Journal of Mathematics Research; Vol. 9, No. 3; June 2017
ISSN 1916-9795 E-ISSN 1916-9809
Published by Canadian Center of Science and Education

Symmetric Boundary Condition for Laplacian on Net of Regular Hexagons

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Received: April 8, 2017 Accepted: May 18, 2017 Online Published: May 25, 2017

doi:10.5539/jmr.v9n3p46 URL: https://doi.org/10.5539/jmr.v9n3p46

Abstract

Hexagonal grid methods are found useful in many research works, including numerical modeling in spherical coordinates, in atmospheric and ocean models, and simulation of electrical wave phenomena in cardiac tissues. Almost all of these used standard Laplacian and mostly on one configuration of regular hexagons. In this work, discrete symmetric boundary condition and energy product for anisotropic Laplacian are investigated firstly on general net of regular hexagons, and then generalized to its most extent in two- or three-dimensional cell-center finite difference applications up to the usage of symmetric stencil in central differences. For analysis of Laplacian related applications, this provides with an approach in addition to the M-matrix theory, series method, functional interpolations and Fourier vectors.

Keywords: Bilinear form, Cell-center finite difference, Discrete Laplacian, Hexagonal grid method.

1. Introduction

Hexagonal (Hex) grid methods are of interest in many research studies: (Pickering,1986) on direct method, (Makarov, Mararov & Moskal'kov, 1993) giving a formula without proof, (Bystrytskyi & Mosklkov, 2001) on seven-point method on rectangular grid with explicit form of eigenpairs, (Zhou & Fulton, 2009) with periodic boundary condition (BC), (Heikes & Randall, 1995, part I,II) and (Heikes, Randall & Konor, 2013) on numerical modeling in spherical coordinates, (van Eck & Kors, 2005) on action potential in heart modeling via algebraic method without using diffusion in form of differential equation, (Nickovic,Gavrilov & Tosic, 2002) showing advantages of Hex grids over commonly used square grids for use in atmospheric and ocean models. In the article by (Lee,Tien,Luo and Luk,2014), Hex grid finite difference (FD) methods are derived in a finite volume (FV) approach involving standard Laplacian, and used in the simulation of electrical wave phenomena propagated in two-dimensional reversed-C type cardiac tissues, exhibiting both linear and spiral waves more efficiently than similar computation carried on rectangular FVs. We note these cited works all used standard Laplacian and mostly on one configuration of regular hexagons.

In two-dimensional applications of configurations consisting of (subset of) Cartesian type regular hexagons, we denote the radius of hexagons by r, the height by $h(=\frac{\sqrt{3}}{2}r)$, and the center-to-center distance by $d(=2h)$. Near a typical center node, $P_0=(x_0,y_0)$, the six neighbor (center) nodes are

$$P_j=(x_j,y_j)=(x_0,y_0)+d(\cos\xi_j,\sin\xi_j),\quad \xi_j=\varphi+\frac{j\pi}{3}+\frac{\pi}{6},\quad 1\le j\le 6. \tag{1}$$

Here the *phase angle*, φ, is the configurarion parameter. Two particular instances are called type I ($\varphi=0$) and type II ($\varphi=\frac{-\pi}{6}$) for convenience. Hexagon centers in lattices of these two types are indexed as for an orthogonal Cartesian mesh as shown in Table 1, while the geometry and neighborhood of a general Hex FV shown in Table 2. Indexing rules are illustrated in Figs. 1, 2, 3 and 4.

For convenience, we abuse the notations and denote FV centers in a neighborhood (Figs. 3 and 4) by an *ordered list*,

$$\begin{aligned}\text{Type I}:\ \{P_j\}_{j=0}^{6}&=\{P,\ P_{N},\ P_{NW},\ P_{SW},\ P_{S},\ P_{SE},\ P_{NE}\},\\ \text{Type II}:\ \{P_j\}_{j=0}^{6}&=\{P,\ P_{NE},\ P_{NW},\ P_{W},\ P_{SW},\ P_{NW},\ P_{E}\}.\end{aligned}\tag{2}$$

We note for applications that a two-dimensional irregular domain may be approximated by a sequence of (not necessarily Cartesian) nets of hexagons. Actually, our work in numerical modeling of ECG depends on this (Algorithm 1 in (Lee,Tien,Luo & Luk, 2014)).

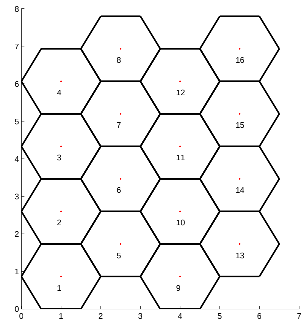

Figure 1. Lattice of type I regular hexagons in natural order by columns

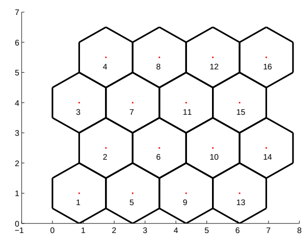

Figure 2. Lattice of type II regular hexagons in natural order by columns

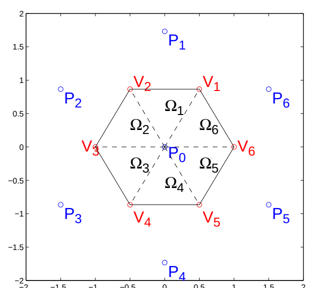

Figure 3. Type I regular hexagonal FV neighborhood

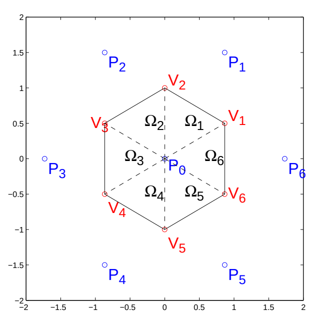

Figure 4. Type II regular hexagonal FV neighborhood

Table 1. Lattices of type I and II regular hexagons

Phase angle	Type I, $\varphi = 0$		Type II, $\varphi = -\pi/6$	
Center point	i^{even}	i^{odd}	j^{even}	j^{odd}
$cx(i, j)$	$(1.5i - 0.5)r$		$2ih$	$(2i - 1)h$
$cy(i, j)$	$2jh$	$(2j - 1)h$	$(1.5j - 0.5)r$	

Table 2. Local geometry at a regular hexagon : six vertices and six neighbor centers

Phase angle	$\varphi \in \mathbb{R}$
Vertices	$V_k = (vx(*, k), vy(*, k))\,,\quad k = 1, 2, \cdots, 6.$
$vx(*, k)$	$cx(*) + r\cos(\varphi + \frac{k\pi}{3})$
$vy(*, k)$	$cy(*) + r\sin(\varphi + \frac{k\pi}{3})$
Neighbor centers	$P_k = V_k + V_{k+1} - P_0, \qquad k = 1, 2, \cdots, 6.$

Concerning the negative anisotropic Laplacian

$$-Lap\,(f) := -D_1 f_{xx} - D_2 f_{yy} \tag{3}$$

with positive constant diffusivities D_1 and D_2, we observe the following.

Lemma 1 (Reflection principle for anisotropic Laplacian.) The two configurations, type I and II regular hexagons centered at the origin together with the anisotropic Laplacian, are convertible from each other by applying reflection with respect to the main diagonal in the xy-plane, and therefore interchanging the two symbol lists (Figs. 3 and 4)

$$\left\{x, y, D_1, D_2, N, NW, SW, S, SE, NE\right\} \qquad \text{and} \qquad \left\{y, x, D_2, D_1, E, SE, SW, W, NW, NE\right\}.$$

With a general phase angle, the reflection interchanges

$$\left\{\,(\varphi),\ (P_j)_{j=1}^{6}\,\right\} \qquad \text{and} \qquad \left\{\,(\frac{\pi}{2} - \varphi),\ (P_{6-j\%6})_{j=1}^{6}\,\right\}.$$

Here $(P_{6-j\%6})_{j=1}^{6}$ refers to the outcome of the order-2 permutation $\binom{1\,2\,3\,4\,5\,6}{5\,4\,3\,2\,1\,6}$ of the indices.

The focus in subsequent discussion is on net of type I hexagons.

We note that spectral analysis of iterative methods solving the discrete anisotropic Laplacian on a net of hexagons seems not as easy as the analysis on square grids (Suli,1993) and (Karaa & Zhang, 2003), since finite trigonometric series is incomplete for the error analysis (even) on a single regular hexagon (McCartin,2002,2003).

The analysis of solving Laplacian related applications on net of (regular) hexagons may be based on series method (Lee, Tien, Luo & Luk, 2014), M-matrix theory (Lee, Tien, Luo & Luk, 2014) and (Lee, August 2017), functional interpolation (Lee, 2015), or Fourier vectors (Lee, August 2017). The current work discusses the Laplacian through discrete *symmetric boundary condition* (Sections 3 and 4).

In the *world* of differential equations, for example (Strauss, 2008), the term *symmetric boundary condition* is defined so as to make a (real) operator *symmetric*. On the other hand, as a practice for long time in the engineering literatures, the phrase *symmetric boundary condition* may mean, differently, that the computational domain is reduced by halving and the numerical BC on the virtual separating edge is of homogeneous Neumann type : (Kim & Huh, 2000), (Xu & Soares, 2013), and (Pal, Lan, Li, Hirleman & Ma, 2015). Same as such with spherical (reflexive) symmetric boundary condition in similar situations.

We are with the operator-theoretic view (Eqs. (5, 20 and 24) in current work).

As for the remaining sections, symmetric boundary condition for the Laplacian is introduced for smooth scalar functions in Section 2, with detailed discussion in Section 3. The theory is generalized and simplified in Section 4 with simple assumption and argument. Discussed in Section 5 are many examples of symmetric boundary condition for Laplacian, including non-product type pairs (generators) for an invariant subspace of some operator on type I Hex grid.

2. Function Symmetric Boundary Condition for Laplacian

We focus here on standard Laplacian (Eq. (3) with $D_1 = D_2 = 1$) and recall the Green's first and second identities,

$$\begin{aligned}
-\iint_\Omega f(x,y)\nabla^2 g(x,y)\,dxdy &= \iint_\Omega \nabla f(x,y)\nabla g(x,y)\,dxdy - \int_{\partial\Omega} f\frac{\partial g}{\partial\vec{n}}\,d\gamma(t)\\
-\iint_\Omega g(x,y)\nabla^2 f(x,y)\,dxdy &= \iint_\Omega \nabla f(x,y)\nabla g(x,y)\,dxdy - \int_{\partial\Omega} g\frac{\partial f}{\partial\vec{n}}\,d\gamma(t)\\
\iint_\Omega (f\nabla^2 g - g\nabla^2 f)\,dxdy &= \int_{\partial\Omega} \Big(f\frac{\partial g}{\partial\vec{n}} - g\frac{\partial f}{\partial\vec{n}}\Big)d\gamma \qquad (4)
\end{aligned}$$

in which Ω is a domain with $\partial\Omega$ its piecewise smooth boundary such that these formulas are valid. The outward normal on the boundary is denoted by $\partial\vec{n}$.

Definition 1. A pair of (distinct) functions $f, g \in C^2(\overline{\Omega})$ satisfies symmetric boundary condition (for the Laplacian), if

$$\int_{\partial\Omega} \Big(f\frac{\partial g}{\partial\vec{n}} - g\frac{\partial f}{\partial\vec{n}}\Big)\,d\gamma = 0, \qquad (5)$$

so that the Laplacian is symmetric on f and g, $\langle f, \nabla^2 g\rangle = \langle \nabla^2 f, g\rangle$.

If every pair in a family of functions satisfies the symmetric boundary condition, we say the Laplacian is symmetric on the family.

Notice that, with or without satisfication of the symmetric boundary condition, we may consider symmetrization of the *energy product*,

$$\langle f, g\rangle_L := \frac{1}{2}\Big(\langle\, f,\, -\nabla^2 g\,\rangle + \langle\, g,\, -\nabla^2 f\,\rangle\Big) = \iint_\Omega \nabla f(x,y)\nabla g(x,y)\,dxdy - B_2(f,g) \qquad (6)$$

in which the *boundary functional* is

$$B_2(f,g) := \frac{1}{2}\int_{\partial\Omega} \frac{\partial}{\partial\vec{n}}(fg)\,d\gamma(t) = \frac{1}{2}\int_{\partial\Omega} (f\frac{\partial g}{\partial\vec{n}} + g\frac{\partial f}{\partial\vec{n}})\,d\gamma(t) \qquad (7)$$

Assuming the symmetric boundary condition, there may exist simplification of the boundary functional and the energy product.

Example 1. Some particular cases assume

$$\partial\Omega =: \Gamma = \Gamma_D \cup \Gamma_N, \quad \Gamma_D \cap \Gamma_N = \phi,$$

then the symmetric B.C. is satisfied, provided that

$$f\big|_{\Gamma_D} = g\big|_{\Gamma_D} = \frac{\partial f}{\partial\vec{n}}\Big|_{\Gamma_N} = \frac{\partial g}{\partial\vec{n}}\Big|_{\Gamma_N} = 0.$$

Accordingly, the energy product is

$$\langle\, f,\, -\nabla^2 g\,\rangle = \langle\, g,\, -\nabla^2 f\,\rangle = \iint_\Omega \nabla f(x,y)\nabla g(x,y)\,dxdy \qquad (8)$$

Two classical examples include pairs both satisfying homogeneous Dirichlet or homogeneous Neumann BC.

Example 2. A pair satisfying Robin BC that

$$\frac{\partial f}{\partial\vec{n}}(x) = -c(x)f(x), \qquad \frac{\partial g}{\partial\vec{n}}(x) = -c(x)g(x) \qquad (9)$$

provides another example which satisfies the symmetric boundary condition, owing to

$$\int_{\partial\Omega} f\,\frac{\partial g}{\partial\vec{n}}\,d\gamma(t) = -\int_{\partial\Omega} c(x(t))f(x(t))g(x(t))\,d\gamma(t) = \int_{\partial\Omega} g\,\frac{\partial f}{\partial\vec{n}}\,d\gamma(t),$$

The corresponding energy product

$$\langle f, -\nabla^2 g \rangle = \langle g, -\nabla^2 f \rangle = \iint_\Omega \nabla f(x,y) \nabla g(x,y)\, dxdy + \int_{\partial\Omega} c(x) f(x) g(x)\, d\gamma$$

is then positive definite, under an additional assumption that $c(x) > 0$ on $\partial\Omega$.

Very general results in discrete symmetric boundary condition are presented in Section 4. For the motivation, we discuss next the discretization (Fig. 1) of a Cartesian net of type I regular hexagons.

3. Discrete Symmetric Boundary Condition on Net of Regular Hexagons

The type I neighborhood topology (Fig. 3) and the geometry (Eq. (2)) are detailed below.

$$\begin{array}{rcll}
\Omega & := & \{ (i,j) \mid 1 \le i \le n_x,\ 1 \le j \le n_y \}, & \text{interior nodes} \\
\partial_i & := & \{ (i,j) \in \Omega \mid (i-1)(j-1)(i-n_x)(j-n_y) = 0 \}, & \text{interior boundary} \\
\partial_e & := & \{ (0,0), (n_x+1, n_y+1) \} & \\
 & & \cup \{ (i,j) \mid i = 0,\ n_x+1,\ 1 \le j \le n_y \} & \\
 & & \cup \{ (i,j) \mid j = 0,\ n_y+1,\ 1 \le i \le n_x \}, & \text{exterior (ghost) boundary} \\
\overline{\Omega} & := & \Omega \cup \partial_e, & \text{interior and exterior} \\
\overline{\Omega}_S & := & \{ S(P), SE(P), SW(P) \mid P \in \Omega \}, & \text{non-top-most part} \\
\overline{\Omega}_N & := & \{ N(P), NE(P), NW(P) \mid P \in \Omega \}, & \text{non-lowest part} \\
\partial_S & := & \partial_e \cap \overline{\Omega}_S, & \text{southern boundary} \\
\partial_N & := & \partial_e \cap \overline{\Omega}_N, & \text{northern boundary}
\end{array}$$

With $P = (i,j) \in \Omega$,

$$\begin{array}{rcrcl}
S & \equiv & S(P) & = & (i, j-1) \\
N & \equiv & N(P) & = & (i, j+1) \\
SW & \equiv & SW(P) & = & \begin{cases} (i-1, j-1), & \text{with odd } i \\ (i-1, j \quad\ ), & \text{with even } i \end{cases} \\
SE & \equiv & SE(P) & = & \begin{cases} (i+1, j-1), & \text{with odd } i \\ (i+1, j \quad\ ), & \text{with even } i \end{cases} \\
NW & \equiv & NW(P) & = & \begin{cases} (i-1, j \quad\ ), & \text{with odd } i \\ (i-1, j+1), & \text{with even } i \end{cases} \\
NE & \equiv & NE(P) & = & \begin{cases} (i+1, j \quad\ ), & \text{with odd } i \\ (i+1, j+1), & \text{with even } i \end{cases}
\end{array}$$

For the symmetry of the negative hexagonal seven-point Laplacian

$$(L_7 f)_P := 6f_P - f_N - f_S - f_{NW} - f_{SE} - f_{NE} - f_{SW}$$

we use *backward* (in vertical direction) differences to derive

$$\begin{aligned}
\langle L_7 f, g \rangle = & \textstyle\sum_{P\in\Omega} \Big(g_P(f_P - f_S) - g_P(f_N - f_P) + g_P(f_P - f_{SW}) - g_P(f_{NE} - f_P) \\
& \qquad\qquad\qquad\qquad + g_P(f_P - f_{NW}) - g_P(f_{SE} - f_P) \Big) \\
= & \textstyle\sum_{P\in\Omega} \Big((f_P - f_S)(g_P - g_S) + (f_P - f_{SW})(g_P - g_{SW}) + (f_P - f_{NW})(g_P - g_{NW}) \Big) \\
& - \textstyle\sum_{N\in\partial_e} g_P(f_N - f_P) + \sum_{S\in\partial_e} g_S(f_P - f_S) \\
& - \textstyle\sum_{NE\in\partial_e} g_P(f_{NE} - f_P) + \sum_{SW\in\partial_e} g_{SW}(f_P - f_{SW}) \\
& - \textstyle\sum_{SE\in\partial_e} g_P(f_{SE} - f_P) + \sum_{NW\in\partial_e} g_{NW}(f_P - f_{NW})
\end{aligned} \tag{10}$$

Similarly, by interchanging f and g,

$$\begin{aligned}\langle f, L_7 g\rangle = &\ \textstyle\sum_{P\in\Omega}\Big(f_P(g_P-g_S)-f_P(g_N-g_P)+f_P(g_P-g_{SW})-f_P(g_{NE}-g_P)\\ &\qquad +f_P(g_P-g_{NW})-f_P(g_{SE}-g_P)\Big)\\ = &\ \textstyle\sum_{P\in\Omega}\Big((f_P-f_S)(g_P-g_S)+(f_P-f_{SW})(g_P-g_{SW})+(f_P-f_{NW})(g_P-g_{NW})\Big)\\ &-\textstyle\sum_{N\in\partial_e} f_P(g_N-g_P)+\sum_{S\in\partial_e} f_S(g_P-g_S)\\ &-\textstyle\sum_{NE\in\partial_e} f_P(g_{NE}-g_P)+\sum_{SW\in\partial_e} f_{SW}(g_P-g_{SW})\\ &-\textstyle\sum_{SE\in\partial_e} f_P(g_{SE}-g_P)+\sum_{NW\in\partial_e} f_{NW}(g_P-g_{NW})\end{aligned}\tag{11}$$

Setting the goal $\langle L_7 f, g\rangle - \langle f, L_7 g\rangle = 0$ leads to backward difference version of the symmetric boundary condition,

$$\begin{aligned}&\textstyle\sum_{N\in\partial_e}(f_P(g_N-g_P)-g_P(f_N-f_P))-\sum_{S\in\partial_e}(f_S(g_P-g_S)-g_S(f_P-f_S))\\ &+\textstyle\sum_{NE\in\partial_e}(f_P(g_{NE}-g_P)-g_P(f_{NE}-f_P))-\sum_{SW\in\partial_e}(f_{SW}(g_P-g_{SW})-g_{SW}(f_P-f_{SW}))\\ &+\textstyle\sum_{SE\in\partial_e}(f_P(g_{SE}-g_P)-g_P(f_{SE}-f_P))-\sum_{NW\in\partial_e}(f_{NW}(g_P-g_{NW})-g_{NW}(f_P-f_{NW}))\\ &=0\end{aligned}\tag{12}$$

Alternatively, we can make use of *forward* (in vertical direction) differences.

$$\begin{aligned}\langle L_7 f, g\rangle = &\ \textstyle\sum_{P\in\Omega}\Big((f_N-f_P)(g_N-g_P)+(f_{NE}-f_P)(g_{NE}-g_P)+(f_{SE}-f_P)(g_{SE}-g_P)\Big)\\ &-\textstyle\sum_{N\in\partial_e} g_N(f_N-f_P)+\sum_{S\in\partial_e} g_P(f_P-f_S)\\ &-\textstyle\sum_{NE\in\partial_e} g_{NE}(f_{NE}-f_P)+\sum_{SW\in\partial_e} g_P(f_P-f_{SW})\\ &-\textstyle\sum_{SE\in\partial_e} g_{SE}(f_{SE}-f_P)+\sum_{NW\in\partial_e} g_P(f_P-f_{NW})\end{aligned}\tag{13}$$

Also, by interchanging f and g,

$$\begin{aligned}\langle f, L_7 g\rangle = &\ \textstyle\sum_{P\in\Omega}\Big((f_N-f_P)(g_N-g_P)+(f_{NE}-f_P)(g_{NE}-g_P)+(f_{SE}-f_P)(g_{SE}-g_P)\Big)\\ &-\textstyle\sum_{N\in\partial_e} f_N(g_N-g_P)+\sum_{S\in\partial_e} f_P(g_P-g_S)\\ &-\textstyle\sum_{NE\in\partial_e} f_{NE}(g_{NE}-g_P)+\sum_{SW\in\partial_e} f_P(g_P-g_{SW})\\ &-\textstyle\sum_{SE\in\partial_e} f_{SE}(g_{SE}-g_P)+\sum_{NW\in\partial_e} f_P(g_P-g_{NW})\end{aligned}\tag{14}$$

Comparison of the last two equations leads to forward difference version of the symmetric boundary condition

$$\begin{aligned}&\textstyle\sum_{N\in\partial_e}(f_N(g_N-g_P)-g_N(f_N-f_P))-\sum_{S\in\partial_e}(f_P(g_P-g_S)-g_P(f_P-f_S))\\ &+\textstyle\sum_{NE\in\partial_e}(f_{NE}(g_{NE}-g_P)-g_{NE}(f_{NE}-f_P))-\sum_{SW\in\partial_e}(f_P(g_P-g_{SW})-g_P(f_P-f_{SW}))\\ &+\textstyle\sum_{SE\in\partial_e}(f_{SE}(g_{SE}-g_P)-g_{SE}(f_{SE}-f_P))-\sum_{NW\in\partial_e}(f_P(g_P-g_{NW})-g_P(f_P-f_{NW}))\\ &=0\end{aligned}\tag{15}$$

Taking average of Eqs. (10 and 13), (11 and 14), respectively, leads to

$$\begin{aligned}\langle L_7 f, g\rangle = \tfrac{1}{2}&\ \textstyle\sum_{P\in\Omega}\Big((f_P-f_S)(g_P-g_S)+(f_P-f_{SW})(g_P-g_{SW})+(f_P-f_{NW})(g_P-g_{NW})\Big)\\ +\tfrac{1}{2}&\ \textstyle\sum_{P\in\Omega}\Big((f_N-f_P)(g_N-g_P)+(f_{NE}-f_P)(g_{NE}-g_P)+(f_{SE}-f_P)(g_{SE}-g_P)\Big)\\ -&\ \textstyle\sum_{N\in\partial_e}\frac{(g_N+g_P)}{2}(f_N-f_P)+\sum_{S\in\partial_e}\frac{(g_P+g_S)}{2}(f_P-f_S)\\ -&\ \textstyle\sum_{NE\in\partial_e}\frac{(g_{NE}+g_P)}{2}(f_{NE}-f_P)+\sum_{SW\in\partial_e}\frac{(g_P+g_{SW})}{2}(f_P-f_{SW})\\ -&\ \textstyle\sum_{SE\in\partial_e}\frac{(g_{SE}+g_P)}{2}(f_{SE}-f_P)+\sum_{NW\in\partial_e}\frac{(g_P+g_{NW})}{2}(f_P-f_{NW})\end{aligned}\tag{16}$$

$$
\begin{aligned}
\langle f, L_7 g\rangle = \tfrac{1}{2} & \textstyle\sum_{P\in\Omega}\Big((f_P - f_S)(g_P - g_S) + (f_P - f_{SW})(g_P - g_{SW}) + (f_P - f_{NW})(g_P - g_{NW})\Big) \\
+\tfrac{1}{2} & \textstyle\sum_{P\in\Omega}\Big((f_N - f_P)(g_N - g_P) + (f_{NE} - f_P)(g_{NE} - g_P) + (f_{SE} - f_P)(g_{SE} - g_P)\Big) \\
- & \textstyle\sum_{N\in\partial_e} \frac{(f_N+f_P)}{2}(g_N - g_P) + \sum_{S\in\partial_e}\frac{(f_P+f_S)}{2}(g_P - g_S) \\
- & \textstyle\sum_{NE\in\partial_e} \frac{(f_{NE}+f_P)}{2}(g_{NE} - g_P) + \sum_{SW\in\partial_e}\frac{(f_P+f_{SW})}{2}(g_P - g_{SW}) \\
- & \textstyle\sum_{SE\in\partial_e} \frac{(f_{SE}+f_P)}{2}(g_{SE} - g_P) + \sum_{NW\in\partial_e}\frac{(f_P+f_{NW})}{2}(g_P - g_{NW})
\end{aligned}
\tag{17}
$$

To summarize in compact form. Let P' represent a member in the neighborhood of $P \in \Omega$, that is, symbolically,

$$P' \in \left\{ P_{_N},\ P_{_{NW}},\ P_{_{SW}},\ P_{_S},\ P_{_{SE}},\ P_{_{NE}} \right\}$$

Then, in terms of *backward* differences (using three lower neighbors, Eq. (10)),

$$\langle L_7 f, g\rangle = \sum_{P'\in\Omega_S}(g_P - g_{P'})(f_P - f_{P'}) + \sum_{P'\in\partial_S} g_{P'}(f_P - f_{P'}) - \sum_{P'\in\partial_N} g_P(f_{P'} - f_P)$$

and, in terms of *forward* differences (using three upper neighbors, Eq. (13)),

$$\langle L_7 f, g\rangle = \sum_{P'\in\Omega_N}(g_{P'} - g_P)(f_{P'} - f_P) + \sum_{P'\in\partial_S} g_P(f_P - f_{P'}) - \sum_{P'\in\partial_N} g_{P'}(f_{P'} - f_P)$$

Taking average of these two leads to a compact form of Eq. (16),

$$\langle L_7 f, g\rangle = \frac{1}{2}\sum_{P\in\Omega}(g_P - g_{P'})(f_P - f_{P'}) - \sum_{P'\in\partial_e}\frac{g_P + g_{P'}}{2}(f_{P'} - f_P) \tag{18}$$

Similarly, with f and g interchanged, we obtain compact forms of Eqs. (11 and 14),

$$
\begin{aligned}
\langle f, L_7 g\rangle &= \sum_{P'\in\Omega_S}(f_P - f_{P'})(g_P - g_{P'}) + \sum_{P'\in\partial_S} f_{P'}(g_P - g_{P'}) - \sum_{P'\in\partial_N} f_P(g_{P'} - g_P) \\
\langle f, L_7 g\rangle &= \sum_{P'\in\Omega_N}(f_{P'} - f_P)(g_{P'} - g_P) + \sum_{P'\in\partial_S} f_P(g_P - g_{P'}) - \sum_{P'\in\partial_N} f_{P'}(g_{P'} - g_P)
\end{aligned}
$$

and their average, now as a compact form of Eq. (17),

$$\langle f, L_7 g\rangle = \frac{1}{2}\sum_{P\in\Omega}(f_P - f_{P'})(g_P - g_{P'}) - \sum_{P'\in\partial_e}\frac{f_P + f_{P'}}{2}(g_{P'} - g_P) \tag{19}$$

In summary.

Theorem 2 (Symmetric boundary condition and energy product for negative seven-point Laplacian on Cartesian net of type I regular hexagons.)

$$
\begin{aligned}
\langle g, L_7 f\rangle - \langle f, L_7 g\rangle = 0 \quad &\Leftrightarrow \quad \textstyle\sum_{P'\in\partial_e}\left(\frac{(f_P+f_{P'})}{2}(g_{P'} - g_P) - \frac{(g_P+g_{P'})}{2}(f_{P'} - f_P)\right) = 0 \\
&\Leftrightarrow \quad \textstyle\sum_{P'\in\partial_e}(f_P g_{P'} - f_{P'} g_P) = 0
\end{aligned}
\tag{20}
$$

If the above (implied) symmetric boundary condition is satisfied, then the bilinear form

$$\langle f, g\rangle_{L_7} := \langle L_7 f, g\rangle = \langle f, L_7 g\rangle = \frac{1}{2}\sum_{P\in\Omega}(f_{P'} - f_P)(g_{P'} - g_P) + \frac{1}{2}\sum_{P'\in\partial_e}(f_P g_P - f_{P'} g_{P'}) \tag{21}$$

is well-defined and symmetric.

Proof. Taking difference of Eqs. (19 and 18) yields the symmetric boundary condition, while taking average leads to the discrete product. □

Remark 1. The Theorem is valid on a general (not necessarily Cartesian) net of type I hexagons, because there is no usage of integral indices in the relevant discussion. Even more general case is applicable with central differencing in a proper setup, as presented in Section 4.

Example 3. (*Stencil-truncation.*) Assume cell-average Dirichlet BC that the grid data vanish at ghost nodes, $f_{P'} = g_{P'} = 0, \forall P' \in \partial_e$, the symmetric boundary condition (Eq. (20)) is then satisfied. The simplified energy product

$$\langle f, g \rangle_{L_7} = \frac{1}{2} \sum_{P\in\Omega} (f_{P'} - f_P)(g_{P'} - g_P) + \frac{1}{2} \sum_{P\in\partial_i} f_P g_P$$

is certainly positive-definite. We note the boundary functional is defined with multiplicities at interior boundary nodes.

Example 4. (*Torus.*) A Cartesian net of hexagons (Fig. 1), as a *computational domain* with periodic BC, corresponds to a torus with no exterior boundary (ghost) node. The symmetric boundary condition for Laplacian is satisfied. The boundary functional vanishes and the discrete energy product is positive semi-definite. $\langle f, f \rangle_{L_7} = 0$ if and only if f is a (single) constant with the discrete topology being path-connected.

There are more examples along this line, with the periodic BC replaced by twist BC or by mixing of periodic and twist, resulting in applications of dynamical systems for the real projective plane or a Klein bottle. Open field problems subject to homogeneous Dirichlet or Neumann BC are discussed as corollaries to the general result in the next section.

4. Symmetric Boundary Condition for Discrete Laplacian by Cell-center Finite Difference

For applications involving discrete (negative) Laplacian in the form

$$L(f) := \sum_{P'\in\mathcal{N}(P)} A_{P'}(f_P - f_{P'}),$$

with Ω and ∂_e denoting respectively the (disjoint) set of interior grid nodes and ghost nodes, we assume very general assumptions that

(i) the discrete neighborhood topology is *reflexive* so that *being-neighbor-to* is a symmetric relation among interior nodes,

$$P, Q \in \Omega, \quad Q \in \mathcal{N}(P) \iff P \in \mathcal{N}(Q),$$

(ii) the central difference (CD) stencil is *symmetric*, assuming proper orientation (ordering) consistently in all (local) neighbor lists, such that

$$\begin{aligned} A :=& \left\{ A_{P'} \mid P' \in \mathcal{N}(P) \right\} && \text{(independent of } P \in \Omega) \\ \equiv& \left\{ A(P, Q) \mid P \in \Omega,\ Q \in \mathcal{N}(P) \subset \Omega \cap \partial_e \right\}, && A(P, Q) = A(Q, P) \text{ if } P, Q \in \Omega. \end{aligned}$$

As an example, consider standard Laplacian on a net of type I regular hexagons (Figs. 1 and 3, and Eq. (3)), the homogeneous discrete *neighborhood* is the relation

$$\mathcal{N} := \left\{ (P, N(P)), (P, NW(P)), (P, SW(P)), (P, S(P)), (P, SE(P)), (P, NE(P)) \right\} \subset \Omega \times (\Omega \cup \partial_e)$$

which is symmetric among interior nodes. We abuse the notation slightly and use

$$\mathcal{N}(P) \equiv \left\{ N(P), NW(P), SW(P), S(P), SE(P), NE(P) \right\}$$

or, with implied dependence,

$$\mathcal{N} = \left\{ N, NW, SW, S, SE, NE \right\}, \qquad \forall P \in \Omega.$$

The consistently ordered homogeneous symmetric stencil (Lee,2015) is,

$$A := \left\{ A_N, A_{NW}, A_{SW}, A_S, A_{SE}, A_{NE} \right\} = \left\{ \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{6} \right\}, \quad \forall P \in \Omega,$$

and, *in order*,

$$\begin{aligned} \forall P \in \Omega, \quad P' \in& \left\{ N, NW, SW, S, SE, NE \right\} \\ A_{P'} \in& \left\{ A_N, A_{NW}, A_{SW}, A_S, A_{SE}, A_{NE} \right\} = \left\{ \tfrac{1}{6}, \tfrac{1}{6}, \tfrac{1}{6}, \tfrac{1}{6}, \tfrac{1}{6}, \tfrac{1}{6} \right\}. \end{aligned}$$

We add in passing, for anisotropic negative Laplacian (Eq. (3) on type I Hex net, that (Lee,2015)

$$A \sim \left\{3D_2 - D_1,\, 2D_1,\, 2D_1,\, 3D_2 - D_1,\, 2D_1,\, 2D_1\right\}$$

The following relations are helpful.

Lemma 3

$$\sum_{P\in\Omega}\sum_{P'\in N(P)\cap\Omega} A_{P'}(f_P g_{P'} - f_{P'} g_P) = 0 \tag{22}$$

$$\sum_{P\in\Omega}\sum_{P'\in N(P)\cap\Omega} A_{P'}(f_P g_P - f_{P'} g_{P'}) = 0 \tag{23}$$

We establish a very general result, as follows.

Theorem 4 The symmetric boundary condition for $\langle Lf,\, g\rangle = \langle Lg,\, f\rangle$ is

$$\sum_{P\in\Omega,\; P'\in N(P)\cap\partial_e} A_{P'}(f_P g_{P'} - f_{P'} g_P) = 0, \tag{24}$$

and up to satisfication of which, the resulting energy product is

$$\langle f, g\rangle_L = \sum_{P\in\Omega}\sum_{P'\in N(P)} A_{P'}(f_{P'} - f_P)(g_{P'} - g_P) + \sum_{P\in\Omega,\; P'\in N(P)\cap\partial_e} (f_P g_P - f_{P'} g_{P'}) \tag{25}$$

Proof. Note that

$$\begin{aligned}
\langle Lf,\, g\rangle &= \sum_{P\in\Omega}\sum_{P'\in N(P)} A_{P'}(f_P - f_{P'})g_P \\
&= \sum_{P\in\Omega}\sum_{P'\in N(P)\cap\Omega} A_{P'}(f_P - f_{P'})g_P + \sum_{P\in\Omega}\sum_{P'\in N(P)\cap\partial_e} A_{P'}(f_P - f_{P'})g_p \\
\langle Lg,\, f\rangle &= \sum_{P\in\Omega}\sum_{P'\in N(P)\cap\Omega} A_{P'}(g_P - g_{P'})f_P + \sum_{P\in\Omega}\sum_{P'\in N(P)\cap\partial_e} A_{P'}(g_P - g_{P'})f_P
\end{aligned}$$

By taking difference of the last two equations and using Eq. (22), we obtain

$$\begin{aligned}
\langle Lf,\, g\rangle - \langle Lg,\, f\rangle &= \sum_{P\in\Omega}\sum_{P'\in N(P)\cap\partial_e} A_{P'}(f_P g_{P'} - f_{P'} g_P) \\
\text{(also)} \qquad &= \sum_{P\in\Omega}\sum_{P'\in N(P)\cap\partial_e} A_{P'}\Big(\frac{f_{P'} + f_P}{2}(g_{P'} - g_P) - \frac{g_{P'} + g_P}{2}(f_{P'} - f_P)\Big)
\end{aligned} \tag{26}$$

which yields the symmetric boundary condition (Eq. (24)), while taking the average and using Eq. (23),

$$\begin{aligned}
\langle f, g\rangle_L :=& \frac{1}{2}(\langle Lf,\, g\rangle + \langle Lg,\, f\rangle) = \langle Lf, g\rangle = \langle Lg, f\rangle \\
=& \frac{1}{2}\sum_{P\in\Omega}\sum_{P'\in N(P)\cap\Omega} A_{P'}(f_P g_P + f_{P'} g_{P'} - f_P g_{P'} - f_{P'} g_P) + \frac{1}{2}\sum_{P\in\Omega}\sum_{P'\in N(P)\cap\in\partial_e} A_{P'}(2f_P g_P - f_P g_{P'} - f_{P'} g_P) \\
=& \frac{1}{2}\sum_{P\in\Omega}\sum_{P'\in N(P)\cap(\Omega\cup\partial_e)} A_{P'}(f_{P'} - f_P)(g_{P'} - g_P) - \frac{1}{2}\sum_{P\in\Omega}\sum_{P'\in N(P)\cap\partial_e} A_{P'}\Big((f_{P'} - f_P)(g_{P'} - g_P) - 2f_P g_P + f_P g_{P'} + f_{P'} g_P\Big) \\
=& \frac{1}{2}\sum_{P\in\Omega}\sum_{P'\in N(P)} A_{P'}(f_{P'} - f_P)(g_{P'} - g_P) + B(f, g)
\end{aligned}$$

with boundary functional

$$B(f, g) := \frac{1}{2}\sum_{P\in\Omega,\, P'\in N(P)\cap\partial_e} (f_P g_P - f_{P'} g_{P'}) \tag{27}$$

Thus ends the proof. □

Remark 2. A second-order central difference approximation to the contour integral term (Eq. (5)) predicts correctly the discrete symmetric boundary condition (Eqs. (26 and 20)).

Corollary 5 Suppose every exterior (ghost) boundary node, $P' \in \partial_e$, is of homogeneous Dirichlet, homogeneous Neumann or Robin type such that, respectively,

$$\begin{array}{llllll} \text{either} & f_P + f_{P'} & = & g_P + g_{P'} & = & 0, \\ \text{or} & f_P - f_{P'} & = & g_P - g_{P'} & = & 0, \\ \text{or} & \frac{f_P + f_{P'}}{f_P - f_{P'}} & = & \frac{g_P + g_{P'}}{g_P - g_{P'}} & = & \text{const}_{P'}, \ \text{ at each pair } \ (P, P'), \end{array}$$

then the symmetric boundary condition (Eq. (24)) is satisfied.

Corollary 6

(i) If a mixed type homogeneous BC consists of at least one Dirichlet and some Neumann node(s) with vanishing boundary functional (owing to $f_{P'}/f_P = f_{P'}/f_P = \pm 1$ at boundary), then the energy product simplifies to

$$\langle f, g \rangle_L = \langle f, Lg \rangle = \langle Lf, g \rangle = \frac{1}{2} \sum_{P \in \Omega} \sum_{P' \in N(P)} (f_{P'} - f_P)(g_{P'} - g_P) \tag{28}$$

and is (symmetric and) positive-definite.

(ii) If pure homogeneous Neumann BC ($f_{P'} - f_P = g_{P'} - g_P = 0$) holds, then the symmetric boundary condition is satisfied, the boundary functional vanishes, the energy product is reduced (to Eq. (28)) and is positive semi-definite such that $\langle f, f \rangle_L = 0$ if and only if f is constant in each (path-)connected component of Ω.

(iii) In case of (function) Robin BC (Eq. (9)) with $c(x) > 0$ on $\partial\Omega$, the central difference approximation

$$\frac{f_{P'} - f_P}{2h} = -c \frac{f_{P'} + f_P}{2}$$

with $2h$ being the node-to-node distance, implies

$$\frac{f_{P'}}{f_P} = \frac{1 - ch}{1 + ch} = \frac{g_{P'}}{g_P}.$$

Therefore, the energy product (Eq. (25))

$$\langle f, g \rangle_L = \frac{1}{2} \sum_{P \in \Omega} (f_{P'} - f_P)(g_{P'} - g_P) + \frac{1}{2} \sum_{(P,P') \in \Omega \times (N(P) \cap \partial_e)} (f_P g_P \frac{4ch}{(1 + ch)^2}) \tag{29}$$

is positive definite, up to $c := c_{(P+P')/2} > 0$ in practice.
We note the boundary functional is defined with various multiplicities at ghost nodes.

4.1 Symmetric Boundary Condition for Five-point Laplacian

In a setup of rectangular grid, the scaled negative five-point Laplacian reads

$$Lf_{i,j} = 4f_{i,j} - f_{i-1,j} - f_{i+1,j} - f_{i,j-1} - f_{i,j+1},$$

in which $1 \le i \le n_x,\ 1 \le j \le n_y$ at interior nodes, and $i = 0, n_x + 1,\ j = 0, n_y + 1$ at ghost nodes. The general theory (Eqs. (24 and 25)) specializes as follows.

Theorem 7 Let the indices run through all interior nodes, $1 \le i \le n_x,\ 1 \le j \le n_y$.

(i) The discrete 2D symmetric boundary condition for five-point Laplacian is

$$\begin{aligned} & \sum_i \left(f_{i,0} g_{i,1} - f_{i,1} g_{i,0} + f_{i,n_y+1} g_{i,n_y} - f_{i,n_y} g_{i,n_y+1} \right) \\ + & \sum_j \left(f_{0,j} g_{1,j} - f_{1,j} g_{0,j} + f_{n_x+1,j} g_{n_x,j} - f_{n_x,j} g_{n_x+1,j} \right) = 0. \end{aligned} \tag{30}$$

(ii) Suppose the above symmetric boundary condition is satisfied, then the following expression

$$\begin{aligned}\langle f, g\rangle_L := \langle Lf, g\rangle = \langle f, Lg\rangle = \tfrac{1}{2} & \sum_{i,j}\Big(\triangle_i f_{i,j} \triangle_i g_{i,j} + \triangle_j f_{i,j} \triangle_j g_{i,j} + \nabla_i f_{i,j} \nabla_i g_{i,j} + \nabla_j f_{i,j} \nabla_j g_{i,j}\Big) \\ + & \sum_i \Big(f_{i,1} g_{i,1} - f_{i,0} g_{i,0}\Big) + \sum_i \Big(f_{i,n_y} g_{i,n_y} - f_{i,n_y+1} g_{i,n_y+1}\Big) \\ + & \sum_j \Big(f_{1,j} g_{1,j} - f_{0,j} g_{0,j}\Big) + \sum_j \Big(f_{n_x,j} g_{n_x,j} - f_{n_x+1,j} g_{n_x+1,j}\Big)\end{aligned} \tag{31}$$

defines a symmetric bilinear form.

The above theory were actually studied firstly in details, and motivated the discussion of Hex grid case (Section 3) and then the very general case (Section 4). We omit any meta-analysis in deriving Eqs. (30 and 31). Instead, we specialize for a commonly encountered application on rectangular grid.

Theorem 8 *(Product-form symmetric boundary condition.)* Suppose that the application data are (separable) in product forms,

$$(a_i b_j)_{i,j} \equiv (f_{i,j})_{i,j} \neq (g_{i,j})_{i,j} \equiv (c_i d_j)_{i,j}, \tag{32}$$

then the symmetric boundary condition (Eq. (30)) simplifies to

$$\begin{aligned} & (b_0 d_1 - b_1 d_0 + b_{n_y+1} d_{n_y} - b_{n_y} d_{n_y+1}) \sum_{i=1}^{n_x} a_i c_i \\ + \quad & (a_0 c_1 - a_1 c_0 + a_{n_x+1} c_{n_x} - a_{n_x} c_{n_x+1}) \sum_{j=1}^{n_y} b_j d_j = 0, \end{aligned} \tag{33}$$

which is satisfied if any of the following four conditions holds

$$b_0 d_1 - b_1 d_0 + b_{n_y+1} d_{n_y} - b_{n_y} d_{n_y+1} = a_0 c_1 - a_1 c_0 + a_{n_x+1} c_{n_x} - a_{n_x} c_{n_x+1} = 0 \tag{34}$$

$$b_0 d_1 - b_1 d_0 + b_{n_y+1} d_{n_y} - b_{n_y} d_{n_y+1} = \sum_{j=1}^{n_y} b_j d_j = 0 \tag{35}$$

$$a_0 c_1 - a_1 c_0 + a_{n_x+1} c_{n_x} - a_{n_x} c_{n_x+1} = \sum_{i=1}^{n_x} a_i c_i = 0 \tag{36}$$

$$\sum_{i=1}^{n_x} a_i c_i = \sum_{j=1}^{n_y} b_j d_j = 0 \tag{37}$$

5. Discussion

We give here examples of sets of (basis) vectors which all satisfy pairwisely the symmetric boundary condition for discrete Laplacian. The *private* BC in each case is indicated when it is convenient.

We consider 2D half-integral nodes

$$x_i = \frac{i - 0.5}{n_x}, \quad 1 \le i \le n_x, \qquad y_j = \frac{j - 0.5}{n_y}, \quad 1 \le j \le n_y,$$

with extensions to ghost nodes. Depending on applications, several Cartesian type bases exist as summarized in Table 3, in which the one-dimensional components are defined next.

5.1 One-dimensional Fourier Vectors

With (n, k, t_k) denoting (n_x, i, x_i) or (n_y, j, y_j), the Fourier half-wave *Sine* and *Cosine*, and quarter-wave *Sine* and *Cosine* vectors are, respectively,

$$v_k^\ell := \sin(\ell\pi t_k), \quad u_k^\ell := \cos((\ell - 1)\pi t_k), \quad w_k^\ell := \sin((\ell - 0.5)\pi t_k), \quad z_k^\ell := \cos((\ell - 0.5)\pi t_k), \qquad 1 \le k, \ell \le n \tag{38}$$

The implied boundary values ($k = 0, n$) satisfy *private* BCs that

$$v_0^\ell + v_1^\ell = v_{n+1}^\ell + v_n^\ell = u_0^\ell - u_1^\ell = u_{n+1}^\ell - u_n^\ell = w_0^\ell + w_1^\ell = w_{n+1}^\ell - w_n^\ell = z_0^\ell - z_1^\ell = z_{n+1}^\ell + z_n^\ell = 0, \qquad \forall \ell \tag{39}$$

We allow the extension that $v_i^0 = u_i^{n+1} \equiv 0$ and refer to Figs. 5 and 6 for several low degree instances of these vectors. The bases defined by Eq. (38) satisfy many properties, among which we mention the following.

(1) *(Central-)Even-odd symmetry in half-wave vectors.*

With $f = v^\ell$ or u^ℓ, $f_{n+1-i}^\ell = (-1)^{\ell+1} f_i^\ell$. That is,

$$\begin{array}{rclrcl} v_{n+1-i}^{2\ell-1} & = & v_i^{2\ell-1}, & v_{n+1-i}^{2\ell} & = & -v_i^{2\ell}, \\ u_{n+1-i}^{2\ell-1} & = & u_i^{2\ell-1}, & u_{n+1-i}^{2\ell} & = & -u_i^{2\ell}, \end{array} \qquad 1 \le i,\, 2\ell \le n. \tag{40}$$

In particular,

$$\begin{array}{rclrcl} v_n^{2\ell-1} & = & v_1^{2\ell-1}, & v_n^{2\ell} & = & -v_1^{2\ell}, \\ u_n^{2\ell-1} & = & u_1^{2\ell-1}, & u_n^{2\ell} & = & -u_1^{2\ell}, \end{array}$$

and therefore as twist and periodic BCs, respectively, that

$$\left\{ \begin{array}{l} v_{n+1}^{2\ell-1} = -v_n^{2\ell-1} = -v_1^{2\ell-1} = v_0^{2\ell-1}, \\ u_{n+1}^{2\ell} = u_n^{2\ell} = -u_1^{2\ell} = -u_0^{2\ell}. \end{array} \right. \quad \left\{ \begin{array}{l} v_{n+1}^{2\ell} = -v_n^{2\ell} = v_1^{2\ell} = -v_0^{2\ell}, \\ u_{n+1}^{2\ell-1} = u_n^{2\ell-1} = u_1^{2\ell-1} = u_0^{2\ell-1}. \end{array} \right. \tag{41}$$

(2) *Symmetry in quarter-wave vectors.*

With $i + i' = \ell + \ell' = n + 1$,

$$\begin{array}{rclclcl} w_i^\ell & = & (-1)^{\ell+1}\, z_{i'}^\ell & = & (-1)^{i+1}\, z_i^{\ell'} & = & (-1)^{\ell+1+i} w_{i'}^{\ell'} \\ z_i^\ell & = & (-1)^{\ell+1} w_{i'}^\ell & = & (-1)^{\ell+1} w_{i'}^\ell & = & (-1)^{\ell+1+i}\, z_{i'}^{\ell'} \end{array} \tag{42}$$

(3) *1D orthogonality.*

$$\langle v^\ell, v^p \rangle = \left\{ \begin{array}{ll} n, & \ell = p = n, \\ \frac{n}{2}, & 1 \le \ell = p < n, \\ 0, & 1 \le \ell \ne p \le n, \end{array} \right. \qquad \langle u^\ell, u^p \rangle = \left\{ \begin{array}{ll} n, & 1 = \ell = p, \\ \frac{n}{2}, & 1 < \ell = p \le n, \\ 0, & 1 \le \ell \ne p \le n. \end{array} \right. \tag{43}$$

$$\langle\, w^\ell,\ w^p\, \rangle = \langle\, z^\ell,\ z^p\, \rangle \quad = \quad \frac{n}{2} \delta_{\ell,p} \tag{44}$$

(4) *1D cross-product.*

$$\langle\, v^\ell,\, u^p\, \rangle = \left\{ \begin{array}{ll} 0, & \text{if } \ell - p \text{ is odd,} \\ \frac{1}{2}(\csc \frac{(\ell+p-1)\pi/2}{n} + \csc \frac{(\ell-p+1)\pi/2}{n}), & \text{if } \ell - p \text{ is even.} \end{array} \right. \tag{45}$$

$$\langle\, w^\ell,\, z^p\, \rangle = \left\{ \begin{array}{rclll} -\langle\, w^p,\, z^\ell\, \rangle & = & \frac{1}{2} \csc \frac{(\ell-p)\pi}{2n}, & \text{if } \ell - p \text{ is odd,} \\ \langle\, w^p,\, z^\ell\, \rangle & = & \frac{1}{2} \csc \frac{(\ell+p-1)\pi}{2n}, & \text{if } \ell - p \text{ is even,} \end{array} \right. \tag{46}$$

Orthogonal bases exist in various forms. We state a few.

Lemma 9 Every set in the following generates an orthogonal basis of $\mathbb{R}^n$.

$$\begin{array}{ll} (1)\ \{\, v^\ell \ \mid\ 1 \le \ell \le n\,\}, & (3)\ \{\, u^{2\ell-1},\quad v^{2\ell} \ \mid\ 1 \le \ell \le \frac{n}{2}\,\}, \\ (2)\ \{\, u^\ell \ \mid\ 1 \le \ell \le n\,\}, & (4)\ \{\, v^{2\ell-1},\quad u^{2\ell} \ \mid\ 1 \le \ell \le \frac{n}{2}\,\}. \end{array}$$

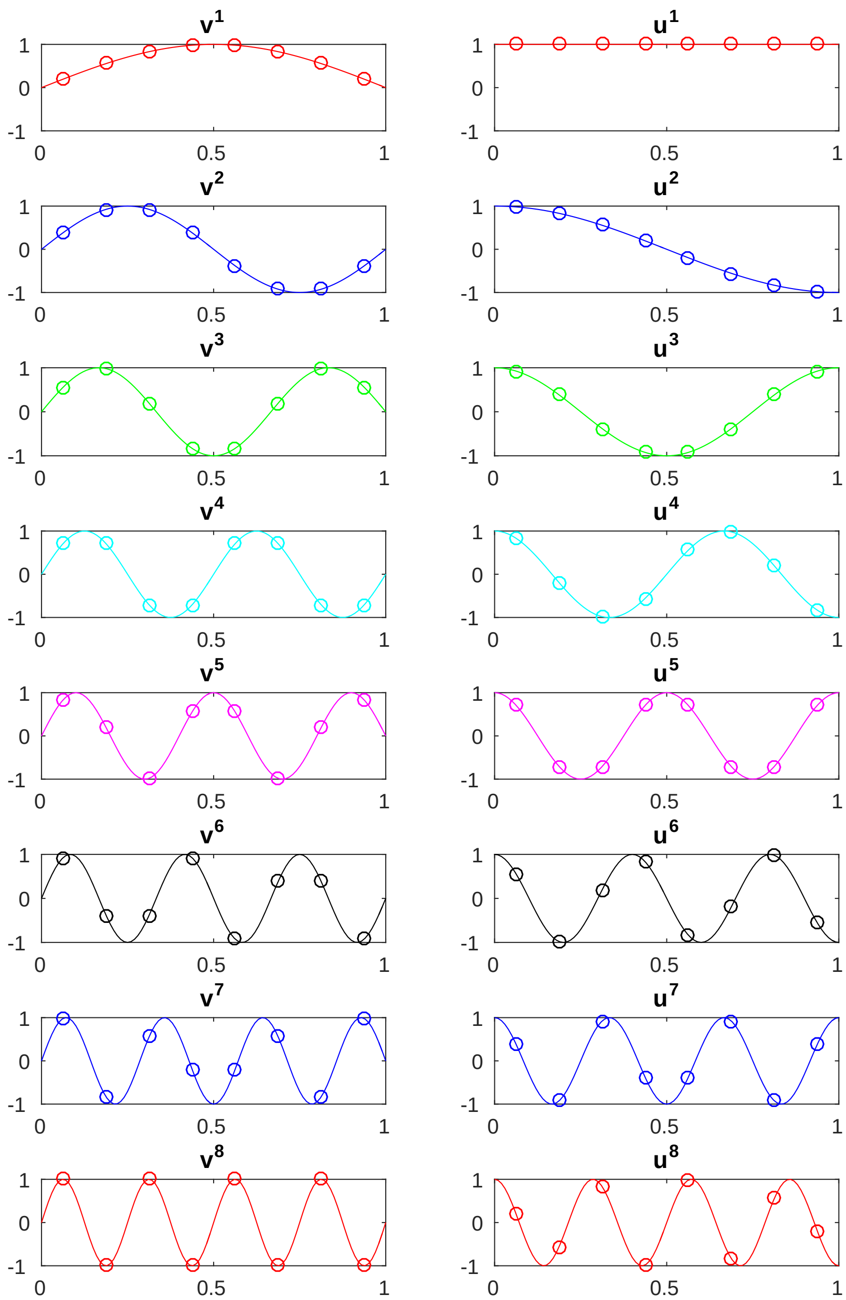

Figure 5. Fourier half-wave Sine and Cosine vectors of degrees up to eight

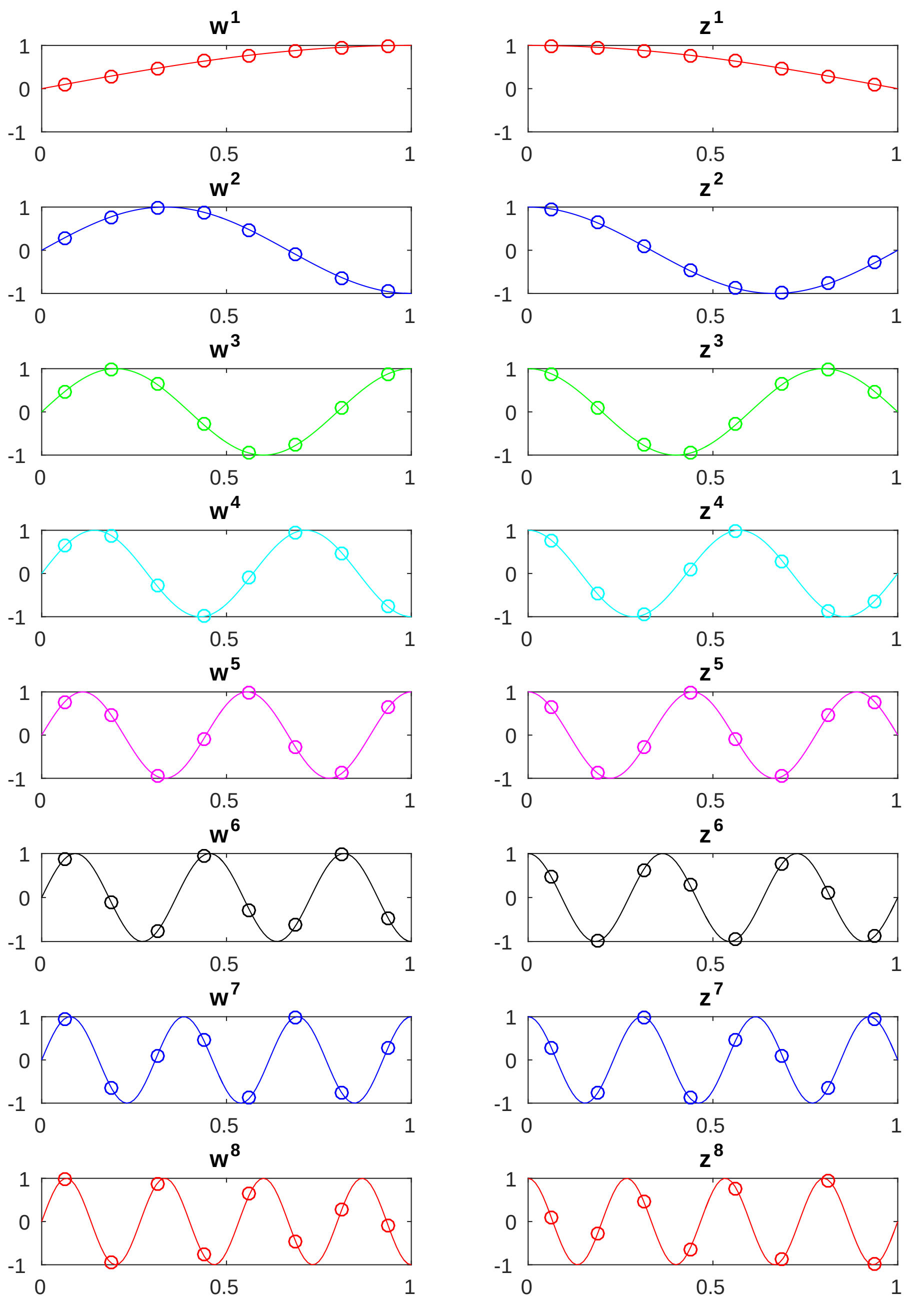

Figure 6. Fourier quarter-wave Sine and Cosine vectors of degrees up to eight

Remark 3. These four algebraic bases are also eigenbases of the 1D three-point Laplacian subject to separable or non-separable BCs of types (D)irichlet, (N)eumann, (P)eriodic and (T)wist, respectively, as follows.

$$\begin{array}{lll} \text{(i) Dirichlet :} & f_0 = -f_1, & f_{n+1} = -f_n \\ \text{(ii) Neumann :} & f_0 = \ \ f_1, & f_{n+1} = \ \ f_n \\ \text{(iii) Periodic :} & f_0 = \ \ f_n, & f_{n+1} = \ \ f_1 \\ \text{(iv) Twist :} & f_0 = -f_n, & f_{n+1} = -f_1 \end{array} \tag{47}$$

The corresponding BCs, for *smooth* functions, are

$$\begin{array}{llll} \text{(i) Dirichlet :} & f(0) & = f(1) & = 0 \\ \text{(ii) Neumann :} & f'(0) & = f'(1) & = 0 \\ \text{(iii) Periodic :} & f(0) - f(1) & = f'(0^+) - f'(1^-) & = 0 \\ \text{(iv) Twist :} & f(0) + f(1) & = f'(0^+) + f'(1^-) & = 0 \end{array}$$

The *Twist* subcase suggests that the dynamics of a BVP solution be realized on a Mobius strip, while on a circle with the periodic one.

5.2 Two-dimensional Fourier Vectors

With admissible indices $1 \le \ell, i \le n_x,\ 1 \le m, j \le n_y$ and extension to ghost nodes, we define 2D Fourier Sine, Cosine and two mixed type vectors, respectively,

$$\begin{array}{rlrl} v^{\ell,m} \equiv & (v^{\ell,m}_{i,j})_{i,j}, & v^{\ell,m}_{i,j} := & v^{\ell}_i\, v^m_j = \sin(\ell\pi x_i)\, \sin(m\pi y_j), \\ u^{\ell,m} \equiv & (u^{\ell,m}_{i,j})_{i,j}, & u^{\ell,m}_{i,j} := & u^{\ell}_i\, u^m_j = \cos((\ell-1)\pi x_i)\, \cos((m-1)\pi y_j), \\ (v^{\ell}u^m)_{i,j} \equiv & (v^{\ell}_i u^m_j)_{i,j}, & & v^{\ell}_i\, u^m_j = \sin(\ell\pi x_i)\, \cos((m-1)\pi y_j), \\ (u^{\ell}v^m)_{i,j} \equiv & (u^{\ell}_i v^m_j)_{i,j}, & & u^{\ell}_i\, v^m_j = \cos((\ell-1)\pi x_i)\, \sin(m\pi y_j), \end{array} \tag{48}$$

with the convention that

$$v^{\ell,m} \equiv 0, \text{ if } \ell m = 0, \quad \text{and} \quad u^{\ell,m} \equiv 0, \text{ if } \ell = n_x + 1 \text{ or } m = n_y + 1.$$

Another four bases of mixed type are

$$\begin{array}{ll} w^{\ell,m} \equiv (w^{\ell,m}_{i,j})_{i,j}, & w^{\ell,m}_{i,j} := w^{\ell}_i w^m_j = \sin\frac{(\ell-0.5)(i-0.5)\pi}{n_x} \sin\frac{(m-0.5)(j-0.5)\pi}{n_y} \\ z^{\ell,m} \equiv (z^{\ell,m}_{i,j})_{i,j}, & z^{\ell,m}_{i,j} := z^{\ell}_i\, z^m_j = \cos\frac{(\ell-0.5)(i-0.5)\pi}{n_x} \cos\frac{(m-0.5)(j-0.5)\pi}{n_y} \end{array} \tag{49}$$

and

$$\begin{array}{ll} (w^{\ell}_i z^m_j)_{i,j} & := \left(\sin\frac{(\ell-0.5)(i-0.5)\pi}{n_x} \cos\frac{(m-0.5)(j-0.5)\pi}{n_y}\right)_{i,j} \\ (z^{\ell}_i w^m_j)_{i,j} & := \left(\cos\frac{(\ell-0.5)(i-0.5)\pi}{n_x} \sin\frac{(m-0.5)(j-0.5)\pi}{n_y}\right)_{i,j} \end{array} \tag{50}$$

Appropriate BCs in applications with these bases (Eqs. (48,49 and 50)), among others, are shown in Table 3. The associated *priviate* BCs can be expressed collectively, with $1 \le \ell \le n_x,\ 1 \le m \le n_y$, as

$$\begin{array}{l} \frac{v^{\ell}_0}{v^{\ell}_1} = \frac{v^m_0}{v^m_1} = \frac{w^{\ell}_0}{w^{\ell}_1} = \frac{w^m_0}{w^m_1} = \frac{v^{\ell}_{n_x+1}}{v^{\ell}_{n_x}} = \frac{v^m_{n_y+1}}{v^m_{n_y}} = \frac{z^{\ell}_{n_x+1}}{z^{\ell}_{n_x}} = \frac{z^m_{n_y+1}}{z^m_{n_y}} = -1 \\ \frac{u^{\ell}_0}{u^{\ell}_1} = \frac{u^m_0}{u^m_1} = \frac{z^{\ell}_0}{z^{\ell}_1} = \frac{z^m_0}{z^m_1} = \frac{u^{\ell}_{n_x+1}}{u^{\ell}_{n_x}} = \frac{u^m_{n_y+1}}{u^m_{n_y}} = \frac{w^{\ell}_{n_x+1}}{w^{\ell}_{n_x}} = \frac{w^m_{n_y+1}}{w^m_{n_y}} = 1 \end{array} \tag{51}$$

More bases and BCs appear in Tables 4 and 5, in which the types of BC are consistent with usage in Remark 3, except for a new type: *A*(lternating between D and N). Discrete symmetric boundary condition and energy product for five-point Laplacian are discussed next.

Table 3. Fourier bases on rectangular half-integral nodes and associated BCs

Basis	BC_w	BC_e	BC_s	BC_n
DD-DD, $\left\{(v_i^\ell v_j^m)_{i,j}\right\}_{\ell,m}$	$v_0^\ell = -v_1^\ell$	$v_{n_x+1}^\ell = -v_{n_x}^\ell$	$v_0^m = -v_1^m$	$v_{n_y+1}^m = -v_{n_y}^m$
NN-NN, $\left\{(u_i^\ell u_j^m)_{i,j}\right\}_{\ell,m}$	$u_0^\ell = u_1^\ell$	$u_{n_x+1}^\ell = u_{n_x}^\ell$	$u_0^m = u_1^m$	$u_{n_y+1}^m = u_{n_y}^m$
DD-NN, $\left\{(v_i^\ell u_j^m)_{i,j}\right\}_{\ell,m}$	$v_0^\ell = -v_1^\ell$	$v_{n_x+1}^\ell = -v_{n_x}^\ell$	$u_0^m = u_1^m$	$u_{n_y+1}^m = u_{n_y}^m$
NN-DD, $\left\{(u_i^\ell v_j^m)_{i,j}\right\}_{\ell,m}$	$u_0^\ell = u_1^\ell$	$u_{n_x+1}^\ell = u_{n_x}^\ell$	$v_0^m = -v_1^m$	$v_{n_y+1}^m = -v_{n_y}^m$
DN-DN, $\left\{(w_i^\ell w_j^m)_{i,j}\right\}_{\ell,m}$	$w_0^\ell = -w_1^\ell$	$w_{n_x+1}^\ell = w_{n_x}^\ell$	$w_0^m = -w_1^m$	$w_{n_y+1}^m = w_{n_y}^m$
ND-ND, $\left\{(z_i^\ell z_j^m)_{i,j}\right\}_{\ell,m}$	$z_0^\ell = z_1^\ell$	$z_{n_x+1}^\ell = -z_{n_x}^\ell$	$z_0^m = z_1^m$	$z_{n_y+1}^m = -z_{n_y}^m$
DN-ND, $\left\{(w_i^\ell z_j^m)_{i,j}\right\}_{\ell,m}$	$w_0^\ell = -w_1^\ell$	$w_{n_x+1}^\ell = w_{n_x}^\ell$	$z_0^m = z_1^m$	$z_{n_y+1}^m = -z_{n_y}^m$
ND-DN, $\left\{(z_i^\ell w_j^m)_{i,j}\right\}_{\ell,m}$	$z_0^\ell = z_1^\ell$	$z_{n_x+1}^\ell = -z_{n_x}^\ell$	$w_0^m = -w_1^m$	$w_{n_y+1}^m = w_{n_y}^m$
DD-DN, $\left\{(v_i^\ell w_j^m)_{i,j}\right\}_{\ell,m}$	$v_0^\ell = -v_1^\ell$	$v_{n_x+1}^\ell = -v_{n_x}^\ell$	$w_0^m = -w_1^m$	$w_{n_y+1}^m = w_{n_y}^m$
DD-ND, $\left\{(v_i^\ell z_j^m)_{i,j}\right\}_{\ell,m}$	$v_0^\ell = -v_1^\ell$	$v_{n_x+1}^\ell = -v_{n_x}^\ell$	$z_0^m = z_1^m$	$z_{n_y+1}^m = -z_{n_y}^m$
NN-DN, $\left\{(u_i^\ell w_j^m)_{i,j}\right\}_{\ell,m}$	$u_0^\ell = u_1^\ell$	$u_{n_x+1}^\ell = u_{n_x}^\ell$	$w_0^m = -w_1^m$	$w_{n_y+1}^m = w_{n_y}^m$
NN-ND, $\left\{(u_i^\ell z_j^m)_{i,j}\right\}_{\ell,m}$	$u_0^\ell = u_1^\ell$	$u_{n_x+1}^\ell = u_{n_x}^\ell$	$z_0^m = z_1^m$	$z_{n_y+1}^m = -z_{n_y}^m$
DN-DD, $\left\{(w_i^\ell v_j^m)_{i,j}\right\}_{\ell,m}$	$w_0^\ell = -w_1^\ell$	$w_{n_x+1}^\ell = w_{n_x}^\ell$	$v_0^m = -v_1^m$	$v_{n_y+1}^m = -v_{n_y}^m$
DN-NN, $\left\{(w_i^\ell u_j^m)_{i,j}\right\}_{\ell,m}$	$w_0^\ell = -w_1^\ell$	$w_{n_x+1}^\ell = w_{n_x}^\ell$	$u_0^m = u_1^m$	$u_{n_y+1}^m = u_{n_y}^m$
ND-DD, $\left\{(z_i^\ell v_j^m)_{i,j}\right\}_{\ell,m}$	$z_0^\ell = z_1^\ell$	$z_{n_x+1}^\ell = -z_{n_x}^\ell$	$v_0^m = -v_1^m$	$v_{n_y+1}^m = -v_{n_y}^m$
ND-NN, $\left\{(z_i^\ell u_j^m)_{i,j}\right\}_{\ell,m}$	$z_0^\ell = z_1^\ell$	$z_{n_x+1}^\ell = -z_{n_x}^\ell$	$u_0^m = u_1^m$	$u_{n_y+1}^m = u_{n_y}^m$

Table 4. Eigenpairs of negative 5-point Laplacian, Part I

Case	Basis	Types of BCs in i and j	Eigenvalue
1a	$v_i^\ell v_j^m$	D, D	$\lambda_{\ell,m} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$
1b	$u_i^\ell u_j^m$	N, N	$\lambda_{\ell,m} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$
1c	$v_i^\ell u_j^m$	D, N	$\lambda_{\ell,m} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$
1d	$u_i^\ell v_j^m$	N, D	$\lambda_{\ell,m} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$
2a	$v_i^\ell v_j^{2m-1}$,	A, T	$\lambda_{\ell,2m-1} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$,
	$u_i^\ell u_j^{2m}$		$\lambda_{\ell,2m} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$
2b	$u_i^\ell v_j^{2m-1}$,	A, T	$\lambda_{\ell,2m-1} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$,
	$v_i^\ell u_j^{2m}$		$\lambda_{\ell,2m} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$
2c	$v_i^\ell v_j^{2m-1}$,	D, T	$\lambda_{\ell,2m-1} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$,
	$v_i^\ell u_j^{2m}$		$\lambda_{\ell,2m} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$
2d	$u_i^\ell v_j^{2m-1}$,	N, T	$\lambda_{\ell,2m-1} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$,
	$u_i^\ell u_j^{2m}$		$\lambda_{\ell,2m} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$
2e	$v_i^\ell u_j^{2m-1}$,	A, P	$\lambda_{\ell,2m-1} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{(2m-2)\pi}{n_y}$,
	$u_i^\ell v_j^{2m}$		$\lambda_{\ell,2m} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{2m\pi}{n_y}$
2f	$u_i^\ell u_j^{2m-1}$,	A, P	$\lambda_{\ell,2m-1} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{(2m-2)\pi}{n_y}$,
	$v_i^\ell v_j^{2m}$		$\lambda_{\ell,2m} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{2m\pi}{n_y}$
2g	$v_i^\ell u_j^{2m-1}$,	D, P	$\lambda_{\ell,2m-1} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{(2m-2)\pi}{n_y}$,
	$v_i^\ell v_j^{2m}$		$\lambda_{\ell,2m} = 4 - 2\cos\frac{\ell\pi}{n_x} - 2\cos\frac{2m\pi}{n_y}$
2h	$u_i^\ell u_j^{2m-1}$,	N, P	$\lambda_{\ell,2m-1} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{(2m-2)\pi}{n_y}$,
	$u_i^\ell v_j^{2m}$		$\lambda_{\ell,2m} = 4 - 2\cos\frac{(\ell-1)\pi}{n_x} - 2\cos\frac{2m\pi}{n_y}$
3a	$v_i^{2\ell-1} v_j^m$,	T, A	$\lambda_{2\ell-1,m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$,
	$u_i^{2\ell} u_j^m$		$\lambda_{2\ell,m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$
3b	$v_i^{2\ell-1} u_j^m$,	T, A	$\lambda_{2\ell-1,m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$,
	$u_i^{2\ell} v_j^m$		$\lambda_{2\ell,m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$

Table 5. Eigenpairs of negative 5-point Laplacian, Part II

Case	Basis	Types of BCs in i and j	Eigenvalue
3c	$v_i^{2\ell-1} v_j^m$,	T, D	$\lambda_{2\ell-1,m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$,
	$u_i^{2\ell} v_j^m$		$\lambda_{2\ell,m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$
3d	$v_i^{2\ell-1} u_j^m$,	T, N	$\lambda_{2\ell-1,m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$,
	$u_i^{2\ell} u_j^m$		$\lambda_{2\ell,m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$
3e	$u_i^{2\ell-1} v_j^m$,	P, A	$\lambda_{2\ell-1,m} = 4 - 2\cos\frac{(2\ell-2)\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$,
	$v_i^{2\ell} u_j^m$		$\lambda_{2\ell,m} = 4 - 2\cos\frac{2\ell\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$
3f	$u_i^{2\ell-1} u_j^m$,	P, A	$\lambda_{2\ell-1,m} = 4 - 2\cos\frac{(2\ell-2)\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$,
	$v_i^{2\ell} v_j^m$		$\lambda_{2\ell,m} = 4 - 2\cos\frac{2\ell\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$
3g	$u_i^{2\ell-1} v_j^m$,	P, D	$\lambda_{2\ell-1,m} = 4 - 2\cos\frac{(2\ell-2)\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$,
	$v_i^{2\ell} v_j^m$		$\lambda_{2\ell,m} = 4 - 2\cos\frac{2\ell\pi}{n_x} - 2\cos\frac{m\pi}{n_y}$
3h	$u_i^{2\ell-1} u_j^m$,	P, N	$\lambda_{2\ell-1,m} = 4 - 2\cos\frac{(2\ell-2)\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$,
	$v_i^{2\ell} u_j^m$		$\lambda_{2\ell,m} = 4 - 2\cos\frac{2\ell\pi}{n_x} - 2\cos\frac{(m-1)\pi}{n_y}$
4a	$v_i^{2\ell-1} v_j^{2m-1}$,	T, T	$\lambda_{2\ell-1,2m-1}$
	$v_i^{2\ell-1} u_j^{2m}$,		$= \lambda_{2\ell-1,2m}$
	$u_i^{2\ell} v_j^{2m-1}$,		$= \lambda_{2\ell,2m-1}$
	$u_i^{2\ell} u_j^{2m}$		$= \lambda_{2\ell,2m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$,
4b	$u_i^{2\ell-1} v_j^{2m-1}$,	P, T	$\lambda_{2\ell-1,2m-1}$
	$u_i^{2\ell-1} u_j^{2m}$,		$= \lambda_{2\ell-1,2m} = 4 - 2\cos\frac{(2\ell-2)\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$,
	$v_i^{2\ell} v_j^{2m-1}$,		$\lambda_{2\ell,2m-1}$
	$v_i^{2\ell} u_j^{2m}$		$= \lambda_{2\ell,2m} = 4 - 2\cos\frac{2\ell\pi}{n_x} - 2\cos\frac{(2m-1)\pi}{n_y}$,
4c	$v_i^{2\ell-1} u_j^{2m-1}$,	T, P	$\lambda_{2\ell-1,2m-1}$
	$u_i^{2\ell} u_j^{2m-1}$,		$= \lambda_{2\ell,2m-1} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{(2m-2)\pi}{n_y}$,
	$v_i^{2\ell-1} v_j^{2m}$,		$\lambda_{2\ell-1,2m}$
	$u_i^{2\ell} v_j^{2m}$		$= \lambda_{2\ell,2m} = 4 - 2\cos\frac{(2\ell-1)\pi}{n_x} - 2\cos\frac{(2m)\pi}{n_y}$,
4d	$u_i^{2\ell-1} u_j^{2m-1}$,	P, P	$\lambda_{2\ell-1,2m-1} = 4 - 2\cos\frac{(2\ell-2)\pi}{n_x} - 2\cos\frac{(2m-2)\pi}{n_y}$,
	$u_i^{2\ell-1} v_j^{2m}$,		$\lambda_{2\ell-1,2m} = 4 - 2\cos\frac{(2\ell-2)\pi}{n_x} - 2\cos\frac{2m\pi}{n_y}$,
	$v_i^{2\ell} u_j^{2m-1}$,		$\lambda_{2\ell,2m-1} = 4 - 2\cos\frac{2\ell\pi}{n_x} - 2\cos\frac{(2m-2)\pi}{n_y}$,
	$v_i^{2\ell} v_j^{2m}$		$\lambda_{2\ell,2m} = 4 - 2\cos\frac{2\ell\pi}{n_x} - 2\cos\frac{2m\pi}{n_y}$,

5.3 Discrete Two-dimensional Symmetric Boundary Condition

Following the general usage of the vector notations (Eq. (32)), we note the following.

Example 5. The product-form symmetric boundary condition (Eq. (33)) is satisfied by all the 16 bases in Table 3.

Proof. With the specified component bases (and $f \neq g$), each of the individual BCs (Eq. (51)) implies

$$\left\{ \frac{a_1}{a_0} = \frac{c_1}{c_0}, \frac{a_{n_x+1}}{a_{n_x}} = \frac{c_{n_x+1}}{c_{n_x}}, \frac{b_1}{b_0} = \frac{d_1}{d_0}, \frac{b_{n_y+1}}{b_{n_y}} = \frac{d_{n_y+1}}{d_{n_y}} \right\} \subset \left\{ \pm 1 \right\}.$$

Hence the assertion, by Eq. (34).

An alternative argument exists as follows. For $ab = f \neq g = cd$,

$$\begin{aligned} &\text{if } a \neq c, b \neq d, \text{ then } \langle a, c\rangle = \langle b, d\rangle = 0, \\ &\text{if } a \neq c, b = d, \text{ then } \langle a, c\rangle = b_0 d_1 - b_1 d_0 + b_{n_y+1} d_{n_y} - b_{n_y} d_{n_y+1} = 0, \\ &\text{if } a = c, b \neq d, \text{ then } \langle b, d\rangle = a_0 c_1 - a_1 c_0 + a_{n_y+1} c_{n_y} - a_{n_y} c_{n_y+1} = 0. \end{aligned}$$

All Eqs. (34, 35 and 36) are thus satisfied in these 16 cases. □

Discussion of cases in the next example makes use of (i) Eqs. (35 and 36), (ii) the respective BCs (Eq. (39)) of 1D Fourier vectors, and (iii) the even-odd symmetry (Eqs. (40 and 47)) that

$$\begin{aligned} \left(v_0^{2\ell-1}, v_1^{2\ell-1}, v_{n_x}^{2\ell-1}, v_{n_x+1}^{2\ell-1} \right) &= v_1^{2\ell-1}\left(-1, \ 1, \ 1, -1 \right), \\ \left(v_0^{2\ell}, v_1^{2\ell}, v_{n_x}^{2\ell}, v_{n_x+1}^{2\ell} \right) &= v_1^{2\ell}\left(-1, \ 1, -1, \ 1 \right), \\ \left(u_0^{2\ell-1}, u_1^{2\ell-1}, u_{n_x}^{2\ell-1}, u_{n_x+1}^{2\ell-1} \right) &= u_1^{2\ell-1}\left(1, \ 1, \ 1, \ 1 \right), \\ \left(u_0^{2\ell}, u_1^{2\ell}, u_{n_x}^{2\ell}, u_{n_x+1}^{2\ell} \right) &= u_1^{2\ell}\left(1, \ 1, -1, -1 \right), \end{aligned}$$

and the same holds with (l, n_x) replaced by (m, n_y).

Example 6. We justify the symmetric boundary condition (Eq. (33)) for all 24 bases listed in Tables 4 and 5.

(1) The first four (1a-1d) options of bases are covered in the previous example.

(2) For bases (2a-2d), we note

$$b_j = v_j^{2m-1}, \quad d_j = u_j^{2m}, \qquad \langle\, b, \ d \,\rangle = \langle\, v^{2m-1}, \ u^{2m} \,\rangle = 0$$

and

$$\begin{aligned} (\, b_0 d_1, \ -b_1 d_0, \ b_{n_y+1} d_{n_y}, \ -b_{n_y} d_{n_y+1} \,) &= (\, v_0^{2m-1} u_1^{2m}, \ -v_1^{2m-1} u_0^{2m}, \ v_{n_y+1}^{2m-1} u_{n_y}^{2m}, \ -v_{n_y}^{2m-1} u_{n_y+1}^{2m} \,) \\ &= v_1^{2m-1} u_1^{2m} (-1, -1, 1, 1). \end{aligned}$$

(3) For bases (2e-2h),

$$b_j = u_j^{2m-1}, \quad d_j = v_j^{2m}, \qquad \langle\, b, \ d \,\rangle = \langle\, u^{2m-1}, \ v^{2m} \,\rangle = 0,$$

and

$$\begin{aligned} (\, b_0 d_1, \ -b_1 d_0, \ b_{n_y+1} d_{n_y}, \ -b_{n_y} d_{n_y+1} \,) &= (\, u_0^{2m-1} v_1^{2m}, \ -u_1^{2m-1} v_0^{2m}, \ u_{n_y+1}^{2m-1} v_{n_y}^{2m}, \ -u_{n_y}^{2m-1} v_{n_y+1}^{2m} \,) \\ &= u_1^{2m-1} v_1^{2m} (1, 1, -1, -1). \end{aligned}$$

(4) Same argument applies to bases (3a-3h), as does for (2a-2h), by an interchange of the two symbol lists

$$\{\, j, m, n_y, b, d \,\} \qquad \text{and} \qquad \{\, i, \ell, n_x, a, c \,\}.$$

(5) It is similar for bases (4a-4d). We mention for basis set (4a), by Eq. (41), that

$$f \in \left\{ v_i^{2\ell-1} v_j^{2m-1},\ \ v_i^{2\ell-1} u_j^{2m},\ \ u_i^{2\ell} v_j^{2m-1},\ \ u_i^{2\ell} u_j^{2m} \right\},$$
$$f_{0,j} = \epsilon f_{n_x,j}, \quad f_{n_x+1,j} = \epsilon f_{1,j}, \quad f_{i,0} = \epsilon f_{i,n_y}, \quad f_{i,n_y+1} = \epsilon f_{i,1}.$$

with $\epsilon = -1$. Note that $\epsilon = 1$ works for basis 4(d).

5.4 Two-dimensional Non-product Type Pairs

This is an example on type I Hex grid. For convenience, we label components of the symmetric boundary condition (Eq. (30)) as follows,

$$\begin{aligned} 0 &= \text{1st-sum} + \text{2nd-sum} + \text{3rd-sum} + \text{4th-sum} \\ &\equiv \sum_{i=1}^{n_x} (f_{i,0} g_{i,1} - f_{i,1} g_{i,0}) + \sum_{i=1}^{n_x} (f_{i,n_y+1} g_{i,n_y} - f_{i,n_y} g_{i,n_y+1}) \\ &\quad + \sum_{j=1}^{n_y} (f_{0,j} g_{1,j} - f_{1,j} g_{0,j}) + \sum_{j=1}^{n_y} (f_{n_x+1,j} g_{n_x,j} - f_{n_x,j} g_{n_x+1,j}) \end{aligned} \tag{52}$$

and consider three *non-product type* families (and members),

$$\begin{aligned} &\text{Pair 1.} && f, g \in \left\{ z_i^{\ell} z_j^m + w_i^{\ell'} w_j^m \right\}_{\ell,m}, \\ &\text{Pair 2.} && f, g \in \left\{ z_i^{\ell} z_j^m - w_i^{\ell'} w_j^m \right\}_{\ell,m}, \\ &\text{Pair 3.} && f \in \left\{ z_i^{\ell} z_j^m + w_i^{\ell'} w_j^m \right\}_{\ell,m}, \quad g \in \left\{ z_i^{\ell} z_j^m - w_i^{\ell'} w_j^m \right\}_{\ell,m}. \end{aligned}$$

We note these are invariant under some operator, Q_4^H (Lee,(2016,submitted)), on a net of type I Hex grid.

In above and below, the admissible indices satisfy

$$1 \le i, \ell, \ell', p, p' \le n_x, \qquad \ell + \ell' = p + p' = n_x + 1, \qquad 1 \le j, m, q \le n_y.$$

Theorem 10 (Pair 1 and pair 2.) Let

$$f_{i,j} = z_i^{\ell} z_j^m \pm w_i^{\ell'} w_j^m, \qquad g_{i,j} = z_i^p z_j^q \pm w_i^{p'} w_j^q.$$

If (i) $q = m$, or (ii) $p = \ell'$ and $m - q$ is odd, then the symmetric boundary condition (Eq. (30)) is satisfied on both pairs.

Proof. With respect to Eq. (52), it is straight forward to derive the following,

$$\begin{aligned} \text{1st-sum} &= \begin{cases} \pm \sec \frac{(\ell+p-1)\pi}{2n_x} \sin \frac{(q-m)\pi}{2n_y}, & \text{if } \ell - p \text{ is even} \\ \pm \sec \frac{(\ell-p)\pi}{2n_x} \sin \frac{(q-m)\pi}{2n_y}, & \text{if } \ell - p \text{ is odd} \end{cases} \\ \text{2nd-sum} &= (-1)^{q-m} \cdot (\text{1st-sum}) \\ \text{3rd-sum} &= \begin{cases} 0, & \text{if } q - m \text{ is even} \\ \pm 2 \csc \frac{(q-m)\pi}{2n_y} \cos \frac{(\ell-0.5)\pi}{2n_x} \cos \frac{(p-0.5)\pi}{2n_x}, & \text{if } q - m \text{ is odd} \end{cases} \\ \text{4th-sum} &= \begin{cases} 0, & \text{if } q - m \text{ is even} \\ \pm 2 \csc \frac{(q-m)\pi}{2n_y} (-1)^{\ell+p} \sin \frac{(\ell-0.5)\pi}{2n_x} \sin \frac{(p-0.5)\pi}{2n_x}, & \text{if } q - m \text{ is odd} \end{cases} \end{aligned}$$

This ends the proof. □

Theorem 11 (Pair 3.) Let

$$f_{i,j} = z_i^{\ell} z_j^m + w_i^{\ell'} w_j^m, \qquad g_{i,j} = z_i^p z_j^q - w_i^{p'} w_j^q.$$

If $p = \ell'$ and $m - q$ is even, then the symmetric boundary condition (Eq. (30)) is satisfied.

Proof. The following are obtained.

$$
\begin{aligned}
\text{1st-sum} &= \begin{cases} -\sec\frac{(\ell+p-1)\pi}{2n_x}\sin\frac{(m+q-1)\pi}{2n_y}, & \text{if } \ell-p \text{ is even} \\ -\sec\frac{(\ell-p)\pi}{2n_x}\sin\frac{(m+q-1)\pi}{2n_y}, & \text{if } \ell-p \text{ is odd} \end{cases} \\
\text{2nd-sum} &= \quad (-1)^{m-q}\cdot(\text{1st-sum}) \\
\text{3rd-sum} &= \begin{cases} -2\csc\frac{(m+q-1)\pi}{2n_y}\cos\frac{(\ell-0.5)\pi}{2n_x}\cos\frac{(p-0.5)\pi}{2n_x}, & \text{if } m-q \text{ is even} \\ 0, & \text{if } m-q \text{ is odd} \end{cases} \\
\text{4th-sum} &= \begin{cases} (-1)^{\ell+p}2\csc\frac{(m+q-1)\pi}{2n_y}\sin\frac{(\ell-0.5)\pi}{2n_x}\sin\frac{(p-0.5)\pi}{2n_x}, & \text{if } m-q \text{ is even} \\ 0, & \text{if } m-q \text{ is odd} \end{cases}
\end{aligned}
$$

□

We note all the calculations of discrete inner-products involving finite trigonometric series are derived by hands and also verified by C-codes.

6. Conclusions

Cell-centered hexagonal finite volume based finite difference method were confirmed effective in Poisson problems and also in time-dependent problems such as to exhibit successfully linear and spiral waves. The hexagonal seven-point Laplacian is analyzed in this work by using symmetric boundary condition. The developed theory, together with some examples, are readily generalized to many two- and three-dimensional applications up to usage of symmetric central differences. Further generalizations to biharmonic and self-adjoint operators are expected.

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