AN IMMERSED INTERFACE METHOD FOR SOLVING
ANISOTROPIC ELLIPTIC BOUNDARY VALUE PROBLEMS IN 3D *

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Abstract. We have developed a first-order stable Cartesian grid discretization that uses only interior grid points for inhomogeneous anisotropic elliptic operators subject to Neumann boundary condition on a bounded non-rectangular geometry in 3D. For this discretization method, a necessary and sufficient condition depending on the mesh size $h$ for the existence of this first-order stable scheme at a regular (i.e. interior) grid point is found in terms of the anisotropy matrix. For this discretization method, a way to analyze the existence of a first-order stable scheme at an irregular (i.e. boundary) grid point is also given. The arguments are identical to those for the 2D case [2]; only the details change. Unlike in [2], discussion for Dirichlet and Robin boundary conditions are also included. In particular, it is shown that the Gerschgorin condition does not impose sign restrictions on irregular grid points stencil coefficients as in the Neumann case.

Key words. Immersed interface method, anisotropic Laplacian, Gerschgorin criterion, linear programming.

AMS subject classifications. 65N06, 65N12.

1. Introduction. This paper is a generalization to 3D domains of [2]. That is, we develop a first-order stable discretization to find an approximate solution of the elliptic second-order partial differential equation in its divergence form

$$-\nabla \cdot (\mathbf{D}(x, y, z) \nabla v) + \mathbf{u}(x, y, z) \cdot \nabla v + w(x, y, z)v = f(x, y, z),$$

in a three dimensional irregular bounded domain $\Omega$, subject to the boundary condition

$$\beta (\mathbf{n} \cdot \mathbf{D} \nabla v) + \alpha v = g,$$

on $\Gamma = \partial \Omega$. $\Gamma$ is assumed to be smooth and could be composed of several disconnected surfaces. $\mathbf{n}$ is the outward unit normal vector to $\Gamma$; $\alpha$ and $\beta$ are nonnegative constants such that $\alpha + \beta > 0$; $\mathbf{u}(x, y, z) = (u_1(x, y, z), u_2(x, y, z), u_3(x, y, z))$ and $\mathbf{D} = \mathbf{D}(x, y, z)$ at the point $(x, y, z)$ is a symmetric positive definite $3 \times 3$ matrix of the form

$$\mathbf{D}(x, y, z) = 
\begin{pmatrix}
D_{11}(x, y, z) & D_{12}(x, y, z) & D_{13}(x, y, z) \\
D_{12}(x, y, z) & D_{22}(x, y, z) & D_{23}(x, y, z) \\
D_{13}(x, y, z) & D_{23}(x, y, z) & D_{33}(x, y, z)
\end{pmatrix}.$$ 

The regularity assumed for $\mathbf{D}, \mathbf{u}, f$ and $w$ are as follows: $D_{ij}$ are $C^1(\Omega)$ functions for $i, j = 1, 2, 3$; $u_1, u_2, u_3$ are continuous functions in $\overline{\Omega}$; $f$ is continuous in $\overline{\Omega}$ and $w(x, y, z)$ is nonnegative and continuous in $\overline{\Omega}$.

It is also assumed that $g$ is $C^1(\overline{\Omega})$ for Neumann and Robin boundary conditions and $C^2(\overline{\Omega})$ for Dirichlet boundary conditions.

Given the finite domain $\Omega$, we embed $\Omega$ in a box $R$ and take a Cartesian equally-spaced grid for $R$. Grid points $(ih, jh, kh)$ which lie inside $\Omega$ are called interior grid points. Exterior grid points are the remaining grid points.

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There are two types of interior grid points. A grid point \((x, y, z)\) is a regular grid point if all the grid points in certain set \(K\) lie inside \(\Omega\). If at least one point in \(K\) is outside \(\Omega\) then the point \((x, y, z)\) is called an irregular grid point. In this paper we consider two different sets \(K\), namely

\[
K_1(x, y, z) = \{(x + i_1h, y + j_1h, z + k_1h), i_1, j_1, k_1 \in \{-1, 0, 1\}\},
\]

\[
K_2(x, y, z) = \{(x + i_1h, y + j_1h, z + k_1h) \in K_1(x, y, z); i_1j_1k_1 = 0\}.
\]

Observe that \(K_2(x, y, z) \subset K_1(x, y, z)\). The set \(K_1(x, y, z)\) includes all the nearest neighbors of \((x, y, z)\) with the topology defined by the infinity norm (a cube). The set \(K_2(x, y, z)\) does not include the corners in the discrete ‘cube’ \(K_1(x, y, z)\). We consider two different stencils depending on which set \(K_1(x, y, z)\) or \(K_2(x, y, z)\) is used to define interior and exterior grid points. We refer to these as \(K_1\) stencils and \(K_2\) stencils. In our simulations we will use \(K_1\) stencils of points defined by \(K_1\). \(K_2\) stencils are included for their theoretical interest.

The Immersed Interface Method (IIM) was developed by LeVeque and Li [5] for the scalar anisotropic Laplacian on an irregular domain in 2D with interfaces across which the anisotropy has jump discontinuities or Dirac delta functions. Li extended the method to scalar anisotropic Laplacians in 3D [6]. In [4] Fogelson and Keener used the treatment of irregular grid points of IIM [6] to approximate the Laplace operator for Neumann problems. They included stability considerations and solved the linear system with a multigrid solver.

Finite Element [9] and Finite Volume [8] discretizations are the only other non-adaptive mesh refinement methods that have been developed to solve (1.1)-(1.2) with a general nondiagonal anisotropic matrix \(D\) in 3D.

The content of the remainder of this paper is as follows: In section 2 weakly diagonal dominant (w.d.d.) first-order schemes for a regular grid point are found for both \(K_1\) and \(K_2\) stencils. In section 3 a linear programming approach to find the weights of the schemes for a regular interior grid point is presented. The idea of solving a programming problem to obtain finite difference schemes is also utilized in [10]. There, sign restrictions are imposed to find schemes that satisfy the discrete maximum principle [7] for irregular grid points.

In section 4 w.d.d. first-order stencils for an irregular grid point depending on the boundary condition type imposed are found for each stencil. Sufficient conditions for the existence of solutions to those systems are presented in section 5. The arguments in all sections are identical to those for the 2D case; only the details change.

In section 6 we present some numerical results illustrating the method. Conclusions are included in section 7.

2. The scheme at a regular interior grid point. In this section, we seek a discretization of (1.1) at a regular interior grid point using \(K_1\) and \(K_2\) stencils. Consider an interior point \((x, y, z) = (ih, jh, kh)\), for some integers \(i, j, k\) where the grid size is \(h\). The operator \(\nabla \cdot (D \nabla v) - vw\) evaluated at this point can be written as

\[
\nabla \cdot (D \nabla v) - vw = -uw + P v_x + Q v_y + R v_z + D_{11} v_{xx} + D_{22} v_{yy} + D_{33} v_{zz} + 2D_{12} v_{xy} + 2D_{13} v_{xz} + 2D_{23} v_{yz}.
\]

(2.1)

where \(P = (D_{11})_x + (D_{12})_y + (D_{13})_z - u_1\), \(Q = (D_{12})_x + (D_{22})_y + (D_{23})_z - u_2\), \(R = (D_{13})_x + (D_{23})_y + (D_{33})_z - u_3\).

Our goal is to find a discretization of this operator with first-order local truncation error (LTE) at the interior point \((x, y, z)\). The presence of mixed derivatives suggests
that we consider a 27 point stencil. These 27 points are the points in \( K_1(x, y, z) \). We label the points in \( K_1(x, y, z) \) by the following rule: \( ijk \) corresponds to \( (x + ih, y + jh, z + kh) \), where \( i, j, k = -1, 0, 1 \).

We wish to approximate the differential operator (2.1) at \((x, y, z)\) using the linear combination of values on the grid of immediate neighbors \( L[v] = \sum_{i,j,k=-1}^{1} \tilde{c}_{ijk} v_{ijk} \) where \( v_{ijk} = v(x + ih, y + jh, z + kh) \), \( i, j, k = -1, 0, 1 \).

The linear combination is taken over the immediate neighbors of \((x, y, z)\), for \( h \) small enough each term of the linear combination is approximated by a second-order Taylor expansion centered at \((x, y, z)\). It follows that

\[
L[v] = (\tilde{c}_.)v + (\tilde{c}_{1.} - \tilde{c}_{-.1})hv_x + (\tilde{c}_{1.1} - \tilde{c}_{-.1.1})hv_y + (\tilde{c}_{1.1.1} - \tilde{c}_{-.1.1.1})hv_z + \frac{h^2}{2} (\tilde{c}_{11} - \tilde{c}_{-.11} + \tilde{c}_{1-1} - \tilde{c}_{-11})v_{xx} + \frac{h^2}{2} (\tilde{c}_{11.1} - \tilde{c}_{-.11.1} + \tilde{c}_{1-1.1} - \tilde{c}_{-11.1})v_{yy} + \frac{h^2}{2} (\tilde{c}_{111} - \tilde{c}_{-.111} + \tilde{c}_{1-11} - \tilde{c}_{-111})v_{zz} + h^3 \sum_{i,j,k=-1,0,1} q_{ijk} \tilde{c}_{ijk}.
\]

For \( L[v] \) to approximate \( \nabla \cdot (D \nabla v) - wv \) for arbitrary \( v \), we must match terms corresponding to the same derivative in the two different expressions, i.e., we require

\[
\tilde{c}_. = -w; \quad \tilde{c}_{1.} - \tilde{c}_{-.1} = \frac{P}{h}; \quad \tilde{c}_{1.1} - \tilde{c}_{-.1.1} = \frac{Q}{h}; \quad \tilde{c}_{1.1.1} - \tilde{c}_{-.1.1.1} = \frac{R}{h}.
\]

The system is equivalent to

\[
\begin{align*}
(2.2) & \quad c_{1.} = D_{11} + P \\
(2.3) & \quad c_{-.1} = D_{11} - P \\
(2.4) & \quad c_{1.1} = D_{22} + Q \\
(2.5) & \quad c_{-.1.1} = D_{22} - Q \\
(2.6) & \quad c_{1.1.1} = D_{33} + R \\
(2.7) & \quad c_{-.1.1.1} = D_{33} - R \\
(2.8) & \quad c_{11.} - c_{1-1} + c_{-.1-1} - c_{-.11} = 2D_{12} \\
(2.9) & \quad c_{1.1} - c_{1-1} + c_{1-1.1} - c_{-.11} = 2D_{13} \\
(2.10) & \quad c_{11.1} - c_{11-1} + c_{11-1.1} - c_{11-.11} = 2D_{23} \\
(2.11) & \quad c_{-} = -h^2 w
\end{align*}
\]

where \( c_{ijk} = h^2 \tilde{c}_{ijk}, i, j, k = -1, 0, 1 \); \( P = \frac{h}{2} P \) and \( Q = \frac{h}{2} Q \), \( R = \frac{h}{2} R \).

If these conditions for weights \( c_{ijk}, i, j, k = -1, 0, 1 \) can be satisfied, then our approximation will have first-order LTE since \( h^2 \sum_{i,j,k} q_{ijk} \tilde{c}_{ijk} = h \sum_{i,j,k} q_{ijk} c_{ijk} \).

Since \( \nabla \cdot (D \nabla v) - wv \) is a non-positive definite operator it is desirable that its discretization be the same. It can be proved that the Gerschgorin criterion \([11]\),

\[
-\alpha_{000} \geq \sum_{ijk \neq 000} |c_{ijk}| is sufficient to guarantee that the discretization matrix is nonpositive definite. Nonpositive definiteness of the discretization matrix enforces \( c_{000} \leq 0 \).

According to (2.11) with \( w(x, y, z) \equiv 0 \), the sum of the weights in the 27-point stencil must be zero. So \( \alpha_{000} = \sum_{ijk \neq 000} c_{ijk} \). Hence the Gerschgorin criterion becomes \( \sum_{ijk \neq 000} c_{ijk} \geq \sum_{ijk \neq 000} |c_{ijk}| \). This can be guaranteed if and only if \( c_{ijk} \geq 0 \) for all \( ijk \neq 000 \).
When the non-homogeneous term \( w(x, y, z) \) is not zero, it is possible to have \( c_{ijk} < 0 \) for some \( ijk \neq 000 \). It is sufficient to set \( c_{000} = -w - \sum_{ijk \neq 000} c_{ijk} \) where \( c_{ijk} \geq 0, ijk \neq 000 \). Therefore, to get a stable first-order scheme it is sufficient to find a solution of the system (2.2)-(2.11) such that

\[
(2.12) \quad c_{000} \leq 0, \quad c_{ijk} \geq 0, \quad ijk \neq 000.
\]

In other words, for regular grid points \((x, y, z)\), the Gerschgorin criterion implies that the scheme must be weakly diagonal dominant (w.d.d.). So we are interested in w.d.d. first-order schemes. Such a scheme will be called a weakly diagonal dominant first-order scheme (or w.d.d. first-order scheme).

It is well known that if at a regular point \((x, y, z)\) the discretization of a linear elliptic operator under homogeneous Dirichlet boundary conditions is w.d.d, then the order of accuracy of the discretization method at \((x, y, z)\) coincides with the order of the LTE at \((x, y, z)\) (see Chapter 6 in [7]).

A necessary and sufficient condition to find a w.d.d. first-order \( K_1 \) stencil is given in the next theorem.

**Theorem 2.1.** Suppose \( D(x, y, z) \) is a symmetric positive definite matrix for all \((x, y, z)\) in the domain \( \Omega \). Then it is possible to find a w.d.d. first-order \( K_2 \) stencil scheme for (1.1) at a regular interior grid point \((x_0, y_0, z_0)\) if and only if \( D(x_0, y_0, z_0) \) is weakly diagonal dominant.

**Proof** A 3 \( \times \) 3 symmetric positive definite matrix is said to be weakly diagonal dominant if the diagonal elements are larger than or equal to the absolute values of the off-diagonal entries. Before giving the proof of the sufficiency and necessity it is convenient to find an equivalent form of the system (2.2)-(2.11) which is easier to deal with.

The system (2.2)-(2.11) is a linear system of 10 equations and 27 unknowns, so at least 17 of the unknowns can be viewed as parameters, or independent variables. If we consider \( c_{100}, c_{-100}, c_{010}, c_{010}, c_{001}, c_{-110}, c_{100}, c_{-110}, c_{011}, c_{011}, c_{000} \) as dependent variables then the system (2.2)-(2.11) can be rewritten in terms of the remaining variables as

\[
\begin{align*}
c_{100} &= (D_{11} + 2D_{13} + P) - c_{1-1-1} - c_{1-10} - c_{1-11} \\
&\quad -2c_{101} - c_{11-1} - c_{110} - c_{111} - c_{-10-1} + c_{-101} \geq 0, \\
c_{-100} &= (D_{11} + 2D_{12} - P) - c_{-1-1-1} - 2c_{-1-10} - c_{-1-11} \\
&\quad -c_{-10-1} - c_{-101} - c_{-11-1} + c_{-110} - c_{110} + c_{1-10} \geq 0, \\
c_{010} &= (D_{22} + 2D_{12} + Q) - c_{-11-1} - c_{-111} - c_{01-1} \\
&\quad -c_{011} - c_{01-1} - 2c_{010} - c_{011} - c_{-1-10} - c_{-1-11} + c_{010} \geq 0, \\
c_{010} &= (D_{22} + 2D_{12} + Q) - c_{-11-1} - c_{-111} - c_{01-1} \\
&\quad -2c_{01-1} - c_{01-1} - c_{010} - c_{011} - c_{-1-10} + c_{011} \geq 0, \\
c_{001} &= (D_{33} + 2D_{23} + R) - c_{-11-1} - 2c_{011} - c_{-111} \\
&\quad -c_{01-1} + c_{011} - c_{11-1} - c_{110} - c_{111} + c_{-101} \geq 0, \\
c_{001} &= (D_{33} + 2D_{13} - R) - c_{-11-1} - c_{01-1} - c_{11-1} \\
&\quad -2c_{-10-1} - c_{11-1} - c_{01-1} - c_{110} - c_{111} - c_{-101} \geq 0, \\
c_{-110} &= -2D_{12} + c_{-1-10} + c_{110} - c_{1-10} + c_{111} + c_{011} \\
&\quad -c_{11-1} - c_{110} - c_{111} + c_{-1-10} - c_{-111} - c_{-1-11} \geq 0, \\
c_{10} &= -2D_{13} + c_{-10-1} + c_{101} - c_{-101} + c_{111} + c_{111}
\end{align*}
\]
\[-c_{11} - c_{1-1-1} + c_{-1-1-1} + c_{-1-1-1} - c_{-1-11} - c_{-1-11} \geq 0,\]
\[c_{0-11} = -2D_{23} + c_{0-1-1} + c_{011} - c_{01-1} + c_{111} + c_{-111},\]
\[-c_{11-1} - c_{-11-1} + c_{1-1-1} - c_{-1-1-1} - c_{-11-1} - c_{-11-1} \geq 0,\]
\[c_{000} = -2(D_{33} + D_{22} + D_{11} + D_{12} + D_{13} + D_{23} - \frac{h^2w}{2})\]
\[+ 2(c_{-1-10} + c_{110} + c_{-1-1-1} + c_{-1-11} + c_{-10-1})\]
\[+ c_{1-11} + c_{-111} + c_{111} + c_{011} + c_{11-1}\]
\[+ c_{11-1} + c_{-111} + c_{111} + c_{011} + c_{11-1} \leq 0.\]

(2.13)

By choosing axes appropriately, without loss of generality \(D_{11} \geq D_{22} \geq D_{33}\).

If \(D_{12} < 0\) then instead of using \(c_{-110}\) in (2.8) as dependent variable, we can use \(c_{-1-10}\) as dependent variable. Therefore, if we define \(P = P, Q = -Q, R = R, D_{11} = D_{11}, D_{22} = D_{22}, D_{33} = D_{33}, D_{12} = -D_{12}, D_{13} = D_{13}, D_{23} = D_{23}\) and \(\hat{c}_{ijk} = c_{-1-jk}, \hat{c}_{0jk} = c_{0jk}, \hat{c}_{-1jk} = c_{-1jk}\) then the system for the \(\hat{c}_{ijk}\) variables is exactly the system (2.13) but with \(\hat{c}_{ijk}\) instead of \(c_{ijk}\). A similar argument can be used for the cases \(D_{13} < 0\) and \(D_{23} < 0\). Therefore we can assume without loss of generality that \(D_{11} \geq D_{22} \geq D_{33}\) and \(D_{12}, D_{13}, D_{23} \geq 0\).

The \(K_2\) stencil has no corners i.e., we must have \(c_{ijk} = 0, ijk \neq 0\). The 10 inequalities in (2.13) can be written as

\[
\begin{align*}
\text{(2.14)} & \quad -c_{-10-1} - c_{-101} + c_{10-1} + 2c_{101} + c_{110} \leq D_{11} + 2D_{13} + P, \\
\text{(2.15)} & \quad 2c_{-10-1} + c_{10-1} + c_{101} + c_{110} - c_{1-10} \leq D_{11} + 2D_{12} - P, \\
\text{(2.16)} & \quad c_{01-1} + c_{011} + 2c_{110} + c_{-1-10} - c_{1-10} \leq D_{22} + 2D_{12} + Q, \\
\text{(2.17)} & \quad c_{-101} + 2c_{00-1} + c_{1-10} + c_{011} - c_{01-1} \leq D_{22} + 2D_{23} - Q, \\
\text{(2.18)} & \quad 2c_{101} + c_{011} + c_{010} + c_{0-1-1} - c_{01-1} \leq D_{33} + 2D_{23} + R, \\
\text{(2.19)} & \quad 2c_{-10-1} + c_{0-1-1} + c_{01-1} + c_{101} - c_{1-10} \leq D_{34} + 2D_{13} - R, \\
\text{(2.20)} & \quad c_{1-10} + c_{110} - c_{1-10} \geq 2D_{12}, \\
\text{(2.21)} & \quad c_{-10-1} + c_{101} - c_{101} \geq 2D_{13}, \\
\text{(2.22)} & \quad c_{0-1-1} + c_{011} - c_{01-1} \geq 2D_{23}, \\
\text{(2.23)} & \quad c_{-1-10} + c_{110} + c_{10-1} + c_{011} + c_{0-1-1} + c_{101} \leq D_{000},
\end{align*}
\]

where \(D_{000} = D_{11} + D_{22} + D_{33} + D_{12} + D_{13} + D_{23} + \frac{h^2w}{2}\).

Since \(D\) is positive definite, \(D_{11} = e_1^TDe_1 > 0, D_{22} = e_2^TDe_2 > 0\) and \(D_{33} = e_3^TDe_3 > 0\), where \(e_1, e_2\) and \(e_3\) are the standard basis of \(\mathbb{R}^3\). Since \(D\) is weakly diagonal dominant, \(D_{12} + D_{13} \leq D_{11}, D_{12} + D_{23} \leq D_{22}\) and \(D_{13} + D_{23} \leq D_{33}\).

A solution of the system (2.14)-(2.23) (where the variables \(c_{ijk}\) \(ijk \neq 0\) have been previously set to zero) is given by

\[
\begin{align*}
\text{(2.24)} & \quad c_{1-10} = 0, \quad c_{-101} = 0, \quad c_{01-1} = 0
\end{align*}
\]
provided \( h \) is sufficiently small.

Observe that in the case of the Laplacian operator \( D_{11} = D_{22} = D_{33} = 1 \) and 
\( D_{12} = D_{13} = D_{23} = P = Q = R = 0 \). Therefore \( c_{ijk} = 0 \), \( i, j, k = -1, 1 \) and \( c_{ijk} = 0 \) for \( i = 0 \) or \( j = 0 \) or \( k = 0 \). In addition, \( c_{000} = -6 \) and \( c_{ijk} = 1 \) for exactly one among \( i, j, k \) different than zero, which is exactly the classic 7-point stencil.

**sufficiency**

Suppose that \( D \) is not weakly diagonal dominant. Without loss of generality assume that

\[
D_{33} < D_{13} + D_{23}.
\]

Equations (2.18) and (2.19) can be written as

\[
2c_{011} + c_{101} + c_{0-1-1} \leq D_{33} + 2D_{23} + R - c_{-101} + c_{01-1},
\]

\[
2c_{-10-1} + c_{0-1-1} + c_{101} \leq D_{33} + 2D_{13} - R - c_{01-1} + c_{-101},
\]

respectively. From equations (2.21) and (2.22), it follows that

\[
-c_{-10-1} - c_{101} \leq -2D_{13} - c_{-101} \leq -2D_{13},
\]

\[
-c_{0-1-1} - c_{011} \leq -2D_{23} - c_{01-1} \leq -2D_{23}.
\]

Therefore \( \frac{1}{2} ((2.18) + (2.19)) + (2.28) + (2.29) \) is

\[
0 \leq D_{33} - D_{13} - D_{23}
\]

or equivalently \( D_{13} + D_{23} \leq D_{33} \), which is a contradiction to (2.25). The other two cases \( D_{11} < D_{12} + D_{13} \) and \( D_{22} < D_{12} + D_{23} \) can be treated similarly. ♦

From the proof of the theorem it follows that the necessity condition of theorem 2.1 also holds for \( K_1 \) stencils.

**3. A linear programming approach.** A first-order discretization of \( \nabla \cdot (D \nabla v) - uv \) always exists for regular interior grid points (using centered differences). When it is not possible to find Gerschgorin stable schemes for all regular interior grid points in the domain then at least a solution to the system of equations (2.2)-(2.11) can always be found.

Since it is desirable that the center of the Gerschgorin circle be negative and in absolute value as large as possible, the weights of the scheme should be the solution of the following linear programming problem (LPP)

\[
\text{min } c_{000},
\]

subject to the first-order restrictions (2.2)-(2.11) and the Gerschgorin condition (2.12) when a \( K_1 \) stencil is used.

Linear programming techniques can be used to find the weights of the scheme for regular interior grid points even when there is a w.d.d. scheme. The restrictions of the LPP are the equations in the first-order LTE system (2.2)-(2.11) along with Gerschgorin stability condition (2.12).

In the case of the Laplacian it can be shown that this optimal solution is the classical 1, 1, -6, 1, 1 discretization. For, from the formula for \( c_{000} \) in (2.13),

\[
c_{000} = 2(c_{-1-10} + c_{110} + c_{-1-1-1} + c_{-1-11} + c_{-10-1} + c_{-11-1} + c_{-111} + c_{011} + c_{11-1} + c_{1-11} + c_{0-1-1} + c_{010}) - 6.
\]
If we use (2.14)-(2.23) then the LPP defined by the objective function (3.1), the LTE restrictions (2.2)-(2.11) and the sign restrictions triggered by the Gerschgorin condition (2.12) become
\[
\begin{align*}
\min & \ (c_{-1-10} + c_{110} + c_{-1-1-1} + c_{-1-11} + c_{-10-1} + c_{-11-1} + c_{-111}) \\
\text{subject to} & \\
\ & \ (c_{-1-1-1} + c_{1-10} + c_{-11} + 2c_{101} + c_{110} + c_{111} \leq 1 + c_{-101}) \\
\ & \ (c_{-1-1-1} + 2c_{-1-10} + c_{-1-11} + c_{-10-1} + c_{-111} + c_{-111} + c_{110} \leq 1 + c_{-10}) \\
\ & \ (c_{-1-1-1} + c_{-111} + c_{011} + c_{11-1} + 2c_{110} + c_{111} + c_{-1-10} \leq 1 + c_{-10}) \\
\ & \ (c_{-1-1-1} + c_{-1-10} + c_{-1-11} + c_{-10-1} + c_{11-1} + c_{-111} + c_{110} \leq 1 + c_{-10}) \\
\ & \ (c_{1-10} + c_{110} \geq c_{-10}) \\
\ & \ (c_{-10-1} + c_{101} \geq c_{-101}) \\
\ & \ (c_{0-1-1} + c_{011} \geq c_{01-1}) \\
\ & \ (c_{111} + c_{011} + c_{11-1} + c_{-111} + c_{-1-1-1} + c_{-1-11} + c_{-10-1} + c_{-111} + c_{110} \leq 3), \\
\ & \ (c_{ijk} \geq 0, \ i,j,k = -1,1; \ c_{0ll} \geq 0, \ c_{0ll} \geq 0, \ c_{0ll} \geq 0, \ l = -1,1).
\end{align*}
\]

To minimize \(c_{000}\) we need to assign the smallest possible values to the nonnegative variables in the objective function. Inequalities (3.9)-(3.11) are the only ones that might prevent zero values from being assigned to all the variables in the objective function. Nevertheless, it is possible to make all the variables in the objective function zero if \(c_{1-10} = c_{-101} = c_{01-1} = 0\). In this way, not only are all inequalities (3.3)-(3.13) satisfied, but it is impossible to find another point in the feasibility region where the objective function \(c_{000}\) achieves a lower value. From (2.13), \(c_{100} = 1, c_{-100} = 1, c_{010} = 1, c_{0-10} = 1, c_{001} = 1, c_{00-1} = 1, c_{-110} = 0, c_{10-1} = 0, c_{01-1} = 0, c_{00} = -6\.

It is not difficult to show that the feasibility region of this LPP is bounded.

4. The scheme at an irregular interior grid point. At an irregular point, not all of the points in the \(K_1\) stencil are interior to the domain. At these points we seek to incorporate boundary information into the discretization.

The goal at an irregular interior grid point is to find an approximate equation that discretizes (2.1) at a boundary point \((x^*, y^*, z^*)\) of \(\Gamma\) that is close to the irregular grid point \((x, y, z)\).

To approximate the operator \((\nabla \cdot (D \nabla v) - wv)(x^*, y^*, z^*)\) on the set of functions that satisfy exactly (1.2) we use
\[
\sum_{k \in K^+} \gamma_{kk} v(x_k, y_k, z_k) - C
\]
for appropriate chosen coefficients \(\gamma_{kk}\) where \(k = rst\), where \(r, s, t = -1,0,1\) (as in Figure 4.1), \(K^+ = K_1^+\) is the set of immediate neighbors which are also interior points.
and $C$ is a constant yet to be determined. The local truncation error at an irregular interior point using this approximation is

\[(4.2) \quad LTE = (\nabla \cdot (D\nabla v) - wv)_{(x^*, y^*, z^*)} - \sum_{k \in K^+} \gamma_k v(x_k, y_k, z_k) + C.\]

At this point the Taylor expansion of $v(x_k, y_k, z_k)$ around $(x^*, y^*, z^*)$ should be calculated. However, before doing this it is convenient to introduce a local change of coordinates near $(x^*, y^*, z^*)$. This is given by (see Figure 1)

\[(4.3) \quad \begin{bmatrix} \xi \\ \eta \\ \mu \end{bmatrix} = \begin{bmatrix} \cos \theta \sin \phi & \sin \theta \sin \phi & \cos \phi \\ -\sin \theta & \cos \theta & 0 \\ \cos \theta \cos \phi & \sin \theta \cos \phi & -\sin \phi \end{bmatrix} \begin{bmatrix} (x - x^*) \\ (y - y^*) \\ (z - z^*) \end{bmatrix},\]

where $\xi$ is along the exterior normal to $(x^*, y^*, z^*)$.

In this new coordinate system $(x^*, y^*, z^*)$ has coordinates $(0, 0, 0)$ and $\Gamma$ can be described locally near $(x^*, y^*, z^*)$ by $\xi = \chi(\eta, \mu)$ such that $\chi(0, 0) = 0, \chi_{\eta}(0, 0) = 0, \chi_{\mu}(0, 0) = 0$ ($\xi$ is taken to be the normal exterior vector at $(x^*, y^*, z^*)$) and $\chi_{\eta\mu}(0, 0) = 0$ (because of the symmetry of the Gaussian curvature tensor).

The Taylor expansion of $v$ at $(x_k, y_k, z_k)$ for $k \in K^+$ becomes

\[(4.4) \quad v(x_k, y_k, z_k) = v + v_\xi \xi_k + v_\eta \eta_k + v_\mu \mu_k + \frac{1}{2} v_{\xi\xi} \xi_k^2 + \frac{1}{2} v_{\eta\eta} \eta_k^2 + \frac{1}{2} v_{\mu\mu} \mu_k^2 + v_{\xi\eta} \xi_k \eta_k + v_{\xi\mu} \xi_k \mu_k + v_{\eta\mu} \eta_k \mu_k + O(h^3),\]

with $v$ taking limiting values at points of $\Gamma$ from the inside of $\Omega$.

The operator $\nabla \cdot (D\nabla v) - wv$ can be written in the new coordinates as

\[(4.5) \quad \nabla \cdot (D\nabla v) - wv = -wv + d_1 v_\xi + d_2 v_\eta + d_1 v_\eta + d_2 v_\eta + d_3 v_\mu + 2d_1 v_\xi + 2d_2 v_\eta + 2d_3 v_\mu,\]
where \( d_i = r_1 D_\xi r_i^T + r_2 D_\eta r_i^T + r_3 D_\mu r_i^T - u \cdot r_i^T, \ i = 1, 2, 3 \) and \( d_{ij} = r_i r_j^T, \ i, j = 1, 2, 3 \) with \( D_\xi \) indicates the matrix whose components are \( \frac{\partial D_{ij}}{\partial \xi} \) and where \( r_i \) is the \( i \)-th row of the rotation matrix (4.3). Notice that \( d_{ii} > 0, i = 1, 2, 3 \).

The next step is to use the exact boundary condition to get a linear relation among the values \( v, v_\xi, v_\eta, v_\mu, v_{\xi\xi}, v_{\eta\eta}, v_{\mu\mu}, v_{\xi\eta}, v_{\xi\mu}, v_{\eta\mu} \). For Neumann or Robin boundary conditions, the operator \( \mathbf{n} \cdot (\mathbf{D} \nabla v) \) is needed and can be expressed as

\[
(4.6) \quad \mathbf{n} \cdot (\mathbf{D} \nabla v) = (1 + \chi_1^2 + \chi_2^2) - \mathbf{z} (1, -\chi_1 - \chi_2)^T \cdot (D_{11} v_\xi + D_{12} v_\eta + D_{13} v_\mu, \\
D_{12} v_\eta + D_{13} v_\mu, D_{12} v_\eta + D_{13} v_\mu, D_{13} v_\mu)
\]

In addition, if (4.6) is differentiated with respect to \( \eta \) and \( \mu \) at the origin of the new coordinate system we get

\[
(4.7) \quad \frac{\partial \mathbf{n} \cdot (\mathbf{D} \nabla v)}{\partial \eta} = ((D_{11})_\eta - \chi_{11} D_{12}) v_\xi + ((D_{12})_\eta - \chi_{11} D_{22}) v_\eta + \\
(D_{13})_\eta - \chi_{12} D_{13}) v_\mu + D_{11} v_{\xi\eta} + D_{12} v_{\eta\eta} + D_{13} v_{\mu\eta}
\]

\[
(4.8) \quad \frac{\partial \mathbf{n} \cdot (\mathbf{D} \nabla v)}{\partial \mu} = ((D_{11})_\mu - \chi_{22} D_{13}) v_\xi + ((D_{12})_\mu - \chi_{22} D_{23}) v_\eta + \\
(D_{13})_\mu - \chi_{22} D_{33}) v_\mu + D_{11} v_{\xi\mu} + D_{12} v_{\eta\mu} + D_{13} v_{\mu\mu}
\]

Furthermore, at \((x^*, y^*, z^*)\) (4.6) becomes

\[
(4.9) \quad \mathbf{n} \cdot (\mathbf{D} \nabla v) = D_{11} v_\xi + D_{12} v_\eta + D_{13} v_\mu.
\]

For Dirichlet and Robin boundary conditions \( v = v(\xi, \eta, \mu) \) is needed. Its first and second derivatives with respect to \( \eta \) and \( \mu \) are

\[
(4.10) \quad \frac{\partial v}{\partial \eta} = v_\xi \chi_1 + v_\eta, \quad \frac{\partial^2 v}{\partial \eta^2} = (v_\xi \chi_1 + v_\xi \chi_2 + v_\xi \chi_1 + v_\eta), \\
\frac{\partial v}{\partial \mu} = v_\xi \chi_2 + v_\mu, \quad \frac{\partial^2 v}{\partial \eta \partial \mu} = (v_\xi \chi_1 + v_\xi \mu) \chi_1 + v_\xi \chi_2 + v_\eta, \\
\frac{\partial^2 v}{\partial \mu^2} = (v_\xi \chi_2 + v_\xi \mu) \chi_2 + v_\xi \chi_2 + v_\mu
\]

Therefore at \((x^*, y^*, z^*)\) (4.10) become

\[
\frac{\partial v}{\partial \eta} = v_\eta, \quad \frac{\partial v}{\partial \mu} = v_\mu, \quad \frac{\partial^2 v}{\partial \eta^2} = v_\xi \chi_1 + v_\eta, \quad \frac{\partial^2 v}{\partial \eta \partial \mu} = v_\eta, \quad \frac{\partial^2 v}{\partial \mu^2} = v_\xi \chi_2 + v_\mu
\]

To simplify the calculation that follows, we define

\[
\mathbf{V} = (v, v_\xi, v_\eta, v_\mu, v_{\xi\xi}, v_{\eta\eta}, v_{\mu\mu})^T, \\
\mathbf{Z}_k = (1, \xi_k, \eta_k, \mu_k, \frac{1}{2} \xi_k, \eta_k, \xi_k, \eta_k, \frac{1}{2} \xi_k \mu_k, \frac{1}{2} \xi_k \eta_k, \eta_k \mu_k, \eta_k \mu_k)^T, \\
\mathbf{W} = (-w, d_1, d_2, d_3, d_{11}, d_{12}, d_{21}, d_{22}, d_{31}, d_{32}, d_{33}, d_{33})^T.
\]

Then (4.5) becomes \( \nabla \cdot (\mathbf{D} \nabla v) - w v = \mathbf{W}^T \mathbf{V}, \) and (4.4) becomes \( v(x_k, y_k, z_k) = \mathbf{Z}_k^T \mathbf{V} + q_k h^3 \). Hence the LTE can be written as

\[
LTE = \mathbf{W}^T \mathbf{V} - \sum_{k \in K^+} q_k (\mathbf{Z}_k^T \mathbf{V} + q_k h^3) + C
\]
\begin{align}
&= (W - \sum_{k \in K^+} \gamma_k Z)^T V + C + h^3 \sum_{k \in K^+} \gamma_k q_k \\
&= a^T V + C + h^3 \sum_{k \in K^+} \gamma_k q_k,
\end{align}

(4.11)

where the vector $a$ is defined by $a = W - \sum_{k \in K^+} \gamma_k Z_k$ and its components are denoted $a_i, i = 1, \ldots, 10$.

The boundary condition provides several relations among elements of $V$. These relations for Neumann, Dirichlet and Robin boundary conditions are different. These relations will be used to eliminate some components of $V$ by expressing those components as a linear combination of the others as follows.

**4.1. Neumann boundary conditions.** Using the expressions in (4.7)-(4.9), the Neumann boundary condition and its derivative with respect to $\eta$ and $\mu$ can be written as

\begin{align}
(0, (D_{11})_\eta - \chi_{11} D_{12}, (D_{12})_\eta - \chi_{11} D_{22}, (D_{13})_\eta - \chi_{11} D_{23}, 0, D_{11}, D_{12}, 0, 0, D_{13})^T V &= g, \\
(0, (D_{11})_\mu - \chi_{22} D_{13}, (D_{12})_\mu - \chi_{22} D_{23}, (D_{13})_\mu - \chi_{22} D_{33}, 0, 0, D_{11}, D_{13}, D_{12})^T V &= g.
\end{align}

Therefore,

\begin{align}
v_\xi &= D_{11}^{-1}(g - D_{12} v_\eta - D_{13} v_\mu) \\
v_{\xi\eta} &= D_{11}^{-1}(g_\eta - ((D_{11})_\eta - \chi_{11} D_{12}) v_\xi - ((D_{12})_\eta - \chi_{11} D_{22}) v_\eta) \\
&\quad - ((D_{13})_\eta - \chi_{11} D_{23}) v_\mu - D_{12} v_{\eta\eta} - D_{13} v_{\eta\mu}) \\
v_{\xi\mu} &= D_{11}^{-1}(g_\mu - ((D_{11})_\mu - \chi_{22} D_{13}) v_\xi - ((D_{12})_\mu - \chi_{22} D_{23}) v_\eta) \\
&\quad - ((D_{13})_\mu - \chi_{22} D_{33}) v_\eta - D_{13} v_{\mu\mu} - D_{12} v_{\eta\mu}).
\end{align}

Substitution of (4.12)-(4.14) in LTE (4.11) gives

\begin{align}
\text{LTE} &= a_1 v + \{a_3 - a_2 D_{11}^{-1} D_{12} + D_{11}^{-2} D_{12}((D_{11})_\eta - \chi_{11} D_{12}) a_6 \\
&\quad - D_{11}^{-1}((D_{12})_\eta - \chi_{11} D_{22}) a_6 + D_{11}^{-2} D_{12}((D_{11})_\mu - \chi_{22} D_{13}) a_8 \\
&\quad - D_{11}^{-1}((D_{12})_\mu - \chi_{22} D_{23}) a_8 + \{a_4 - a_2 D_{11}^{-1} D_{13} \\
&\quad + D_{11}^{-2} D_{13}((D_{11})_\mu - \chi_{11} D_{12}) a_6 - D_{11}^{-1}((D_{13})_\mu - \chi_{11} D_{23}) a_6 \\
&\quad + D_{11}^{-2} D_{13}((D_{11})_\mu - \chi_{22} D_{13}) a_8 - D_{11}^{-1}((D_{13})_\mu - \chi_{22} D_{33}) a_8\} v_\mu \\
&\quad + a_5 v_{\xi\xi} + \{a_7 - D_{11}^{-1} D_{12} a_6\} v_{\eta\eta} + \{d_3 - D_{11}^{-1} D_{13} a_8\} v_{\eta\mu} \\
&\quad + \{a_9 + D_{11}^{-1} D_{13} a_6 - D_{11}^{-1} D_{12} a_8\} v_{\eta\mu} \\
&\quad + (C + D_{11}^{-1} g a_2 + D_{11}^{-1}(g_\eta - ((D_{11})_\eta - \chi_{11} D_{12}) g D_{11}^{-1}) a_6 \\
&\quad + D_{11}^{-1}(g_\mu - ((D_{11})_\mu - \chi_{22} D_{13}) g D_{11}^{-1}) a_8 + O(h)).
\end{align}

The coefficients $a_i$'s are functions of $\gamma_k$. To get the smallest LTE at $(x^*, y^*, z^*)$, for all $v$ satisfying the boundary condition, all the expressions in brackets must be zero. These are linear relations that must satisfied by the $\gamma_k$'s coefficients and $C$. Using the definition of $a_i$, these equations can be written as

\begin{align}
-w &= \sum_{k \in K^+} \gamma_k \\
D_{11}^2 d_2 - d_1 D_{11} D_{12} + 2d_{12} A + 2d_{13} B &= \sum_{k \in K^+} \gamma_k (D_{11}^2 \eta_k - D_{11} D_{12} \xi_k + \xi_k \eta_k A + \xi_k \mu_k B) \right)
\end{align}
\[
D_{11}^2 d_3 - d_1 D_{11} D_{13} + 2d_{12} C + 2d_{13} D = \sum_{k \in K^+} \gamma_k (D_{11}^2 \mu_k - D_{11} D_{13} \xi_k + \xi_k \eta_k C + \xi_k \mu_k D) \\
2d_{11} = \sum_{k \in K^+} \gamma_k \xi_k^2 \\
D_{11} d_{22} - 2d_{12} D_{12} = \sum_{k \in K^+} \gamma_k \left( \frac{1}{2} D_{11} \eta_k^2 - D_{12} \xi_k \eta_k \right) \\
D_{11} d_{33} - 2d_{13} D_{13} = \sum_{k \in K^+} \gamma_k \left( \frac{1}{2} D_{11} \mu_k^2 - D_{13} \xi_k \mu_k \right) \\
(4.15) 2(D_{11} d_{23} - D_{13} d_{12} - D_{12} d_{13}) = \sum_{k \in K^+} \gamma_k (D_{11} \eta_k \mu_k - D_{13} \xi_k \eta_k - D_{12} \xi_k \mu_k)
\]

where \( A = E + \chi_{11} (D_{11} D_{22} - D_{12}^2), B = F + \chi_{22} (D_{11} D_{23} - D_{12} D_{13}), C = G + \chi_{11} (D_{11} D_{23} - D_{12} D_{13}), D = H + \chi_{22} (D_{11} D_{33} - D_{12}^2), E = D_{12} (D_{11})_{\eta} - D_{11} (D_{12})_{\eta}, F = D_{12} (D_{11})_{\mu} - D_{11} (D_{12})_{\mu}, G = D_{13} (D_{11})_{\eta} - D_{11} (D_{13})_{\eta}, H = D_{13} (D_{11})_{\mu} - D_{11} (D_{13})_{\mu} \).

In the case of the isotropic Laplacian with Neumann boundary condition (4.15) reduces to the system of equations that Fogelson and Keener [4] found when they assigned zero weight for exterior neighbors.

The Gerschgorin stability condition imposes another restriction on the \( \gamma_k \) coefficients. As in the discussion for a regular interior grid point, the first equation of (4.15) and the Gerschgorin criterion for stability translates to \( \gamma_{k00} \leq 0 \) and \( \gamma_k \geq 0, k \in K^+ \setminus \{000\} \).

### 4.2. Dirichlet boundary conditions

Using the expressions in (4.8) the Dirichlet boundary condition and its first two derivatives with respect to \( \eta \) can be written as

\[
(1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0)^T \mathbf{v} = g, \\
(0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0)^T \mathbf{v} = g_\eta, \\
(0, \chi_{11}, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0)^T \mathbf{v} = g_{\eta\eta}, \\
(0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1)^T \mathbf{v} = g_{\eta\mu}.
\]

Therefore,

\[
v = g, \quad v_\eta = g_\eta, \quad v_\mu = g_\mu, \quad v_{\eta\eta} = g_{\eta\eta} - \chi_{11} v_\xi, \quad v_{\eta\mu} = g_{\eta\mu} - \chi_2 v_\xi, \quad v_{\eta\mu} = g_{\eta\mu}.
\]

(4.16)

Substitution of (4.16) in the expression (4.11) gives

\[
\text{LTE} = \{a_2 - \chi_{11} a_7 - \chi_{22} a_9 \} v_\eta + a_5 v_{\eta\eta} + a_6 v_{\eta\xi} + a_8 v_{\xi\mu} + (C + a_1 g + a_3 g_\eta + a_4 g_\mu + a_7 g_{\eta\eta} + a_9 g_{\eta\mu} + a_{10} g_{\eta\mu}) + O(h).
\]

As in the Neumann case, all the expressions in brackets must be zero (they generate linear relations to be satisfied by the coefficients \( \gamma_k \) and \( C \)). Using the definition of \( a_i \) the equations are

\[
2d_{11} = \sum_{k \in K^+} \gamma_k \xi_k^2 \\
2d_{12} = \sum_{k \in K^+} \gamma_k \xi_k \eta_k
\]
\[ 2d_{13} = \sum_{k \in K^+} \gamma_k \xi_k \mu_k \]

(4.17) \[ d_1 - \chi_{11} d_{22} - \chi_{22} d_{33} = \sum_{k \in K^+} \gamma_k \left( \xi_k - \frac{1}{2} \chi_{11} \eta_k^2 - \frac{1}{2} \chi_{22} \mu_k^2 \right). \]

The Gerschgorin stability condition imposes an additional restriction to the \( \gamma_k \) coefficients.

### 4.3. Robin boundary conditions \((\alpha v + \vec{u} \cdot D \nabla v = g)\).

Using the expressions in (4.6)-(4.8) the Robin boundary condition and its derivatives with respect to \( \eta \) and \( \mu \) can be written as

\[
(\alpha, D_{11}, D_{12}, D_{13}, 0, 0, 0, 0, 0, 0)^T \mathbf{V} = g, \\
(0, (D_{11})_\eta - \chi_{11} D_{12}, \alpha + (D_{12})_\eta - \chi_{11} D_{22}, (D_{13})_\eta - \chi_{11} D_{23}, 0, D_{11}, D_{12}, 0, 0, 0, D_{13})^T \mathbf{V} = g_\eta, \\
(0, (D_{11})_\mu - \chi_{22} D_{13}, (D_{12})_\mu - \chi_{22} D_{23}, \alpha + (D_{13})_\mu - \chi_{22} D_{33}, 0, 0, 0, D_{11}, D_{13}, D_{12})^T \mathbf{V} = g_\mu.
\]

Therefore,

\[
v = \alpha^{-1}(g - D_{11} v_\xi - D_{12} v_\eta - D_{13} v_\mu), \\
v_\xi = D_{11}^{-1}(g_\eta - ((D_{11})_\eta - \chi_{11} D_{12}) v_\xi - ((D_{12})_\eta - \chi_{11} D_{22} + \alpha) v_\eta - ((D_{13})_\eta - \chi_{11} D_{23}) v_\mu - D_{12} v_{\eta\eta} - D_{13} v_{\eta\mu}), \\
v_\mu = D_{11}^{-1}(g_\mu - ((D_{11})_\mu - \chi_{22} D_{13}) v_\xi - ((D_{12})_\mu - \chi_{22} D_{23}) v_\eta - ((D_{13})_\mu - \chi_{22} D_{33} + \alpha) v_\mu - D_{13} v_{\mu\mu} - D_{12} v_{\mu\eta}).
\]

(4.18) Substitution of (4.18) in (4.11) gives

\[
L T E = \{-\alpha^{-1}D_{11}a_1 + a_2 + D_{11}^{-1}(\chi_{11} D_{12} - (D_{11})_\eta) a_0 \\
+ D_{11}^{-1}(\chi_{12} D_{13} - (D_{11})_\mu) a_8 \} v_\xi + \{-\alpha^{-1}D_{12}a_1 + a_3 \\
+ D_{11}^{-1}(\chi_{11} D_{22} - (D_{12})_\eta - \alpha) a_6 + D_{11}^{-1}(\chi_{22} D_{23} - (D_{12})_\mu) a_8 \} v_\eta \\
+ \{-\alpha^{-1}D_{13}a_1 + a_4 + D_{11}^{-1}(\chi_{11} D_{23} - (D_{13})_\eta) a_0 \\
+ D_{11}^{-1}(\chi_{22} D_{33} - (D_{13})_\mu - \alpha) a_6 \} v_\mu + a_4 v_\xi \xi + \{-D_{11}^{-1}D_{12} a_6 + a_7 \} v_{\eta\eta} \\
+ \{-D_{11}^{-1}D_{13} a_7 + a_9 \} v_{\mu\mu} + \{a_{10} - D_{11}^{-1}D_{13} a_6 - D_{11}^{-1}D_{12} a_8 \} v_{\eta\mu} \\
+ (C + \alpha^{-1}g a_1 + D_{11}^{-1}g_\eta a_6 + D_{11}^{-1}g_\mu a_8) + O(h).
\]

If all the expressions in brackets are zero, they generate linear relations to be satisfied by the \( \gamma_k \)'s coefficients and \( C \). Using the definition of \( a_i \) the equations can be written as

\[
\alpha^{-1}D_{11}^2 w + D_{11} d_1 + 2d_{12} I + 2d_{13} J = \sum_{k \in K^+} \gamma_k (-D_{11} + D_{11} \xi_k + I \xi_k \eta_k + J \xi_k \mu_k) \\
\alpha^{-1}D_{11} D_{12} w + D_{11} d_2 + 2d_{12} K + 2d_{13} L = \sum_{k \in K^+} \gamma_k (-D_{11} + D_{11} \eta_k + K \xi_k \eta_k + L \xi_k \mu_k) \\
\alpha^{-1}D_{11} D_{13} w + D_{11} d_3 + 2d_{12} M + 2d_{13} N = \sum_{k \in K^+} \gamma_k (-D_{11} + D_{11} \mu_k + M \xi_k \eta_k + N \xi_k \mu_k) \\
2d_{11} = \sum_{k \in K^+} \gamma_k \xi_k^2 \]
\[
D_{11}d_{22} - 2d_{12}D_{12} = \sum_{k \in K^+} \gamma_k \left( \frac{1}{2} D_{11} \eta_k^2 - D_{12} \xi_k \eta_k \right)
\]
\[
D_{11}d_{33} - 2d_{13}D_{13} = \sum_{k \in K^+} \gamma_k \left( \frac{1}{2} D_{11} \mu_k^2 - D_{13} \xi_k \mu_k \right)
\]
(4.19) \[ 2(D_{11}d_{23} - D_{13}d_{12} - D_{12}d_{13}) = \sum_{k \in K^+} \gamma_k (D_{11} \eta_k \mu_k - D_{13} \xi_k \eta_k - D_{12} \xi_k \mu_k), \]

where \( I = \chi_{11}D_{12} - (D_{11})_{\eta}, J = \chi_{22}D_{13} - (D_{11})_{\mu}, K = \chi_{11}D_{22} - (D_{12})_{\eta} - \alpha, L = \chi_{22}D_{23} - (D_{12})_{\mu}, M = \chi_{11}D_{23} - (D_{13})_{\eta}, N = \chi_{22}D_{33} - (D_{13})_{\mu} - \alpha. \) The Gerschgorin stability condition imposes an additional restriction to the \( \gamma_k \) coefficients.

It can be shown that when \( \alpha = 0 \) (4.19) is equivalent to (4.15).

5. Existence of first-order schemes for the Neumann, Dirichlet and Robin cases. It is not evident that a first-order scheme (not necessarily w.d.d.) is always available for an irregular grid point when using only interior grid points. In this section we discuss the possibility of finding a first-order scheme for Neumann, Dirichlet and Robin boundary conditions.

Using the change of variables (4.3) it is possible to calculate the \((\xi_k, \eta_k, \mu_k)\) coordinates. In particular, from Figure 4.1, \( \xi_{000} = -d, \eta_{000} = 0 \) and \( \mu_{000} = 0 \), where \( d \) is the distance between the irregular grid point \((x, y, z)\) and its closest boundary point \((x', y', z')\). If we define \( \xi_k = \xi_{000} + \Delta \xi_k, \eta_k = \eta_{000} + \Delta \eta_k = \Delta \eta_k \) and \( \mu_k = \mu_{000} + \Delta \mu_k = \Delta \mu_k \) it is easier to calculate those values.

Therefore

\[
\sum_{K} \gamma_k \xi_k^2 = d^2 \sum_{K} \gamma_k - 2d \sum_{K} \gamma_k \Delta \xi_k + \sum_{K} \gamma_k (\Delta \xi_k)^2
\]
\[
\sum_{K} \gamma_k \eta_k^2 = \sum_{K} \gamma_k (\Delta \eta_k)^2
\]
\[
\sum_{K} \gamma_k \mu_k^2 = \sum_{K} \gamma_k (\Delta \mu_k)^2
\]
\[
\sum_{K} \gamma_k \xi_k \eta_k = -d \sum_{K} \gamma_k \Delta \eta_k + \sum_{K} \gamma_k (\Delta \xi_k)(\Delta \eta_k)
\]
\[
\sum_{K} \gamma_k \xi_k \mu_k = -d \sum_{K} \gamma_k \Delta \mu_k + \sum_{K} \gamma_k (\Delta \xi_k)(\Delta \mu_k)
\]
\[
\sum_{K} \gamma_k \eta_k \mu_k = \sum_{K} \gamma_k (\Delta \eta_k)(\Delta \mu_k).
\]

Since

\[
\begin{bmatrix}
\xi_k - \xi_{000} \\
\eta_k - \eta_{000} \\
\mu_k - \mu_{000}
\end{bmatrix} = \begin{bmatrix}
\cos \theta \sin \phi & -\sin \theta & \cos \theta \cos \phi \\
\sin \theta \sin \phi & \cos \theta & \sin \theta \cos \phi \\
\cos \phi & 0 & -\sin \phi
\end{bmatrix} \begin{bmatrix}
x_k - x \\
y_k - y \\
z_k - z
\end{bmatrix},
\]

where \( x_k, y_k \) and \( z_k \) are the Cartesian coordinates of the neighbors of \((x, y, z)\), then

(5.1) \[ \Delta \xi_k = r \cos \theta \sin \phi - s \sin \theta + t \cos \theta \sin \phi, \]
(5.2) \[ \Delta \eta_k = r \sin \theta \sin \phi + s \cos \theta + t \sin \theta \cos \phi, \]
(5.3) \[ \Delta \mu_k = r \cos \phi - t \sin \phi, \]

where the index \( k \) denotes the index \( rst, r, s, t = -1, 0, 1. \)
Substituting (5.1)-(5.3) in (5.1) one finds that

\[
\begin{align*}
\sum K \gamma_k \Delta \xi_k &= \cos \theta \sin \phi \Gamma_1 - \sin \theta \Gamma_2 + \cos \theta \cos \phi \Gamma_3 \\
\sum K \gamma_k \Delta \eta_k &= \sin \theta \sin \phi \Gamma_1 + \cos \theta \Gamma_2 + \sin \theta \cos \phi \Gamma_3 \\
\sum K \gamma_k \Delta \mu_k &= \cos \phi \Gamma_1 - \sin \phi \Gamma_3 \\
\sum K \gamma_k (\Delta \xi_k)^2 &= \cos^2 \theta \sin^2 \phi \Gamma_4 + \sin^2 \theta \Gamma_5 + \cos^2 \theta \cos^2 \phi \Gamma_6 - \sin 2\theta \sin \phi \Gamma_7 - \sin 2\theta \\
&+ \cos \phi \Gamma_8 + \cos^2 \theta \sin 2\phi \Gamma_9 \\
\sum K \gamma_k (\Delta \eta_k)^2 &= \sin^2 \theta \sin^2 \phi \Gamma_4 + \cos^2 \theta \Gamma_5 + \sin^2 \theta \cos^2 \phi \Gamma_6 + \sin 2\theta \sin \phi \Gamma_7 + \sin 2\theta \\
&+ \cos \phi \Gamma_8 + \sin^2 \theta \sin 2\phi \Gamma_9 \\
\sum K \gamma_k (\Delta \mu_k)^2 &= \cos^2 \theta \Gamma_4 + \sin^2 \theta \Gamma_6 - \sin 2\phi \Gamma_9 \\
\sum K \gamma_k \Delta \xi_k \Delta \eta_k &= \frac{1}{2} \sin 2\theta \sin^2 \phi \Gamma_4 - \frac{1}{2} \sin 2\theta \Gamma_5 + \frac{1}{2} \sin 2\theta \cos^2 \phi \Gamma_6 + \cos \theta \sin \phi \Gamma_7 \\
&+ \cos 2\theta \cos \phi \Gamma_8 + \frac{1}{2} \sin 2\theta \sin 2\phi \Gamma_9 \\
\sum K \gamma_k \Delta \xi_k \Delta \mu_k &= - \sin \theta \cos \phi \Gamma_7 + \sin \theta \sin \phi \Gamma_8 + \cos \theta \cos 2\phi \Gamma_9 + \frac{1}{2} \cos \theta \sin 2\phi \Gamma_{10} \\
\sum K \gamma_k \Delta \eta_k \Delta \mu_k &= \cos \theta \cos \phi \Gamma_7 - \cos \theta \sin \phi \Gamma_8 + \sin \theta \cos 2\phi \Gamma_9 + \frac{1}{2} \sin \theta \sin 2\phi \Gamma_{10},
\end{align*}
\]

where \( \Gamma_1 = \gamma_{11} - \gamma_{-11}, \Gamma_2 = \gamma_{1.} - \gamma_{-1.}, \Gamma_3 = \gamma_{.1} - \gamma_{-.1}, \Gamma_4 = \gamma_{11} + \gamma_{-11}, \Gamma_5 = \gamma_{1.} + \gamma_{-1.}, \Gamma_6 = \gamma_{1.} + \gamma_{-1.}, \Gamma_7 = \gamma_{1.-1} + \gamma_{-1.1}, \Gamma_8 = \gamma_{1.-1} + \gamma_{-1.1}, \Gamma_9 = \gamma_{1.-1} + \gamma_{1.1} - \gamma_{-1.-1}, \Gamma_{10} = \gamma_{1.-1} + \gamma_{1.1} - \gamma_{-1.-1}. \)

Using (5.4) the Neumann system (4.15), can be written as \( M \gamma = \rho \), where \( \gamma_k \) is the column vector of \( \gamma_k \)'s, \( \rho \) is the column vector of quantities independent of \( \gamma_k \) and \( M \) is a \( 6 \times 26 \) (first equation in (4.15) has been used to reduce the number of coefficients \( \gamma_k \) by 1) matrix which depends on \( D \), curvature, distance from the boundary point to the irregular grid point and the angles \( \theta \) and \( \phi \).

To show the existence of a first-order scheme it is only necessary to find a \( 6 \times 6 \) submatrix of \( M \) (corresponding to interior grid points) whose determinant is different from zero. So, in general, it is possible to find a first-order scheme for an irregular grid point that has as many as 20 exterior neighbors. Stability considerations add sign restrictions to the \( \gamma_k \)'s, as in the 2D case [1].

A similar argument can be used to show that in the Dirichlet case, it is possible in general to find first-order schemes for an irregular grid point with as many as 23 exterior immediate neighbors while in the Robin case, the number of allowed exterior neighbors is reduced to 20.

**5.1. Heuristic arguments for the programming approach for irregular points.** We have seen that with Neumann boundary conditions the Gerschgorin criterion and the first equation of (4.15) imply sign restrictions on the \( \gamma_k \) coeffi-
cents. Hence, for Neumann boundary conditions we can take any linear objective function \( f \) (e.g., \( \min \gamma_{\text{000}} \)) and solve the LPP defined by \( f \) subject to (4.15) and \( \gamma_{\text{000}} \leq 0, \gamma_k \geq 0, k \in K^+ \).

However for Dirichlet and Robin boundary conditions stability must be enforced using the Gerschgorin condition \( |\gamma_{\text{000}}| \geq \sum_{k \in K^+ \setminus \{000\}} |\gamma_k| \) because the systems (4.17) and (4.19) do not contain an equation in terms of only \( \gamma_k \) to incorporate the Gerschgorin criterion like the first equation in (4.15).

For Dirichlet and Robin boundary conditions, we use \( \max |\gamma_{\text{000}}| - \sum_{k \in K^+ \setminus \{000\}} |\gamma_k| \) as the objective function to enforce the Gerschgorin stability criterion (when possible).

Even though the restrictions (4.17) and (4.19) for Dirichlet and Robin boundary conditions are linear, the Gerschgorin criterion \( |\gamma_{\text{000}}| \geq \sum_{k \in K^+ \setminus \{000\}} |\gamma_k| \) is not. However, linear programming techniques can be used to find an optimum solution inside the feasibility region determined by the first-order LTE linear restrictions and the nonlinear Gerschgorin criterion (see [3]).

Sometimes the feasibility region of any of the PP derived for Neumann, Dirichlet or Robin boundary conditions is unbounded and the optimum is at infinity. To achieve a finite solution an appropriate bound is needed for \( |\gamma_k|, k \in K^+ \). If the introduced bound is too large then the discretization matrix will have rows with large coefficients when the feasibility region is unbounded and possibly rows with order 1 coefficients when the row is associated to a regular point. This will give an undesirably large condition number to the full linear system.

A practical strategy is to begin by imposing a modest bound such as \( |\gamma_k| < \frac{1}{h^2}, k \in K^+ \). For this bound, the PP might have no solution but this could be remedied by multiplying the upper bound by some positive constant and trying again, thereby iterating until a first-order Gerschgorin stable scheme is found or the upper bound exceeds an a priori established limit.

For Dirichlet and Robin boundary conditions, the existence of a solution to the PP will follow from finding a submatrix of \( M \) with nonzero determinant. For the Neumann case, the feasibility region could be the empty set. In that case, one can remove the sign restriction on each \( \gamma_k \) and try to solve the LPP \( \max \gamma_{\text{000}} \) subject to (4.15) (to guarantee at least a first-order scheme). Again the feasibility region could be unbounded and successive increasing upper bounds for the variables \( \gamma_k \) might be needed. The existence of a solution to the LPP will follow from finding a \( 3 \times 3 \) submatrix of \( M \) with nonzero determinant. In our computations, we have never found a case of an irregular point that does not have at least a first-order scheme.

6. Numerical Results for the Anisotropic Laplacian. It has been shown that for an isotropic Laplacian our method reproduces the 7-point stencil for a regular point even though our method is only guaranteed to be first-order. To test the actual accuracy of this method, we first consider a problem for which the exact solution is known. We consider the Laplace equation in \( \Omega \) the domain between two concentric spheres of radii \( \frac{1}{2} \) and 1,

\[
\Delta \nu(x, y, z) = 0, \quad (x, y, z) \in \Omega,
\]

\[
\frac{\partial \nu}{\partial n}(1, \theta, \phi) = \cos(\theta) \sin(\phi), \quad \theta \in [0, 2\pi), \phi \in [0, \pi],
\]

\[
\frac{\partial \nu}{\partial n}(\frac{1}{2}, \theta, \phi) = 0, \quad \theta \in [0, 2\pi), \phi \in [0, \pi].
\]
with exact solution given by \( v(x, y, z) = \frac{x}{14} \left( 16 + \frac{1}{(x^2 + y^2 + z^2)^2} \right) \). In Figure 6.1 a log-log plot of the absolute error \( E \) of the numerical solution vs \( h \) is shown. The solid straight lines are the locus of the points \((h, E)\) such that \( \log E = 2 \log h + \log 5 \) and \( \log E = 2 \log h \) respectively. The slope of both lines is two. The circles are the coordinates \((\log h, \log E)\) for the numerical solutions of the isotropic Laplace equation with the mesh size \( h \) varying from 0.04 to 0.13. \( K_1 \) stencils have been used in these computations (which for regular points becomes the 7-point stencil). As expected we do not obtain a straight line because the set of enclosed grid points changes for different values of \( h \). To illustrate this method in an anisotropic case, we solve the anisotropic Laplace’s equation on an irregular domain with inhomogeneous Neumann boundary condition. Let \( \Omega \) be the same domain as in the isotropic case and solve

\[
-\nabla \cdot (\mathbf{D}(x, y, z) \nabla v) = 0, \quad (x, y, z) \in \Omega,
\]

\[
\mathbf{n} \cdot \mathbf{D}(1, \theta, \phi) \nabla v = \cos \theta \sin \phi, \quad \theta \in [0, 2\pi), \phi \in [0, \pi],
\]

\[
\mathbf{n} \cdot \mathbf{D}(\frac{1}{2}, \theta, \phi) \nabla v = 0, \quad \theta \in [0, 2\pi), \phi \in [0, \pi],
\]

where the tensor anisotropy \( \mathbf{D} \) given by

\[
(6.1) \quad \left( \begin{array}{ccc}
D_{11} & D_{12} & D_{13} \\
D_{12} & D_{22} & D_{23} \\
D_{13} & D_{23} & D_{33}
\end{array} \right) = \mathbf{R} \left( \begin{array}{ccc}
1 & 0 & 0 \\
0 & \lambda & 0 \\
0 & 0 & \lambda
\end{array} \right) \mathbf{R}^T,
\]

where \( \theta \) is the polar angle, \( \phi \) is the azimuthal angle and the rotation matrix \( \mathbf{R} \) is given by

\[
\left( \begin{array}{ccc}
\cos \theta \sin \phi & -\sin \theta & \cos \theta \cos \phi \\
\sin \theta \sin \phi & \cos \theta & \sin \theta \cos \phi \\
\cos \phi & 0 & -\sin \phi
\end{array} \right).
\]

The parameter \( \lambda \) measures the relative strength of the anisotropy in the polar and azimuthal directions scaled by the strength of the anisotropy in the radial direction.
Table 6.1  
Minimum real part of eigenvalues of the discretization matrix for several values of $\lambda$ and $h$.

<table>
<thead>
<tr>
<th>$\lambda$</th>
<th>$h = 0.10$</th>
<th>$h = 0.09$</th>
<th>$h = 0.08$</th>
<th>$h = 0.07$</th>
<th>$h = 0.06$</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>1.4096347</td>
<td>1.3395915</td>
<td>1.2927989</td>
<td>1.0467257</td>
<td>0.64804488</td>
</tr>
<tr>
<td>10</td>
<td>1.2761953</td>
<td>1.0948549</td>
<td>1.0224153</td>
<td>0.8875329</td>
<td>0.54919489</td>
</tr>
<tr>
<td>9</td>
<td>1.1514558</td>
<td>0.9493276</td>
<td>0.9053697</td>
<td>0.7524504</td>
<td>0.5022455</td>
</tr>
<tr>
<td>8</td>
<td>0.9720919</td>
<td>0.8246562</td>
<td>0.8497551</td>
<td>0.6702953</td>
<td>0.4923617</td>
</tr>
<tr>
<td>7</td>
<td>0.782107</td>
<td>0.6680941</td>
<td>0.6566986</td>
<td>0.5561247</td>
<td>0.45713473</td>
</tr>
<tr>
<td>6</td>
<td>0.529208</td>
<td>0.4757418</td>
<td>0.4831738</td>
<td>0.3830897</td>
<td>0.24561082</td>
</tr>
<tr>
<td>5</td>
<td>0.4243777</td>
<td>0.4043131</td>
<td>0.3521395</td>
<td>0.3327788</td>
<td>0.17857939</td>
</tr>
</tbody>
</table>

The exact solution of this problem can be found using separation of variables in spherical coordinates. The exact solution is given by $u = x(v(x) - w(x))/v(x))/(\alpha - \beta w(x))$, where $v(x) = (x^2 + y^2 + z^2)^{\frac{1-\alpha}{2}}$, $w(x) = \frac{\alpha}{\beta} (\frac{1}{2})^{\alpha-\beta}$, $\alpha = \frac{-1+\sqrt{1+8\lambda}}{2}$ and $\beta = \frac{-1-\sqrt{1+8\lambda}}{2}$.

For the numerical discretization, the objective function for both regular and irregular grid points was taken to be $\min c_{000}$. A positive minimum real part of the eigenvalues of the discretized linear system indicates that the spectrum of the linear system lies in the right half plane. In particular it implies that the linear system is positive definite.

As one might expect, for a fixed value of $h$, the minimum real part of the eigenvalues of the discretization matrix decreases almost monotonically. This behavior can be seen in Table 6.1. There, the minimum real part of the eigenvalues of the discretization matrix is shown for $0.06 \leq h \leq 0.10$ and $5 \leq \lambda \leq 11$. For a fixed value of $\lambda$, the minimum real part of the eigenvalues of the discretization matrix does not have a definite pattern since the set of grid points included in the interior of the domain varies considerably with $h$.

The lack of monotonicity of the minimum real part of the eigenvalues of the discretization matrix is related to the way bounds were chosen to solve both the LPP associated with first-order non-w.d.d. schemes for regular grid points and the LPP’s associated with irregular grid points (w.d.d. and non-w.d.d. schemes). There the initial bound was $\frac{1}{\sqrt{\lambda}}$. If any LPP with some bound did not have a solution, the bound was incremented by a factor of 2 and the LPP solved again until an optimum solution was found or until the maximum bound of $10^7$ was reached.

When $\lambda$ gets closer to zero, the first term of the exact solution blows up. Therefore, the accuracy of the numerical solution is also expected to deteriorate as $\lambda$ tends to zero.

Figures 6.2, 6.3 and 6.4 show how the absolute error and minimum real part of eigenvalues behave as the parameter $\lambda$ increases for different values of the mesh size $h$. Here, we have taken $\min c_{000}$ as the objective function for both regular and irregular grid points and we have used $K_1$ stencils. In Figure 6.2, the top part shows how the absolute error changes with the parameter $\lambda$ which varies from 0 to 100 and the bottom part is a plot of how the minimum real part of the eigenvalues behaves as $\lambda$ changes from 0 to 100. In both graphs $h = 0.12$. 

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Fig. 6.2. Absolute error (infinity norm) and minimum real part of eigenvalues of the discretization matrix for $h = 0.12$. The parameter $\lambda$ varies from 0.8 and 50 for accuracy and stability.

We observe a similar behavior for the absolute error and the minimum real part of the eigenvalues of the discretization matrix as in the 2D case. The best accuracy is obtained when $\lambda = 1$. The accuracy degrades as $\lambda$ moves from 1. When $\lambda < 1$, the accuracy deteriorates as $\lambda$ gets closer to zero. When $\lambda > 1$, the accuracy degrades until $\lambda$ gets closer to 28. When $\lambda$ is greater than 28 the accuracy improves substantially. However, when $\lambda > 250$ the linear programming algorithm cannot solve some of the optimization problems. The same behavior as in the case for $h = 0.12$ with shifted values of $\lambda$ can be seen in Figures 6.3 and 6.4 where the mesh size is respectively $h = 0.08$ and $h = 0.04$.

The implementation of this discretization method has been done in MATLAB. Linear programming problems were solved using the MATLAB Optimization Toolbox interior point linprog routine. Most of the CPU time was spent solving the linear programming problems that find the weights of the 27-point stencil. However, the CPU time utilized in the discretization can be reduced significatively when the anisotropy matrix is locally constant. In that situation (as in [2]), it is possible not only to show that the discretization is second order accurate but also to find formulas for the optimum solution of the linear programming problems associated to regular grid points when the condition of the theorem 2.1 holds. If the anisotropy matrix does not verify the condition of theorem 2.1 at some regular grid point, then a finite difference discretization of the anisotropic Laplacian can be used. In this way, all linear programming methods for regular grid points can be avoided. The cost of the implementation of this approach for regular grid points is the same as the discretization cost using finite differences. Finding the solution of an LPP (for irregular grid points) is more expensive than using the finite difference boundary approximation. However, this additional cost will not be of major significance since the number of irregular points is of lower order than the order of the number of regular points.

BiCGStab (Bi Conjugate Gradient stable) has been used to solve the discretized linear system.
Fig. 6.3. Absolute error (infinity norm) and minimum real part of eigenvalues of the discretization matrix for $h = 0.08$. The parameter $\lambda$ varies from 0.8 and 25 for accuracy and stability.

Fig. 6.4. Absolute error (infinity norm) and minimum real part of eigenvalues of the discretization matrix for $h = 0.04$. The parameter $\lambda$ varies from 0.8 and 25 for accuracy and stability.

7. Conclusions. The final result of this paper is a first-order stable Cartesian discretization anisotropic, elliptic boundary value problems on irregular bounded domains in 3D, where the resultant linear system is banded and nonsymmetric nonnegative definite.

Finite Difference Methods are accurate but not always stable when applied to the problem (1.1)-(1.2). Our method is stable for a wide range of anisotropic matrices (even for small or large ratios of the eigenvalues corresponding to the anisotropy tensor
Our discretization method does as much as is possible to guarantee nonnegative definiteness of the discretization matrix. In contrast, finite difference schemes are derived in general to guarantee only a certain order of the LTE. Unfortunately, there are circumstances where it is not possible to find a w.d.d. scheme. For instance, if the domain is strongly anisotropic and the direction of anisotropy is not aligned with the Cartesian coordinates at some irregular point, then the linear programming approach might have no solution. Nevertheless, any finite difference method that does not preserve some conservation law will have problems in this situation. In addition, as mentioned in the numerical section, when the anisotropy ratio is too large or too small (for instance, \(\lambda > 250\) for the anisotropic Laplacian) the linear programming algorithm cannot solve some of the optimization problems.

We are currently working to obtain higher order accuracy for anisotropic elliptic boundary value problems for some specific applications.

REFERENCES