cap \Upsilon_{\mathbf{i}}$.

We use the compact notation

$$(\mathbf{x} - \bar{\mathbf{x}})^{\mathbf{p}} = \prod_{d=1}^{D} (x_d - \bar{x}_d)^{p_d}$$
$$\mathbf{p}! = \prod_{d=1}^{D} p_d!$$

Given a *D*-dimensional region of space **i**, and a *D*-dimensional integer vector **p**, we define $m_{\mathbf{i}}^{\mathbf{p}}(\bar{\mathbf{x}})$ to be the \mathbf{p}^{th} moment of **i** to the point $\bar{\mathbf{x}}$.

$$\mathbf{m}_{\mathbf{i}}^{\mathbf{p}}(\bar{\mathbf{x}}) = \int_{\mathbf{i}} (\mathbf{x} - \bar{\mathbf{x}})^{\mathbf{p}} dV^{D}.$$
 (1)

This breaks out into three different cases, volumes, coordinate faces and irregular faces. A coordinate face f_{12} is the area where two volumes (V_1, V_2) intersect. A irregular face f_V is area where the cutting surface intersects the volume V. The volume moment for a particular power \mathbf{p} is given by

$$\mathbf{m}_{V}^{\mathbf{p}} = \int_{\mathbf{i}} (\mathbf{x} - \bar{\mathbf{x}})^{\mathbf{p}} dV \tag{2}$$

The \mathbf{p}^{th} coordinate face moment for the area of where volumes V_1, V_2 intersect is given by

$$\mathbf{m}_{f_{12}}^{\mathbf{p}} = \int_{A(V_1 \cap V_2)} (\mathbf{x} - \bar{\mathbf{x}})^{\mathbf{p}} dA. \tag{3}$$

The cutting surface of the boundary G is given by the zero surface of the implicit function $(I(\mathbf{x}) = 0)$ used in grid generation. The \mathbf{p}^{th} irregular face moment is given by an integral over the intersection of this cutting surface and the Euclidean volume:

$$\mathbf{m}_{V}^{\mathbf{p}} = \int_{A(V \cap G)} (\mathbf{x} - \bar{\mathbf{x}})^{\mathbf{p}} dA. \tag{4}$$

These moments are natural products of the grid generation algorithm in [7].

2 Family of finite volume elliptic operators

Devendran, et al. [4] present an algorithm that solves Poisson's equation to fourth-order accuracy using embedded boundaries. Generalizing somewhat the framework they present, we present a family of elliptic operators.

We are solving Poisson's equation for field ψ , given charge ρ :

$$\nabla \cdot (\nabla \psi) = \rho \tag{5}$$

If we integrate equation 5 and apply the divergence theorem over control volumes we get

$$\int_{V_{\mathbf{i}}} \nabla \cdot (\nabla \psi) dV = \int_{\partial V_{\mathbf{i}}} \nabla \psi \cdot \hat{n} dA = \int_{V_{\mathbf{i}}} \rho dV \tag{6}$$

Without approximation, we can say that the surface integral can be computed by a sum over the faces that comprise the surface of the volume.

$$\sum_{f:f\in\partial V_{\mathbf{i}}} \nabla \psi \cdot \hat{n} dA = \int_{V_{\mathbf{i}}} \rho dV \tag{7}$$

Using equations 3.1 and 3.1, this becomes

$$\sum_{f:f\in\partial V_{\mathbf{i}}} \langle \nabla \psi \cdot \hat{n} \rangle_f A_f = \langle \rho \rangle_{\mathbf{i}} V_{\mathbf{i}}$$
 (8)

A finite volume operator is defined by the algorithm to compute the integral of fluxes at each face. We have three types of face, open faces (the faces between two volumes that are aligned with coordinate directions), domain faces, and cut faces. For now, let's say we have homogeneous Neumann boundary conditions at domain and cut faces $\nabla \psi \cdot \hat{n} = 0 | \partial \Omega$. In this case, to describe the algorithm, we need only describe how to compute $\langle \nabla \psi \cdot \hat{n} \rangle$ on open faces.

3 Open face Poisson flux computation with Neumann boundary conditions

An open face is one that connects two volumes in the solution. These faces are aligned with a coordinate direction. Consider an open face \mathbf{f} aligned with coordinate direction d. We define $\mathbf{n_f}$ to be all the volumes within N_G ghost cells of $\mathbf{f}^{-1}3$].

3.1 Taylor expansion around face

We approximate ψ in the neighborhood of $\bar{\mathbf{x}}$ using a Taylor expansion to order P_T :

$$\psi(\mathbf{x}) = \sum_{p < P_T} C^p (\mathbf{x} - \bar{\mathbf{x}})^p \tag{9}$$

where C^p this appropriate Taylor coefficient. In three dimensions,

$$C^{p} = \frac{1}{p!} \frac{\partial^{p_0}}{\partial x_0} \frac{\partial^{p_1}}{\partial x_1} \frac{\partial^{p_2}}{\partial x_2} (\psi). \tag{10}$$

If we know the local Taylor coefficients, the gradient of the field in direction d is given by

$$\frac{\partial \psi}{\partial x^d} = \sum_{p < P_T} p^d C^p (\bar{\mathbf{x}} - \bar{\mathbf{x}})^{p - e^d}$$
(11)

In finite volume methods, we define grid data to be averages over volumes and fluxes between volumes are averages over the faces between volumes. For the field ψ , the average over the volume **i** is given by

$$V_{\mathbf{i}} < \psi >_{\mathbf{i}} = \int\limits_{V_{\mathbf{i}}} \psi(\mathbf{x}) dV$$

If we insert the Taylor expansion 9, we get a discrete approximation to the smooth function ψ that is accurate to order P_T .

$$<\psi>_{\mathbf{i}} = \frac{1}{V_{\mathbf{i}}} \sum_{p < P_T} C^p \mathbf{m}^p.$$

Similarly, integrating the flux over a d-directional face **f**:

$$<\nabla\psi_d>_{\mathbf{i}} = \frac{1}{A_{\mathbf{f}}}\sum_{p < P_T} p^d C^p \mathbf{m}^{p-e^d}.$$

3.2 Boundary condition equations

To solve for the Taylor coefficients, we use the neighboring volumes' values to form a system of equations (equation 3.1 for each volume $\mathbf{i} \in N_f$, the neighborhood of f). Boundary condition equations are also added to the system. Since we have homogeneous Neumann boundary conditions, for every domain face \mathbf{b} within $\mathbf{n_f}$, we have an equation of the form

$$\langle \frac{\partial \psi}{\partial x^d} \rangle_{\mathbf{b}} = \sum_{p < P_T} p^d C^p \mathbf{m}_{\mathbf{b}}^{p-e^d} = 0.$$
 (12)

Consider a face **c** which is cut by a surface whose normal in direction d is given by $n^d(\mathbf{x})$. We define the normal moments \mathbf{E}^d to be the integral of this product:

$$\mathbf{E}_{\mathbf{c}}^{\mathbf{p},d} = \int_{A(\mathbf{c})} (\mathbf{x} - \bar{\mathbf{x}}) n^d dA. \tag{13}$$

These normal moments are natural products of the [7] grid generation algorithm.

3.3 Moment matrix M and system matrix A

For each c within the n_f , we get an equation of the form

$$\int_{A(\mathbf{c})} \nabla \psi \cdot \hat{n} dA = \sum_{d < D} \int_{A(\mathbf{c})} \sum_{p < P} p_d C^p (\mathbf{x} - \bar{\mathbf{x}})^{p - e^d} dA = \sum_{d < D} \sum_{p < P} p_d C_p \mathbf{E}_{\mathbf{c}}^{p - e^d, d} = 0.$$
(14)

We force there to be enough neighbors so that this system is over-determined. Let's say $\mathbf{n_f}$ contains N_B boundary faces and N_V volumes. To solve for Taylor coefficients, we have a system of the form

$$MC = P$$

where $C = \{C^p\},\$

$$M_{\mathbf{f}} = \left\{ \begin{array}{c} m_{\mathbf{j}}^{p} \\ p^{d} b_{\mathbf{b}}^{p-e^{d}} \\ p^{d} c_{\mathbf{c}}^{p-e^{d}} \end{array} \right\}, \tag{15}$$

and

$$P_{\mathbf{f}} = \left\{ \begin{array}{c} <\psi >_{\mathbf{j}} \\ 0 \\ 0 \end{array} \right\} \tag{16}$$

for every volume \mathbf{j} , cut face \mathbf{c} and domain face \mathbf{b} in $\mathbf{n_f}$. Since the system is over-determined, we can introduce a meaningful weighting matrix W^4 . Choice of W is crucial to the stability of these algorithms ⁵. We multiply and solve

$$WMC = WP$$
.

Since the system is (deliberately) not square, we approximate the solution using a Moore-Penrose pseudo-inverse:

$$C = ((WM)^{T}(WM))^{-1}(WM)^{T}P.$$
(17)

where $A \equiv ((WM)^T(WM))_{\mathbf{f}}$ is the system matrix for face \mathbf{f} .

3.4 Manhattan Distance and the weighting matrix W

All volumes and faces start with an index $\mathbf{i} \in Z^D$. We start from face \mathbf{f} . Say we want to get the distance from \mathbf{f} with index \mathbf{i} to a volume V_1 with index \mathbf{v} . The distance $D_{\mathbf{f}}(V_1)$ is given by the Manhattan distance:

$$D_{\mathbf{f}}(V_1) = \sum_{0 < d < D} |\mathbf{v}^d - \mathbf{i}_0^d|. \tag{18}$$

 $\mathbf{g_f}(V_1)$, the weight of the V_1 equation in \mathbf{f} system is given by

$$\mathbf{g_f}(V_1) \equiv \left(\frac{1}{D_\mathbf{f}(V_1)}\right)^{P_w},\tag{19}$$

where we call P_w the weighting exponent. The weighting matrix $W_{\mathbf{f}} = \{\{\mathbf{w}_{i,j}\}\}\$ is diagonal

$$w_{i,j} = \begin{pmatrix} \mathbf{g_f}(V_i) & \text{if (i==j)} \\ 0 & \text{otherwise} \end{pmatrix}$$
 (20)

Once one has the Taylor coefficients, she can compute the flux through the open face using equation 3.1. Put into matrix form, we define vector $Q_{\mathbf{f}} = \{q_{\mathbf{f}}^p\}$:

$$q_{\mathbf{f}}^p = p^d \mathbf{m}_{\mathbf{f}}^{p-e^d} \tag{21}$$

and the flux at the face is given by

$$\langle \nabla \psi \rangle_{\mathbf{f}} = QCP = Q((WM)^T(WM))^{-1}(WM)^T P. \tag{22}$$

3.5 Stencil formulation

One would like to avoid inverting A every time she wishes to apply an elliptic operator at a point. Since everything in sight is a linear operator, we can simply say that there must exist an equivalent linear operator S such that

$$(SP)_{\mathbf{f}} = \langle \nabla \psi \rangle_{\mathbf{f}} = QC = (Q((WM)^{T}(WM))^{-1}(WM)^{T}P)_{\mathbf{f}}.$$
 (23)

Since this equivalence has to hold for all ψ , the stencil S must be given by:

$$S_{\mathbf{f}} = QC = (Q((WM)^{T}(WM))^{-1}(WM)^{T})_{\mathbf{f}} = QA^{-1}(WM)^{T}.$$
 (24)

4 Solvability of the system matrix A

Overton-Katz, et al. [6] present the above procedure in the absence of boundary condition equations. They show that, for certain values of P_T and P_N , the resulting A matrix can have a severe mismatch between its largest and smallest eigenvalues, signaling that A is poorly conditioned. Their data show the worst solvability issues occur near the domain boundary. It stands to reason that including boundary condition equations could improve the conditioning of the resultant matrices. To test this, we present the same measurement of condition number for several values of P_T and P_N where boundary condition equations are included when they are part of the neighborhood. We present the results for the same three different geometries used in [6]. In figure 4 we show the worst condition numbers where there are no cut cells. In figure 4, we show the worst condition number where we cut the unit domain with a centered sphere of radius 0.45 (this geometry includes very small volumes). Finally, in figure 4, we present results all small volumes have been merged with neighbors.

The data paint a very consistent picture, Though adding boundary condition equations does improve the solvability of A, aggressive choices of P_W and P_T can lead to system matrices that cannot be credibly solved without very high precision numerical arithmetic.

5 Domain face Poisson flux computation with Dirichlet boundary conditions

Neumann boundary conditions are a proscribed flux when solving Poisson's equation. When we have Dirichlet boundary conditions either at the domain

D	P^T	P^W	λ_{max}	λ_{min}	
2	1	1	1.537125e+00	1.150772e-03	7.486517e-04
2	1	2	4.940953e-01	9.196245 e - 05	1.861229 e-04
2	1	3	3.324177e-01	1.064946e-05	3.203639 e-05
2	1	4	2.853322e-01	1.705230 e-06	5.976295 e - 06
2	1	5	2.665812e-01	3.349335e-07	1.256403e- 06
2	2	1	2.407807e+00	1.457063e- 06	6.051408 e-07
2	2	2	4.940956e-01	5.469314 e-08	1.106934e-07
2	2	3	3.324177e-01	2.879583e-09	8.662545 e - 09
2	2	4	2.853323e-01	1.628939e-10	5.708921e-10
2	2	5	2.665812e-01	1.084310e-11	4.067466e-11
2	3	1	2.407807e+00	5.822902e-10	2.418342e-10
2	3	2	9.272889e-01	4.520282e-11	4.874729e-11
2	3	3	3.324177e-01	1.618058e-12	4.867544 e-12
2	3	4	2.853323e-01	7.227717e-14	2.533088e-13
2	3	5	2.665812e-01	3.194386e-15	1.198279e-14
2	4	1	1.880177e+00	1.535955e-25	8.169205 e-26
2	4	2	9.272889e-01	1.098665e-27	1.184814e-27
2	4	3	6.561304e-01	5.104096e-28	7.779089e-28
2	4	4	2.868930e-01	3.731928e-27	1.300808e-26
2	4	5	5.327046e-01	5.118416e-25	9.608357e-25
3	1	1	4.639099e+00	3.887142e-03	8.379088e-04
3	1	2	1.079504e+00	2.369894e-04	2.195354e-04
3	1	3	6.747118e-01	2.359590 e-05	3.497182e-05
3	1	4	5.721834e-01	3.540976e-06	6.188534 e-06
3	1	5	5.333668e-01	6.792558e-07	1.273525 e-06
3	2	1	4.639156e+00	3.176883e-06	6.847975 e - 07
3	2	2	1.079505e+00	1.512048e-07	1.400686e-07
3	2	3	6.747119e-01	6.991076e-09	1.036157e-08
3	2	4	5.721835e-01	3.641527e-10	6.364265 e-10
3	2	5	2.669165e-01	1.146071e-11	4.293744 e-11
3	3	1	4.639157e+00	1.340233e-09	2.888959 e-10
3	3	2	1.079505e+00	7.151353e-11	6.624659 e-11
3	3	3	6.747119e-01	3.977531e-12	5.895155e-12
3	3	4	2.869943e-01	5.757645e-14	2.006188e-13
3	3	5	2.669165e-01	1.723124e-15	6.455665 e-15
3	4	1	6.402997e+00	5.729285 e-26	8.947817e-27
3	4	2	1.079505e+00	1.226846e-27	1.136489e-27
3	4	3	6.907344e-01	1.049444e-28	1.519317e-28
3	4	4	2.903904e-01	8.442770 e-26	2.907386e-25
3	4	5	5.333668e-01	5.987514e-25	1.122588e-24

Table 1: We show the lowest value of \rfloor for an entire Cartesian grid of size 32^D with all boundary conditions homogeneous Neumann. We vary Taylor power P^T , weighting function exponents P^W , and dimensionality D.

D	P^T	P^W	λ_{max}	λ_{min}	
2	1	1	3.244145e+00	5.576001e-03	1.718789e-03
2	1	2	1.108699e+00	5.218520 e-04	4.706884e-04
2	1	3	6.816993e-01	4.992473e-05	7.323570 e-05
2	1	4	5.736425e-01	7.273424e-06	1.267937e-05
2	1	5	5.336857e-01	1.374234e-06	2.574988e-06
2	2	1	2.762140e+00	6.863083 e-06	2.484698e-06
2	2	2	9.453294e-01	7.653732e-07	8.096365 e - 07
2	2	3	6.816994e-01	4.112367e-08	6.032523 e-08
2	2	4	5.736426e-01	3.156232 e-09	5.502089 e-09
2	2	5	5.336858e-01	4.220417e-10	7.908057e-10
2	3	1	2.762140e+00	2.066812e-09	7.482649e-10
2	3	2	9.453294e-01	1.559241e-10	1.649416e-10
2	3	3	6.574277e-01	2.360967e-11	3.591220 e-11
2	3	4	5.705795e-01	4.724557e-12	8.280278e-12
2	3	5	5.336858e-01	2.690617e-13	5.041575e-13
2	4	1	2.762140e+00	3.535738e-13	1.280072e-13
2	4	2	9.453294e-01	3.267022e-14	3.455962e-14
2	4	3	6.574277e-01	3.738186e-15	5.686079 e-15
2	4	4	5.691873e-01	3.830503e- 16	6.729777e-16
2	4	5	5.328410e-01	8.531691e-17	1.601170e-16
3	1	1	7.242861e+00	4.674236e-03	6.453577e-04
3	1	2	1.181250e+00	2.657202 e-04	2.249483e-04
3	1	3	6.863432e-01	3.329115 e-05	4.850511e-05
3	1	4	5.741086e-01	4.562521 e-06	7.947139e-06
3	1	5	5.350591e-01	1.455556e-06	2.720366e-06
3	2	1	7.433403e+00	2.264150e-06	3.045914e-07
3	2	2	1.181248e+00	1.685503e- 07	1.426883e-07
3	2	3	6.804738e-01	1.353871e-08	1.989600e-08
3	2	4	5.806933e-01	2.036542e-09	3.507086e-09
3	2	5	5.350591e-01	1.066432e-10	1.993110e-10
3	3	1	7.433404e+00	8.925217e-10	1.200690e-10
3	3	2	1.182547e+00	8.635683e-11	7.302615e-11
3	3	3	6.804738e-01	4.819403e-12	7.082423e-12
3	3	4	5.729018e-01	3.780488e-13	6.598842e-13
3	3	5	5.350591e-01	6.218451e-14	1.162199e-13
3	4	1	7.433404e+00	1.727339e-13	2.323753e-14
3	4	2	1.182547e+00	2.186136e-14	1.848668e-14
3	4	3	6.804738e-01	1.827956e-15	2.686299e-15
3	4	4	5.728477e-01	7.990908e-17	1.394944e-16
3	4	5	5.338853e-01	1.743421e-17	3.265535e-17

Table 2: We show the lowest value of \rfloor for an entire Cartesian grid of size 32^D with all boundary conditions homogeneous Neumann. The grid covers the unit square and is cut by a sphere of radius 0.45. We vary Taylor power P^T , weighting function exponents P^W , and dimensionality D. This grid includes very small volumes.

D	P^T	P^W	λ_{max}	λ_{min}	
2	1	1	3.110810e+00	6.876828e-04	2.210623e-04
2	1	2	1.820276e+00	2.935551e-04	1.612695 e - 04
2	1	3	6.689318e-01	2.783647e-05	4.161332 e-05
2	1	4	3.112964e-01	3.804498e-06	1.222146e-05
2	1	5	2.931197e-01	4.648824 e - 07	1.585981e-06
2	2	1	4.649575e+00	1.222691e-06	2.629683e-07
2	2	2	2.800875e+00	4.389241e-07	1.567096e-07
2	2	3	1.156823e+00	4.756446e-08	4.111647e-08
2	2	4	1.020254e+00	3.829097e-09	3.753083e-09
2	2	5	9.591803e-01	4.980114e-10	5.192052e-10
2	3	1	8.598864e-01	3.926204 e-10	4.565956e-10
2	3	2	3.682481e+00	6.386263e-10	1.734228e-10
2	3	3	1.036128e+00	1.177339e-11	1.136288e-11
2	3	4	9.070960e-01	5.028483e-13	5.543495e-13
2	3	5	8.510270e-01	3.323827e-14	3.905666e-14
2	4	1	9.197999e-01	3.623068e-14	3.938974e-14
2	4	2	7.945940e-02	1.618085e-15	2.036366e-14
2	4	3	1.186857e+00	4.379402e-15	3.689917e-15
2	4	4	1.039000e+00	3.390648e-16	3.263375 e-16
2	4	5	2.958494e-01	1.292309 e-17	4.368131e-17
3	1	1	5.044398e+00	6.813020e-04	1.350611e-04
3	1	2	2.141787e+00	2.336010 e - 05	1.090683e-05
3	1	3	1.663929e+00	8.355671e-07	5.021651e-07
3	1	4	1.479289e+00	9.414478e-08	6.364192 e-08
3	1	5	3.223939e-01	1.193480e-08	3.701931e-08
3	2	1	6.441253e+00	1.723363e-07	2.675509 e - 08
3	2	2	3.588187e+00	1.066316e-08	2.971741e-09
3	2	3	2.800032e+00	9.932906e-10	3.547425 e-10
3	2	4	2.491816e+00	2.063069e-10	8.279378e-11
3	2	5	6.820526e-01	2.306368e-11	3.381511e-11
3	3	1	2.508964e+00	1.541288e-11	6.143127e-12
3	3	2	4.951047e+00	1.076120e-11	2.173521e-12
3	3	3	3.867831e+00	1.354407e-12	3.501722e-13
3	3	4	2.166936e+00	8.701202e-14	4.015441e-14
3	3	5	2.040600e+00	3.890155e-15	1.906378e-15
3	4	1	2.418622e+00	1.859733e-15	7.689226e-16
3	4	2	1.286816e+00	1.115219e-15	8.666503 e-16
3	4	3	9.013057e-01	9.738926e-17	1.080535e-16
3	4	4	7.856540e-01	2.968168e-17	3.777958e-17
3	4	5	9.668729e-01	1.139377e-17	1.178415e-17

Table 3: We show the lowest value of \rfloor for an entire Cartesian grid of size 32^D with all boundary conditions homogeneous Neumann. The grid covers the unit square and is cut by a sphere of radius 0.45. We vary Taylor power P^T , weighting function exponents P^W , and dimensionality D. This grid has had its small volumes merged with neighboring volumes.

box boundary or at a cut face, we must calculate the flux through that face.

For context, allow us to recap a relevant bit of finite volume formalism. Consider a volume \mathbf{i} bounded by the set of faces $\{f\} = \partial \mathbf{i}$, where the outward-facing normal \hat{n} of each face is known, as is its $V_{\mathbf{i}}$. Given a flux function F, the average divergence $\langle \nabla \cdot F \rangle$ is given by the divergence theorem:

$$\langle \nabla \cdot F \rangle = \frac{1}{V_{\mathbf{i}}} \int_{\mathbf{i}} \nabla \cdot F dV$$

= $\frac{1}{V_{\mathbf{i}}} \int_{\partial \mathbf{i}} F \cdot \hat{n} dA$
= $\frac{1}{V_{\mathbf{i}}} \sum_{f \in \partial \mathbf{i}} \int_{\partial \mathbf{i}} F \cdot \hat{n} dA$. (25)

For all coordinate-aligned faces, the section above's description for how to compute the flux is adequate. What remains are fluxes through cut faces.

We start with a smooth function ψ which we we expand using Taylor (equation 9). At each cut face f with area A_f , we wish to compute the average flux $\langle \nabla \psi \cdot \hat{n} \rangle_f$ through that face.

$$\langle \nabla \psi \cdot \hat{n} \rangle_f = \frac{1}{A_f} \int_f \nabla \psi \cdot \hat{n} dA$$

=
$$\frac{1}{A_f} \int_f \sum_{p \in P} \sum_{0 < =d < D} (p - e^d) C_p \mathbb{E}^{p - e^d} n^d dA$$
 (26)

where the normal moments

$$\mathbf{E}_{\mathbf{c}}^{\mathbf{p},d} = \int_{A(\mathbf{c})} (\mathbf{x} - \bar{\mathbf{x}}) n^d dA \tag{27}$$

are natural products of the [7] grid generation algorithm. Except in that we are using the normal moments, this is semantically the same dance we used to calculate open face fluxes.

5.1 The effect of Dirichlet boundary conditions on system matrix conditioning

In section 3, we discuss how adding Neumann boundary condition equations can improve the conditioning of the system matrix. When the boundary conditions are set to Dirichlet, we get similar results. See tables 5.1, 5.1, and 5.1 for details. Again, boundary conditions help stabilize the system but it is still the case that aggressive choices of P_T or P_W can result in system matrices that cannot be credibly inverted without very high precision numerical arithmetic. Again, this seems less a matter of a particular grid configuration and more a property of the mathematical framework used to generate the stencil.

6 Conclusions

We present a family of elliptic operators and we investigate the solvability of the system matrix used in generating these operators. We find that using boundary condition equations in the system matrix helps its solvability. For aggressive

D	P^T	P^W	λ_{max}	λ_{min}	
2	1	1	1.537125e+00	1.150772e-03	7.486517e-04
2	1	2	4.940953e-01	9.196245 e - 05	1.861229 e-04
2	1	3	3.324177e-01	1.064946e-05	3.203639 e-05
2	1	4	2.853322e-01	1.705230 e-06	5.976295 e - 06
2	1	5	2.665812e-01	3.349335e-07	1.256403e- 06
2	2	1	2.407807e+00	1.457063e- 06	6.051408 e-07
2	2	2	4.940956e-01	5.469314e-08	1.106934e-07
2	2	3	3.324177e-01	2.879583e-09	8.662545 e - 09
2	2	4	2.853323e-01	1.628939e-10	5.708921e-10
2	2	5	2.665812e-01	1.084310e-11	4.067466e-11
2	3	1	2.407807e+00	5.822902e-10	2.418342e-10
2	3	2	9.272889e-01	4.520282e-11	4.874729e-11
2	3	3	3.324177e-01	1.618058e-12	4.867544e-12
2	3	4	2.853323e-01	7.227717e-14	2.533088e-13
2	3	5	2.665812e-01	3.194386e-15	1.198279e-14
2	4	1	2.943604e+00	6.445948e-26	2.189815e-26
2	4	2	9.877639e-01	6.302117e-27	6.380185 e-27
2	4	3	6.561304 e-01	6.778809e-28	1.033150e-27
2	4	4	2.868930e-01	5.733222e-27	1.998383e-26
2	4	5	5.327046e-01	5.117605 e-25	9.606835 e-25
3	1	1	4.639099e+00	3.887142e-03	8.379088e-04
3	1	2	1.079504e+00	2.369894e-04	2.195354e-04
3	1	3	6.747118e-01	2.359590 e-05	3.497182 e- 05
3	1	4	5.721834e-01	3.540976e-06	6.188534 e-06
3	1	5	5.333668e-01	6.792558e-07	1.273525 e-06
3	2	1	4.639156e+00	3.176883e-06	6.847975 e-07
3	2	2	1.079505e+00	1.512048e-07	1.400686e-07
3	2	3	6.747119e-01	6.991076e-09	1.036157e-08
3	2	4	5.721835e-01	3.641527e-10	6.364265 e-10
3	2	5	2.669165 e-01	1.146071e-11	4.293744e-11
3	3	1	4.639157e+00	1.340233e-09	2.888959e-10
3	3	2	1.079505e+00	7.151353e-11	6.624659 e-11
3	3	3	6.747119e-01	3.977531e-12	5.895155e-12
3	3	4	2.869943e-01	5.757645e-14	2.006188e-13
3	3	5	2.669165 e-01	1.723124e-15	6.455665e- 15
3	4	1	3.106689e+00	3.897434e-26	1.254530 e-26
3	4	2	1.171168e+00	3.832896e-28	3.272712e-28
3	4	3	7.002071e-01	3.537134e-28	5.051555e-28
3	4	4	2.903904e-01	8.048694e-26	2.771680e-25

Table 4: We show the lowest value of \rfloor for an entire Cartesian grid of size 32^D with all boundary conditions homogeneous Dirichlet. We vary Taylor power P^T , weighting function exponents P^W , and dimensionality D.

D	P^T	P^W	λ_{max}	λ_{min}	
2	1	1	2.518893e+00	1.601156e-04	6.356588e-05
2	1	2	2.362043e+00	1.461371e-05	6.186896e-06
2	1	3	1.094261e+00	9.635190 e - 07	8.805204 e - 07
2	1	4	1.093340e+00	1.270395e-07	1.161940e-07
2	1	5	1.094367e+00	2.036717e-08	1.861091e-08
2	2	1	1.462450e+00	2.819426e-08	1.927879e-08
2	2	2	1.118414e+00	3.603335e-09	3.221825 e - 09
2	2	3	1.101878e+00	6.259208 e-10	5.680491e-10
2	2	4	1.787419e+00	1.261851e-10	7.059628e-11
2	2	5	1.786900e+00	8.059615e-12	4.510389 e-12
2	3	1	1.463079e+00	5.935296e-12	4.056717e-12
2	3	2	1.119064e+00	1.346836e-12	1.203538e-12
2	3	3	3.180167e+00	2.412859e-13	7.587209e-14
2	3	4	3.171902e+00	1.108072e-14	3.493399e-15
2	3	5	1.101546e+00	1.869284 e-16	1.696964e-16
2	4	1	4.679500e+00	1.267360e-17	2.708324e-18
2	4	2	3.730996e+00	2.933117e-18	7.861486e-19
2	4	3	3.640428e+00	2.031473e-17	5.580313e-18
2	4	4	1.101662e+00	2.052912e-18	1.863468e-18
2	4	5	1.101600e+00	5.403550 e-19	4.905182e-19
3	1	1	5.278503e+00	5.349129e-04	1.013380e-04
3	1	2	2.898423e+00	1.765977e-05	6.092890 e-06
3	1	3	2.480335e+00	5.055998e-07	2.038433e-07
3	1	4	2.468916e+00	2.823132e-08	1.143471e-08
3	1	5	2.528326e+00	3.761767e-09	1.487849e-09
3	2	1	1.845660e+00	1.814540 e - 08	9.831389e-09
3	2	2	4.774894e+00	4.503397e-09	9.431406e-10
3	2	3	2.880922e+00	1.193187e-10	4.141685e-11
3	2	4	2.864876e+00	1.430923e-11	4.994711e-12
3	2	5	4.150386e+00	3.315285e-12	7.987897e-13
3	3	1	1.936290e+00	1.161631e-12	5.999263e-13
3	3	2	2.897250e+00	5.681304e-13	1.960930e-13
3	3	3	3.447497e+00	9.616076e-14	2.789292e-14
3	3	4	2.751616e+00	1.135060e-14	4.125067e-15
3	3	5	2.750524e+00	4.977018e-16	1.809480e-16
3	4	1	2.390817e+00	4.437506e-16	1.856062e-16
3	4	2	4.045567e+00	2.572870e-16	6.359727e-17
3	4	3	2.967273e+00	4.916614e-17	1.656947e-17
3	4	4	6.914527e+00	6.809812e-17	9.848559e-18
3	4	5	6.132492e+00	9.581151e-18	1.562359e-18

Table 5: We show the lowest value of \rfloor for an entire Cartesian grid of size 32^D with all boundary conditions homogeneous Dirichlet. The grid covers the unit square and is cut by a sphere of radius 0.45. We vary Taylor power P^T , weighting function exponents P^W , and dimensionality D. This grid has had its small volumes merged with neighboring volumes.

D	P^T	P^W	λ_{max}	λ_{min}	
2	1	1	2.659761e+00	1.406481e-03	5.287997e-04
2	1	2	1.215453e+00	1.019228e-04	8.385575e-05
2	1	3	1.046275e+00	8.724426e-06	8.338562e-06
2	1	4	1.016321e+00	1.289568e-06	1.268859e-06
2	1	5	1.009826e+00	4.105645e-07	4.065697e-07
2	2	1	2.721312e+00	6.510187e-07	2.392297e-07
2	2	2	1.215454e+00	4.619552e-08	3.800680e-08
2	2	3	1.046439e+00	3.123629e-09	2.985008e-09
2	2	4	1.016267e+00	2.184707e-10	2.149737e-10
2	2	5	1.009758e+00	1.769343e-11	1.752244e-11
2	3	1	2.721312e+00	2.062962e-10	7.580764e-11
2	3	2	1.215454e+00	1.829550 e-11	1.505240 e-11
2	3	3	1.046275e+00	1.297942e-12	1.240537e-12
2	3	4	1.016321e+00	7.989181e-14	7.860883e-14
2	3	5	1.009826e+00	5.099447e-15	5.049829e-15
2	4	1	2.721312e+00	1.944812e-15	7.146596e-16
2	4	2	1.218511e+00	6.245987e-16	5.125916e-16
2	4	3	1.045681e+00	1.558421e-16	1.490342e-16
2	4	4	1.016267e+00	5.658955e-17	5.568374e-17
2	4	5	1.009906e+00	2.092151e-17	2.071630e-17
3	1	1	6.913939e+00	3.982281e-03	5.759786e-04
3	1	2	1.457848e+00	1.829414e-04	1.254873e-04
3	1	3	1.067010e+00	8.920278e-06	8.360072 e-06
3	1	4	1.014179e+00	7.322700 e-07	7.220320e-07
3	1	5	1.003823e+00	1.115560 e-07	1.111311e-07
3	2	1	7.173899e+00	1.868378e-06	2.604411e-07
3	2	2	1.457849e+00	7.351431e-08	5.042654 e-08
3	2	3	1.067007e+00	3.063086e-09	2.870728e-09
3	2	4	1.014193e+00	1.481290 e-10	1.460561e-10
3	2	5	1.003823e+00	8.189605e- 12	8.158418e-12
3	3	1	7.173899e+00	5.736164e-10	7.995881e-11
3	3	2	1.463446e+00	3.367536e-11	2.301099e-11
3	3	3	1.067224e+00	1.254264e-12	1.175258e-12
3	3	4	1.014176e+00	4.631105e-14	4.566371e-14
3	3	5	1.003820e+00	1.806297e-15	1.799424e-15
3	4	1	7.173899e+00	8.925826 e-15	1.244208e-15
3	4	2	1.463446e+00	3.102967e-16	2.120315e-16
3	4	3	1.102822e+00	3.089983e-17	2.801888e-17
3	4	4	1.014074e+00	7.854565e-18	7.745552e-18
3	4	5	5.339547e-01	2.224403e-18	4.165902e-18

Table 6: We show the lowest value of \rfloor for an entire Cartesian grid of size 32^D with all boundary conditions homogeneous Dirichlet. The grid covers the unit square and is cut by a sphere of radius 0.45. We vary Taylor power P^T , weighting function exponents P^W , and dimensionality D. This grid includes very small volumes.

choices of weighting power and Taylor power, however, the system matrix that results is not credibly solvable without high precision arithmetic.

.

References

- [1] M. Adams, P. Colella, D. T. Graves, J. N. Johnson, H. S. Johansen, N. D. Keen, T. J. Ligocki, D. F. Martin, P. W. McCorquodale, D. Modiano, P. O. Schwartz, T. D. Sternberg, and B. Van Straalen. Chombo software package for AMR applications—design document. Technical Report LBNL-6616E, Lawrence Berkeley National Laboratory, 2015.
- [2] P. Colella, D. T. Graves, N.D. Keen, T. J. Ligocki, D. F. Martin, P.W. McCorquodale, D. Modiano, P.O. Schwartz, T.D. Sternberg, and B. Van Straalen. Chombo Software Package for AMR Applications Design Document. Lawrence Berkeley National Laboratory, 2009. https://seesar.lbl.gov/anag/chombo/ChomboDesign-3.0.pdf.
- [3] P. Colella, D. T. Graves, T. J. Ligocki, G. Miller, D. Modiano, P. Schwartz, B. V. Straalen, J. Pillod, D. Trebotich, and M. Barad. EBChombo software package for Cartesian grid, embedded boundary application. Technical Report LBNL-6615E, Lawrence Berkeley National Laboratory, 2014.
- [4] D. Devendran, D. T. Graves, H. Johansen, and T. Ligocki. A fourth-order Cartesian grid embedded boundary method for Poisson's equation. *Comm. App. Math. and Comp. Sci.*, 12(1):51–79, 2017.
- [5] G. H. Miller and D. Trebotich. An embedded boundary method for the navier-stokes equations on a time-dependent domain. *Communications in Applied Mathematics and Computational Science*, 7:1–31, 2012.
- [6] N. Overton-Katz, D. T. Graves, D. Devendran, and O. Antepara. Polynomial expansions of finite volume data in a cut cell context. Technical report. Lawrence Berkeley National Laboratory Technical Report LBNL-2001528.

¹Lawrence Berkeley National Laboratory, Berkeley, CA. Research at LBNL was supported financially by the Office of Advanced Scientific Computing Research of the US Department of Energy under contract number DE-AC02-05CH11231.

²Ford Motor Company, Sunnyvale, CA.

³This includes corner volumes. The neighborhood is formed by taking all the volumes within a grown box. The grown box is formed by growing the box made from the low and high cells of the target face, growing it by N_G and intersecting with the domain. We use the Chombo ([1, 3, 2]) box growth semantic.

 $^{^4}$ If the matrix M is square, a weighting matrix can have no effect and the Moore-Penrose psueudoinverse becomes M^{-1} .

⁵The equations for volumes \mathbf{j} where $\bar{\mathbf{x}}_{\mathbf{j}}$ is large receive higher weights. Diagonal weighting matrices are common. Usually these algorithms define a distance metric $D(\mathbf{i}, \mathbf{j})$ for two volumes \mathbf{i} and \mathbf{j} and make $W_{\mathbf{j},\mathbf{j}}$ decrease strongly with increasing $D(\mathbf{i},\mathbf{j})$. This assign higher importance to the equations for volumes closer to \mathbf{i} . Devendran et al. for example [4], uses a weighting function $W_{\mathbf{i},\mathbf{j}} \approx 1./D(\mathbf{i},\mathbf{j})^5$

[7] P. Schwartz, J. Percelay, T. Ligocki, H. Johansen, D. Graves, D. Devendran, P Colella, and E. Ateljevich. High-accuracy embedded boundary grid generation using the divergence theorem. *Communications in Applied Mathematics and Computational Science*, 10(1):83 – 96, 2015.