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A SPECTRAL METHOD FOR MIXED BOUNDARY VALUE PROBLEMS ON HEXAHEDRONS

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Abstract. In this paper, we investigate a spectral method for mixed boundary value problems defined on hexahedrons. Some results on irrational orthogonal approximation are established, which play important roles in numerical solutions of partial differential equations defined on hexahedrons. As examples of applications, we provide spectral schemes for two model problems, and prove their spectral accuracy. Efficient numerical implementations are described. Numerical results demonstrate the high efficiency of suggested algorithms.

Key words. Irrational orthogonal approximation, spectral method on hexahedrons, mixed boundary value problems.

1. Introduction

Over the past three decades, spectral methods have been increasingly popular in scientific computations. Especially, the Legendre and Chebyshev spectral methods have been widely used for numerical solutions of partial differential equations, see [1, 2, 3, 7, 8, 11, 13, 18] and the references therein. Recently, there was also some work on the Jacobi approximation and the Jacobi spectral method for degenerated problems, see [9, 10, 14, 15, 16]. Most of the problems considered in these papers are defined on bounded rectangular domains. However, it is more practical to deal with problems defined on non-rectangular domains. In particular, it is interesting to develop the spectral method for three-dimensional and non-rectangular domains. Recently, Guo and Jia [12] proposed a spectral method and a spectral element method on polygonal domains. Whereas, so far, there has been little work on spectral and spectral element methods for hexahedrons and polyhedrons.

In this paper, we investigate the spectral method for mixed boundary value problems on hexahedrons. We first recall some recent results on the Legendre orthogonal approximation on the cube in the next section. Then, we introduce the irrational orthogonal approximation on arbitrary convex hexahedrons and establish the basic results on such approximation in Section 3. These results play essential roles in numerical solutions of partial differential equations defined on hexahedrons. As applications of the above results, we propose the spectral method for two model problems on hexahedrons in Section 4. Their spectral accuracy is proved. We describe the numerical implementation of proposed schemes in Section 5, together with some numerical results to demonstrate the high efficiency of our algorithms. The last section is for some concluding remarks. The main idea and techniques

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developed in this work are also applicable to other mixed boundary value problems defined on three-dimensional and non-rectangular domains.

2. Preliminaries

In this section, we recall some recent results on the Legendre orthogonal approximation in three-dimensions. Let the interval $I_j = \{ \xi_j \mid -1 < \xi_j < 1\}$ and the cube $K = \{ \boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3) \mid \xi_j \in I_j,\ 1 \le j \le 3\}$. We denote by $H^r(K)$ and $H_0^r(K)$ the Sobolev spaces as usual with the norm $||u||_{r,K}$. The inner product and the norm of $L^2(K)$ are denoted by $(u, v)_K$ and $||u||_K$, respectively.

For any integer $N > 0, \mathcal{P}_N(I_1)$ stands for the set of all polynomials of degree at most N, and

$$V_N(K) = \mathcal{P}_N(I_1) \otimes \mathcal{P}_N(I_2) \otimes \mathcal{P}_N(I_3).$$

The $L^2(K)-$orthogonal projection $P_{N,K} : L^2(K) \to V_N(K)$ is defined by

$$(u - P_{N,K}u, \phi)_K = 0, \qquad \forall \phi \in V_N(K).$$

For describing the approximation error precisely, we introduce the following quantity with an integer $r \ge 0$,

$$\begin{aligned} \mathbb{A}_{r,K}(u) &= \int_{I_3}\int_{I_2} \|(1-\xi_1^2)^{\frac{r}{2}} \partial_{\xi_1}^r u(\cdot, \xi_2, \xi_3)\|_{I_1}^2 d\xi_2 d\xi_3 \\ &+ \int_{I_3}\int_{I_1} \|(1-\xi_2^2)^{\frac{r}{2}} \partial_{\xi_2}^r u(\xi_1, \cdot, \xi_3)\|_{I_2}^2 d\xi_1 d\xi_3 \\ &+ \int_{I_2}\int_{I_1} \|(1-\xi_3^2)^{\frac{r}{2}} \partial_{\xi_3}^r u(\xi_1, \xi_2, \cdot)\|_{I_3}^2 d\xi_1 d\xi_2. \end{aligned}$$

Throughout this paper, we denote by c a generic constant independent of any function and N. According to Theorem 2.1 of [19], we know that if $u \in L^2(K)$, and $\mathbb{A}_{r,K}(u)$ is finite for integers $r \ge 0, r \le N+1$, then

$$\|P_{N,K}u - u\|_K^2 \le cN^{-2r}\mathbb{A}_{r,K}(u). \tag{1}$$

Next, let $V_N^0(K) = H_0^1(K) \cap V_N(K)$. The $H_0^1(K)-$orthogonal projection $P_{N,K}^{1,0}$: $H_0^1(K) \to V_N^0(K)$ is defined by

$$(\nabla(P_{N,K}^{1,0}u - u), \nabla\phi)_K = 0, \qquad \forall \phi \in V_N^0(K).$$

For any integer $r \ge 1$, we define

$$\mathbb{B}_{r,K}(u) = \mathbb{B}_{r,K}^{(1)}(u) + \mathbb{B}_{r,K}^{(2)}(u) + \mathbb{B}_{r,K}^{(3)}(u), \tag{2}$$

where for $r = 1, 2$,

$$\mathbb{B}_{r,K}^{(1)}(u) = \mathbb{B}_{r,K}^{(2)}(u) = \mathbb{B}_{r,K}^{(3)}(u) = ||u||_{r,K}^2,$$

and for $r \ge 3$,

(3)

$$\mathbb{B}_{r,K}^{(1)}(u) = \int\int\int_K ((1-\xi_1^2)^{r-1}(\partial_{\xi_1}^r u)^2 + (1-\xi_2^2)^{r-1}(\partial_{\xi_2}^r u)^2 + (1-\xi_3^2)^{r-1}(\partial_{\xi_3}^r u)^2) d\xi_1 d\xi_2 d\xi_3,$$

$$\begin{aligned} \mathbb{B}_{r,K}^{(2)}(u) &= \int\int\int_K (1-\xi_1^2)^{r-2}((\partial_{\xi_1}^{r-1}\partial_{\xi_2}u)^2 + (\partial_{\xi_1}^{r-1}\partial_{\xi_3}u)^2) d\xi_1 d\xi_2 d\xi_3 \\ &+ \int\int\int_K (1-\xi_2^2)^{r-2}((\partial_{\xi_1}\partial_{\xi_2}^{r-1}u)^2 + (\partial_{\xi_2}^{r-1}\partial_{\xi_3}u)^2) d\xi_1 d\xi_2 d\xi_3 \\ &+ \int\int\int_K (1-\xi_3^2)^{r-2}((\partial_{\xi_2}\partial_{\xi_3}^{r-1}u)^2 + (\partial_{\xi_1}\partial_{\xi_3}^{r-1}u)^2) d\xi_1 d\xi_2 d\xi_3, \end{aligned} \tag{4}$$

(5)

$$\mathbb{B}^{(3)}_{r,K}(u) = \int\int\int_K ((1-\xi_1^2)^{r-3}(\partial^{r-2}_{\xi_1}\partial_{\xi_2}\partial_{\xi_3}u)^2 + (1-\xi_2^2)^{r-3}(\partial_{\xi_1}\partial^{r-2}_{\xi_2}\partial_{\xi_3}u)^2 + (1-\xi_3^2)^{r-3}(\partial_{\xi_1}\partial_{\xi_2}\partial^{r-2}_{\xi_3}u)^2)d\xi_1 d\xi_2 d\xi_3.$$

According to Theorem 2.3 of [19], we have that if $u \in H^1_0(K)$ and $\mathbb{B}_{r,K}(u)$ is finite for integers $1 \le r \le N+1$, then

$$\|P^{1,0}_{N,K}u - u\|^2_{\mu,K} \le cN^{2\mu-2r}\mathbb{B}_{r,K}(u), \qquad \mu = 0,1. \tag{6}$$

In many practical problems, Neumann or Robin boundary conditions are imposed on certain parts of the boundary of K. For solving such mixed boundary value problems, we need several specific projections. For instance, we set

$$\begin{aligned} {}^0H^1(K) &= \{u \in H^1(K) \mid u(1,\xi_2,\xi_3) = u(\xi_1,1,\xi_3) = u(\xi_1,\xi_2,1) = 0\}, \\ {}^0V_N(K) &= {}^0H^1(K) \cap V_N(K). \end{aligned}$$

The orthogonal projection ${}^0P^1_{N,K} : {}^0H^1(K) \to {}^0V_N(K)$ is given by

$$(\nabla({}^0P^1_{N,K}u - u), \nabla\phi) = 0, \qquad \forall\phi \in {}^0V_{N_K}(K).$$

It was shown in Theorem 2.4 of [19] that if $u \in {}^0H^1(K)$ and $\mathbb{B}_{r,K}(u)$ is finite for integers $1 \le r \le N+1$, then

$$\|{}^0P^1_{N,K}u - u\|^2_{\mu,K} \le cN^{2\mu-2r}\mathbb{B}_{r,K}(u), \qquad \mu = 0,1. \tag{7}$$

Remark 2.1. *In the same manner, we may define the orthogonal projections and derive their error estimates for functions in $H^1(K)$, vanishing on other faces.*

3. Irrational orthogonal approximation on hexahedrons

In this section, we propose the irrational orthogonal approximation on hexahedrons, which serves as the mathematical foundation of spectral method on hexahedrons.

3.1. Variable transformation. Let $\boldsymbol{x} = (x_1, x_2, x_3)$ and Ω be a convex hexahedron with the eight vertices $Q_j = (x_{j1}, x_{j2}, x_{j3}), 1 \le j \le 8$, see Figure 1.

(8)

$$\begin{aligned}
\sigma_1(\xi_1,\xi_2,\xi_3) &= \frac{1}{8}(1-\xi_1)(1-\xi_2)(1-\xi_3), & \sigma_2(\xi_1,\xi_2,\xi_3) &= \frac{1}{8}(1+\xi_1)(1-\xi_2)(1-\xi_3),\\
\sigma_3(\xi_1,\xi_2,\xi_3) &= \frac{1}{8}(1+\xi_1)(1+\xi_2)(1-\xi_3), & \sigma_4(\xi_1,\xi_2,\xi_3) &= \frac{1}{8}(1-\xi_1)(1+\xi_2)(1-\xi_3),\\
\sigma_5(\xi_1,\xi_2,\xi_3) &= \frac{1}{8}(1-\xi_1)(1-\xi_2)(1+\xi_3), & \sigma_6(\xi_1,\xi_2,\xi_3) &= \frac{1}{8}(1+\xi_1)(1-\xi_2)(1+\xi_3),\\
\sigma_7(\xi_1,\xi_2,\xi_3) &= \frac{1}{8}(1+\xi_1)(1+\xi_2)(1+\xi_3), & \sigma_8(\xi_1,\xi_2,\xi_3) &= \frac{1}{8}(1-\xi_1)(1+\xi_2)(1+\xi_3).
\end{aligned}$$

We make a coordinate transformation

$$x_i(\xi_1,\xi_2,\xi_3) = \sum_{j=1}^{8} x_{ji}\sigma_j(\xi_1,\xi_2,\xi_3), \qquad i = 1,2,3. \tag{9}$$

More precisely,

(10)

$$x_i = b_{i0} + b_{i1}\xi_1 + b_{i2}\xi_2 + b_{i3}\xi_3 + b_{i4}\xi_1\xi_2 + b_{i5}\xi_1\xi_3 + b_{i6}\xi_2\xi_3 + b_{i7}\xi_1\xi_2\xi_3, \qquad i = 1,2,3.$$

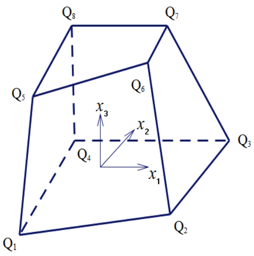

FIGURE 1. Hexahedron Ω.

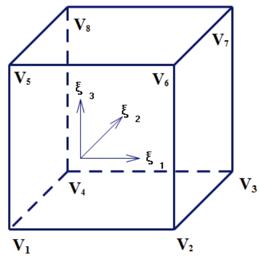

FIGURE 2. Cube K.

where

$$
\begin{aligned}
b_{i0} &= \frac{1}{8}(x_{1i}+x_{2i}+x_{3i}+x_{4i}+x_{5i}+x_{6i}+x_{7i}+x_{8i}),\\
b_{i1} &= \frac{1}{8}(-x_{1i}+x_{2i}+x_{3i}-x_{4i}-x_{5i}+x_{6i}+x_{7i}-x_{8i}),\\
b_{i2} &= \frac{1}{8}(-x_{1i}-x_{2i}+x_{3i}+x_{4i}-x_{5i}-x_{6i}+x_{7i}+x_{8i}),\\
b_{i3} &= \frac{1}{8}(-x_{1i}-x_{2i}-x_{3i}-x_{4i}+x_{5i}+x_{6i}+x_{7i}+x_{8i}),\\
b_{i4} &= \frac{1}{8}(x_{1i}-x_{2i}+x_{3i}-x_{4i}+x_{5i}-x_{6i}+x_{7i}-x_{8i}),\\
b_{i5} &= \frac{1}{8}(x_{1i}-x_{2i}-x_{3i}+x_{4i}-x_{5i}+x_{6i}+x_{7i}-x_{8i}),\\
b_{i6} &= \frac{1}{8}(x_{1i}+x_{2i}-x_{3i}-x_{4i}-x_{5i}-x_{6i}+x_{7i}+x_{8i}),\\
b_{i7} &= \frac{1}{8}(-x_{1i}+x_{2i}-x_{3i}+x_{4i}+x_{5i}-x_{6i}+x_{7i}-x_{8i}).
\end{aligned}
\tag{11}
$$

By the transformation (9), the hexahedron Ω is mapped to the reference cube K with the vertices $V_j = (\xi_{j1}, \xi_{j2}, \xi_{j3})$ corresponding to Q_j for $1 \le j \le 8$, see Figure 2. Indeed, we have

$$
\begin{aligned}
&\begin{pmatrix}
\xi_{11} & \xi_{21} & \xi_{31} & \xi_{41} & \xi_{51} & \xi_{61} & \xi_{71} & \xi_{81}\\
\xi_{12} & \xi_{22} & \xi_{32} & \xi_{42} & \xi_{52} & \xi_{62} & \xi_{72} & \xi_{82}\\
\xi_{13} & \xi_{23} & \xi_{33} & \xi_{43} & \xi_{53} & \xi_{63} & \xi_{73} & \xi_{83}
\end{pmatrix}\\
&= \begin{pmatrix}
-1 & 1 & 1 & -1 & -1 & 1 & 1 & -1\\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & 1\\
-1 & -1 & -1 & -1 & 1 & 1 & 1 & 1
\end{pmatrix}.
\end{aligned}
$$

If Ω is a parallelepiped, then $b_{i\nu} = 0$ for $4 \le \nu \le 7, i = 1, 2, 3$. In this case, the transformation (9) is reduced to an affine mapping.

For simplicity, we denote $\dfrac{\partial x_1}{\partial \xi_1}$ by $\partial_{\xi_1} x_1$, ect.. The Jacobi matrix of transformation of (9) is

$$
M_\Omega(\boldsymbol{\xi}) = \begin{pmatrix}
\partial_{\xi_1} x_1 & \partial_{\xi_1} x_2 & \partial_{\xi_1} x_3\\
\partial_{\xi_2} x_1 & \partial_{\xi_2} x_2 & \partial_{\xi_2} x_3\\
\partial_{\xi_3} x_1 & \partial_{\xi_3} x_2 & \partial_{\xi_3} x_3
\end{pmatrix} =
$$

$$
\begin{pmatrix}
b_{11}+b_{14}\xi_2+b_{15}\xi_3+b_{17}\xi_2\xi_3 & b_{21}+b_{24}\xi_2+b_{25}\xi_3+b_{27}\xi_2\xi_3 & b_{31}+b_{34}\xi_2+b_{35}\xi_3+b_{37}\xi_2\xi_3\\
b_{12}+b_{14}\xi_1+b_{16}\xi_3+b_{17}\xi_1\xi_3 & b_{22}+b_{24}\xi_1+b_{26}\xi_3+b_{27}\xi_1\xi_3 & b_{32}+b_{34}\xi_1+b_{36}\xi_3+b_{37}\xi_1\xi_3\\
b_{13}+b_{15}\xi_1+b_{16}\xi_2+b_{17}\xi_1\xi_2 & b_{23}+b_{25}\xi_1+b_{26}\xi_2+b_{27}\xi_1\xi_2 & b_{33}+b_{35}\xi_1+b_{36}\xi_2+b_{37}\xi_1\xi_2
\end{pmatrix}.
$$

Its Jacobian determinant is denoted by $J_\Omega(\boldsymbol{\xi})$. We assume that hexahedron Ω is convex. Therefore, there exist positive constants δ_Ω and δ_Ω^* such that

$$0 < \delta_\Omega \le J_\Omega(\boldsymbol{\xi}) \le \delta_\Omega^*. \tag{12}$$

The inverse of transformation (9) is given by $\boldsymbol{\xi} = \boldsymbol{\xi}(\boldsymbol{x})$, namely, $\xi_i = \xi_i(x_1, x_2, x_3),\ i = 1, 2, 3$. They are irrational functions generally. The Jacobi matrix of the above inverse transformation is

$$M_K(\boldsymbol{x}) = M_\Omega^{-1}(\boldsymbol{\xi})|_{\boldsymbol{\xi}=\boldsymbol{x}} = \begin{pmatrix} \partial_{x_1}\xi_1 & \partial_{x_1}\xi_2 & \partial_{x_1}\xi_3 \\ \partial_{x_2}\xi_1 & \partial_{x_2}\xi_2 & \partial_{x_2}\xi_3 \\ \partial_{x_3}\xi_1 & \partial_{x_3}\xi_2 & \partial_{x_3}\xi_3. \end{pmatrix}. \tag{13}$$

Its Jacobian determinant is denoted by $J_K(\boldsymbol{x})$. Thanks to (12), we assert that

$$0 < \frac{1}{\delta_\Omega^*} \le J_K(\boldsymbol{x}) = \frac{1}{J_\Omega(\boldsymbol{\xi}(\boldsymbol{x}))} \le \frac{1}{\delta_\Omega}. \tag{14}$$

3.2. $L^2(\Omega)$-irrational orthogonal approximation on hexahedron. We define the spaces $H^r(\Omega)$ and $H_0^r(\Omega)$ in the usual way, with the norm $||u||_{r,\Omega}$. The inner product and the norm of $L^2(\Omega)$ are denoted by $(u, v)_\Omega$ and $||u||_\Omega$, respectively.

For nonnegative integers l, m and n, we introduce the following irrational functions on the hexahedron Ω,

$$\psi_{l,m,n}(\boldsymbol{x}) = L_l(\xi_1(x_1, x_2, x_3))L_m(\xi_2(x_1, x_2, x_3))L_n(\xi_3(x_1, x_2, x_3)). \tag{15}$$

Let

$$V_N(\Omega) = span\{\ \psi_{l,m,n}(\boldsymbol{x}) \mid 0 \le l, m, n \le N\ \}.$$

The $L^2(\Omega)$-irrational orthogonal projection $P_{N,\Omega} : L^2(\Omega) \to V_N(\Omega)$, is defined by

$$(P_{N,\Omega}v - v, \phi)_\Omega = 0, \qquad \forall \phi \in V_N(\Omega). \tag{16}$$

Let d_Ω be the length of the longest edge of Ω. For characterizing the approximation error, we introduce the quantity

$$\mathbb{A}_{r,\Omega}(v) = d_\Omega^{2r} \sum_{i=1}^{3} \sum_{k=0}^{r} \sum_{j=0}^{k} \|(1 - \xi_i^2)^{\frac{r}{2}} \partial_{x_1}^j \partial_{x_2}^{k-j} \partial_{x_3}^{r-k} v\|_\Omega^2.$$

Theorem 3.1. If $v \in L^2(\Omega)$, and $\mathbb{A}_{r,\Omega}(v)$ is finite for integers $r \ge 0$ and $r \le N + 1$, then

$$\|P_{N,\Omega}v - v\|_\Omega^2 \le c\delta_\Omega^* \delta_\Omega^{-1} N^{-2r} \mathbb{A}_{r,\Omega}(v). \tag{17}$$

Proof. By the projection theorem, we have

$$\|P_{N,\Omega}v - v\|_\Omega^2 \le \|\phi - v\|_\Omega^2, \qquad \forall \phi \in V_N(\Omega).$$

Let $u(\boldsymbol{\xi}) = v(x_1(\boldsymbol{\xi}), x_2(\boldsymbol{\xi}), x_3(\boldsymbol{\xi}))$, and

$$\psi(\boldsymbol{\xi}) = P_{N,K}u(\boldsymbol{\xi}), \qquad \phi(\boldsymbol{x}) = \psi(\xi_1(\boldsymbol{x}), \xi_2(\boldsymbol{x}), \xi_3(\boldsymbol{x})) \in V_N(\Omega).$$

By using (1) and (14), we obtain

$$\|\phi - v\|_\Omega^2 = \int\int\int_K (u - P_{N,K}u)^2 J_\Omega(\boldsymbol{\xi}) d\xi_1 d\xi_2 d\xi_3 \le c\delta_\Omega^* N^{-2r} \mathbb{A}_{r,K}(u). \tag{18}$$

By virtue of (10), a direct calculation shows

(19)

$$\partial_{\xi_i}^r u = \sum_{k=0}^{r} \sum_{j=0}^{k} C_r^k C_k^j (\partial_{\xi_i} x_1)^j (\partial_{\xi_i} x_2)^{k-j} (\partial_{\xi_i} x_3)^{r-k} \partial_{x_1}^j \partial_{x_2}^{k-j} \partial_{x_3}^{r-k} v, \quad i = 1, 2, 3.$$

Moreover, we see from (10) that

$$|\partial_{\xi_1} x_1| = |b_{11} + b_{14}\xi_2 + b_{15}\xi_3 + b_{17}\xi_2\xi_3| \le 2d_\Omega, \qquad \text{etc..} \tag{20}$$

Therefore, we use (19), (20) and (14) successively, to derive that $\mathbb{A}_{r,K}(u) \le c\delta_\Omega^{-1}\mathbb{A}_{r,\Omega}(v)$. This, along with (18), leads to the desired result.

Remark 3.1. *In the norms of derivatives $\partial_{x_1}^j \partial_{x_2}^{k-j} \partial_{x_3}^{r-k} v$ involved in the quantity $\mathbb{A}_{r,\Omega}(v)$, there are the weight functions $(1-\xi_1^2)^{\frac{r}{2}}, (1-\xi_2^2)^{\frac{r}{2}}$ or $(1-\xi_3^2)^{\frac{r}{2}}$, which tend to zero simultaneously as the point $Q(x_1, x_2, x_3)$ goes to the vertices of Ω. As a result, $\|P_{N,\Omega}v - v\|_\Omega$ still keeps the order N^{-r}, even if the approximated function has certain weak singularity at the vertices of Ω.*

Remark 3.2 *If $\Omega = K_{a_1,a_2,a_3} = \{(x_1,x_2,x_3) \mid |x_i| < a_i,\ i = 1,2,3\}$, then $x_i = a_i\xi_i,\ i = 1,2,3$. In this case, $J_\Omega = a_1a_2a_3$ and*

$$\|P_{N,\Omega}v - v\|_\Omega^2 \le cN^{-2r} \sum_{i=1}^{3} \|(a_i^2 - x_i^2)^{\frac{r}{2}} \partial_{x_i}^r v\|_\Omega^2.$$

Thus, the $L^2(\Omega)$-irrational orthogonal approximation turns out to be the Legendre orthogonal approximation. It keeps the same spectral accuracy, even if the considered function possesses certain singularity on the faces of Ω.

3.3. Irrational orthogonal approximation in $H_0^1(\Omega)$.

We now turn to the $H_0^1(\Omega)$-irrational orthogonal approximation. According to Poincaré inequality, there exists a positive constant c_Ω such that

$$\|w\|_\Omega \le c_\Omega \|\nabla w\|_\Omega, \qquad \forall w \in H_0^1(\Omega). \tag{21}$$

Let $V_N^0(\Omega) = H_0^1(\Omega) \cap V_N(\Omega)$. The $H_0^1(\Omega)$-irrational orthogonal projection $P_{N,\Omega}^{1,0} : H_0^1(\Omega) \to V_N^0(\Omega)$ is defined by

$$(\nabla(P_{N,\Omega}^{1,0}v - v), \nabla\phi)_\Omega = 0, \qquad \forall \phi \in V_N^0(\Omega). \tag{22}$$

For simplicity of statements, let $x_4 = x_1$ and $x_5 = x_2$. We also introduce the quantity $\mathbb{B}_{r,\Omega}(v)$ as follows,

(23)
$$\begin{aligned} &\mathbb{B}_{1,\Omega}(v) = \delta_\Omega^{-1} d_\Omega^2 |v|_{H^1(\Omega)}^2, \qquad \mathbb{B}_{2,\Omega}(v) = \delta_\Omega^{-1} d_\Omega^4 |v|_{H^2(\Omega)}^2 + \delta_\Omega^{-1} d_\Omega^2 |v|_{H^1(\Omega)}^2, \\ &\mathbb{B}_{r,\Omega}(v) = \mathbb{B}_{r,\Omega}^{(1)}(v) + \mathbb{B}_{r,\Omega}^{(2)}(v) + \mathbb{B}_{r,\Omega}^{(3)}(v), \qquad r \ge 3, \end{aligned}$$

where

$$\mathbb{B}_{r,\Omega}^{(1)}(v) = \delta_\Omega^{-1} d_\Omega^{2r} \sum_{i=1}^{3} \sum_{k=0}^{r} \sum_{j=0}^{k} \|(1-\xi_i^2)^{\frac{r-1}{2}} \partial_{x_1}^j \partial_{x_2}^{k-j} \partial_{x_3}^{r-k} v\|_\Omega^2, \qquad r \ge 3, \tag{24}$$

(25)
$$\begin{aligned} \mathbb{B}_{r,\Omega}^{(2)}(v) \quad &= \delta_\Omega^{-1} d_\Omega^{2r} \sum_{\nu=1}^{3} \sum_{i=1}^{3} \sum_{k=0}^{r-1} \sum_{j=0}^{k} \|(1-\xi_\nu^2)^{\frac{r-2}{2}} \partial_{x_1}^j \partial_{x_2}^{k-j} \partial_{x_3}^{r-k-1} \partial_{x_i} v\|_\Omega^2 \\ &+\delta_\Omega^{-1} d_\Omega^{2r-2} \sum_{\nu=1}^{3} \sum_{i=1}^{3} \sum_{k=0}^{r-2} \sum_{j=0}^{k} \|(1-\xi_\nu^2)^{\frac{r-2}{2}} \partial_{x_1}^j \partial_{x_2}^{k-j} \partial_{x_3}^{r-k-2} \partial_{x_i} v\|_\Omega^2, \quad r \ge 3, \end{aligned}$$

(26)

$$\begin{aligned}
\mathbb{B}^{(3)}_{r,\Omega}(v) &= \delta_\Omega^{-1} d_\Omega^{2r} \sum_{\nu=1}^{3}\sum_{i=1}^{3}\sum_{k=0}^{r-2}\sum_{j=0}^{k}(\|(1-\xi_\nu^2)^{\frac{r-3}{2}}\partial^j_{x_1}\partial^{k-j}_{x_2}\partial^{r-k-2}_{x_3}\partial_{x_i}\partial_{x_{i+1}}v\|^2_\Omega\\
&+\|(1-\xi_\nu^2)^{\frac{r-3}{2}}\partial^j_{x_1}\partial^{k-j}_{x_2}\partial^{r-k-2}_{x_3}\partial^2_{x_i}v\|^2_\Omega + d_\Omega^{-2}\|(1-\xi_\nu^2)^{\frac{r-3}{2}}\partial^j_{x_1}\partial^{k-j}_{x_2}\partial^{r-k-2}_{x_3}\partial_{x_i}v\|^2_\Omega)\\
&+\delta_\Omega^{-1} d_\Omega^{2r-2} \sum_{\nu=1}^{3}\sum_{i=1}^{3}\sum_{k=0}^{r-3}\sum_{j=0}^{k}(\|(1-\xi_\nu^2)^{\frac{r-3}{2}}\partial^j_{x_1}\partial^{k-j}_{x_2}\partial^{r-k-3}_{x_3}\partial_{x_i}\partial_{x_{i+1}}v\|^2_\Omega\\
&+\|(1-\xi_\nu^2)^{\frac{r-3}{2}}\partial^j_{x_1}\partial^{k-j}_{x_2}\partial^{r-k-3}_{x_3}\partial^2_{x_i}v\|^2_\Omega + d_\Omega^{-2}\|(1-\xi_\nu^2)^{\frac{r-3}{2}}\partial^j_{x_1}\partial^{k-j}_{x_2}\partial^{r-k-3}_{x_3}\partial_{x_i}v\|^2_\Omega)\\
&+\delta_\Omega^{-1} d_\Omega^{2r-4} \sum_{\nu=1}^{3}\sum_{i=1}^{3}\sum_{k=0}^{r-4}\sum_{j=0}^{k}(\|(1-\xi_\nu^2)^{\frac{r-3}{2}}\partial^j_{x_1}\partial^{k-j}_{x_2}\partial^{r-k-4}_{x_3}\partial_{x_i}\partial_{x_{i+1}}v\|^2_\Omega\\
&+\|(1-\xi_\nu^2)^{\frac{r-3}{2}}\partial^j_{x_1}\partial^{k-j}_{x_2}\partial^{r-k-4}_{x_3}\partial^2_{x_i}v\|^2_\Omega), \qquad r\ge 4,
\end{aligned}$$

and

$$\mathbb{B}^{(3)}_{3,\Omega}(v) = \delta_\Omega^{-1}\sum_{\lambda=1}^{3} d_\Omega^{2\lambda}|v|^2_{H^\lambda(\Omega)}. \tag{27}$$

Theorem 3.2. If $v\in H^1_0(\Omega)$ and $\mathbb{B}_{r,\Omega}(v)$ is finite for integers $1\le r\le N+1$, then

$$\begin{aligned}
&\|\nabla(P^{1,0}_{N,\Omega}v - v)\|^2_\Omega \le c d_\Omega^4\delta_\Omega^{-1}N^{2-2r}\mathbb{B}_{r,\Omega}(v),\\
&\|P^{1,0}_{N,\Omega}v - v\|^2_\Omega \le c\bar{c}^2_\Omega(c^2_\Omega+1)^2 d_\Omega^{10}(d_\Omega+1)^2\delta_\Omega^{-3}N^{-2r}\mathbb{B}_{r,\Omega}(v),
\end{aligned} \tag{28}$$

where $\bar{c}_\Omega$ is a positive constant determined in (43) of this paper.

Proof. By the projection theorem,

$$\|\nabla(P^{1,0}_{N,\Omega}v - v)\|^2_\Omega \le \|\nabla(\phi - v)\|^2_\Omega, \qquad \forall \phi\in V^0_N(\Omega). \tag{29}$$

Let $u(\boldsymbol{\xi})$ be the same as before, and

$$\psi(\boldsymbol{\xi}) = P^{1,0}_{N,K}u(\boldsymbol{\xi}), \qquad \phi(\boldsymbol{x}) = \psi(\xi_1(\boldsymbol{x}),\xi_2(\boldsymbol{x}),\xi_3(\boldsymbol{x}))\in V^0_N(\Omega).$$

Let $\nabla_K w = (\partial_{\xi_1}w, \partial_{\xi_2}w, \partial_{\xi_3}w)^T$. It can be shown that $\nabla_K w = M_\Omega\nabla w$. Let M^*_Ω be the adjoint matrix of M_Ω. Then $\nabla w = M_\Omega^{-1}\nabla_K w = J_\Omega^{-1}M^*_\Omega\nabla_K w$. Hence, we use (6), (14) and some inequalities like (20), to verify that

$$\begin{aligned}
\|\nabla(\phi - v)\|^2_\Omega &= \int\int\int_K (M^*_\Omega\nabla_K(u - P^{1,0}_{N,K}u))^2 J_\Omega^{-1}(\boldsymbol{\xi})d\xi_1 d\xi_2 d\xi_3\\
&\le c d_\Omega^4\delta_\Omega^{-1}N^{2-2r}\mathbb{B}_{r,K}(u).
\end{aligned} \tag{30}$$

We are going to estimate the upper-bound of $\mathbb{B}_{r,K}(u)$ appearing in (30).

We first deal with the upper-bound of $\mathbb{B}^{(1)}_{r,K}(u)$ for $r\ge 3$, which is defined by (3). Using (14), (19) and some inequalities like (20), we verify that for $r\ge 3$,

$$\mathbb{B}^{(1)}_{r,K}(u) \le c\mathbb{B}^{(1)}_{r,\Omega}(v). \tag{31}$$

Next, we derive an upper-bound of $\mathbb{B}^{(2)}_{r,K}(u)$ for $r \geq 3$, which is defined by (4). A calculation yields that

(32)

$$\begin{aligned}
&\partial_{\xi_1}^{r-1}\partial_{\xi_2}u\\
=\ &\sum_{k=0}^{r-1}\sum_{j=0}^{k} C_{r-1}^k C_k^j(\partial_{\xi_1}x_1)^j(\partial_{\xi_1}x_2)^{k-j}(\partial_{\xi_1}x_3)^{r-1-k}(\partial_{\xi_2}x_1\partial_{x_1}^{j+1}\partial_{x_2}^{k-j}\partial_{x_3}^{r-1-k}v\\
&\quad+\partial_{\xi_2}x_2\partial_{x_1}^{j}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-1-k}v+\partial_{\xi_2}x_3\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k}v)\\
&\quad+(r-1)\sum_{k=0}^{r-2}\sum_{j=0}^{k} C_{r-2}^k C_k^j(\partial_{\xi_1}x_1)^j(\partial_{\xi_1}x_2)^{k-j}(\partial_{\xi_1}x_3)^{r-2-k}\partial_{\xi_1}\partial_{\xi_2}x_1\partial_{x_1}^{j+1}\partial_{x_2}^{k-j}\partial_{x_3}^{r-2-k}v\\
&\quad+\partial_{\xi_1}\partial_{\xi_2}x_2\partial_{x_1}^{j}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-2-k}v+\partial_{\xi_1}\partial_{\xi_2}x_3\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-1-k}v),\\
&\partial_{\xi_1}^{r-1}\partial_{\xi_3}u\\
=\ &\sum_{k=0}^{r-1}\sum_{j=0}^{k} C_{r-1}^k C_k^j(\partial_{\xi_1}x_1)^j(\partial_{\xi_1}x_2)^{k-j}(\partial_{\xi_1}x_3)^{r-1-k}(\partial_{\xi_3}x_1\partial_{x_1}^{j+1}\partial_{x_2}^{k-j}\partial_{x_3}^{r-1-k}v\\
&\quad+\partial_{\xi_3}x_2\partial_{x_1}^{j}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-1-k}v+\partial_{\xi_3}x_3\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k}v)\\
&\quad+(r-1)\sum_{k=0}^{r-2}\sum_{j=0}^{k} C_{r-2}^k C_k^j(\partial_{\xi_1}x_1)^j(\partial_{\xi_1}x_2)^{k-j}(\partial_{\xi_1}x_3)^{r-2-k}(\partial_{\xi_1}\partial_{\xi_3}x_1\partial_{x_1}^{j+1}\partial_{x_2}^{k-j}\partial_{x_3}^{r-2-k}v\\
&\quad+\partial_{\xi_1}\partial_{\xi_3}x_2\partial_{x_1}^{j}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-2-k}v+\partial_{\xi_1}\partial_{\xi_3}x_3\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-1-k}v).
\end{aligned}$$

Moreover, with the aid of (10), we deduce that

$$|\partial_{\xi_1}\partial_{\xi_2}x_1| = |b_{14}+b_{17}\xi_3| \leq d_\Omega, \qquad \text{etc..} \tag{33}$$

Thus, together with (32) and (33), an argument similar to the derivation of (31) leads to

$$\begin{aligned}
&\int\int\int_K (1-\xi_1^2)^{r-2}((\partial_{\xi_1}^{r-1}\partial_{\xi_2}u)^2+(\partial_{\xi_1}^{r-1}\partial_{\xi_3}u)^2)d\xi_1 d\xi_2 d\xi_3\\
&\quad\leq c\delta_\Omega^{-1}d_\Omega^{2r}\sum_{i=1}^{3}\sum_{k=0}^{r-1}\sum_{j=0}^{k}\|(1-\xi_1^2)^{\frac{r-2}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-1}\partial_{x_i}v\|_\Omega^2\\
&\qquad+c\delta_\Omega^{-1}d_\Omega^{2r-2}\sum_{i=1}^{3}\sum_{k=0}^{r-2}\sum_{j=0}^{k}\|(1-\xi_1^2)^{\frac{r-2}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-2}\partial_{x_i}v\|_\Omega^2.
\end{aligned} \tag{34}$$

We could obtain the upper-bounds for the other two terms appearing in (4) similarly, with a modification of replacing the weights in (34) by $(1-\xi_2^2)^{\frac{r-2}{2}}$ or $(1-\xi_3^2)^{\frac{r-2}{2}}$, respectively. Consequently, we reach that

$$\mathbb{B}^{(2)}_{r,K}(u) \leq c\mathbb{B}^{(2)}_{r,\Omega}(v), \qquad r \geq 3. \tag{35}$$

Finally, we derive an upper-bound of $\mathbb{B}^{(3)}_{r,K}(u)$ for $r \geq 3$, which is defined by (5). We have for $r \geq 4$ that

(36)

$$
\begin{aligned}
\partial_{\xi_1}^{r-2}\partial_{\xi_2}\partial_{\xi_3}u = & \sum_{k=0}^{r-2}\sum_{j=0}^{k} C_{r-2}^{k} C_{k}^{j} (\partial_{\xi_1}x_1)^j(\partial_{\xi_1}x_2)^{k-j}(\partial_{\xi_1}x_3)^{r-2-k} \\
& \times(\partial_{\xi_2}x_1\partial_{\xi_3}x_1\partial_{x_1}^{j+2}\partial_{x_2}^{k-j}\partial_{x_3}^{r-2-k}v \\
& +\partial_{\xi_2}x_2\partial_{\xi_3}x_2\partial_{x_1}^{j}\partial_{x_2}^{k+2-j}\partial_{x_3}^{r-2-k}v + \partial_{\xi_2}x_3\partial_{\xi_3}x_3\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k}v \\
& +\partial_{\xi_2}\partial_{\xi_3}x_1\partial_{x_1}^{j+1}\partial_{x_2}^{k-j}\partial_{x_3}^{r-2-k}v + (\partial_{\xi_2}x_1\partial_{\xi_3}x_3 + \partial_{\xi_3}x_1\partial_{\xi_2}x_3)\partial_{x_1}^{j+1}\partial_{x_2}^{k-j}\partial_{x_3}^{r-1-k}v \\
& +\partial_{\xi_2}\partial_{\xi_3}x_2\partial_{x_1}^{j}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-2-k}v + (\partial_{\xi_2}x_2\partial_{\xi_3}x_3 + \partial_{\xi_3}x_2\partial_{\xi_2}x_3)\partial_{x_1}^{j}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-1-k}v \\
& +\partial_{\xi_2}\partial_{\xi_3}x_3\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-1-k}v + (\partial_{\xi_2}x_1\partial_{\xi_3}x_2 + \partial_{\xi_3}x_1\partial_{\xi_2}x_2)\partial_{x_1}^{j+1}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-2-k}v) \\
& +C_{r-2}^{1}\sum_{k=0}^{r-3}\sum_{j=0}^{k} C_{r-3}^{k}C_{k}^{j}(\partial_{\xi_1}x_1)^j(\partial_{\xi_1}x_2)^{k-j} \\
& \times(\partial_{\xi_1}x_3)^{r-3-k}(\partial_{\xi_1}(\partial_{\xi_2}x_1\partial_{\xi_3}x_1)\partial_{x_1}^{j+2}\partial_{x_2}^{k-j}\partial_{x_3}^{r-3-k}v \\
& +\partial_{\xi_1}(\partial_{\xi_2}x_2\partial_{\xi_3}x_2)\partial_{x_1}^{j}\partial_{x_2}^{k+2-j}\partial_{x_3}^{r-3-k}v + \partial_{\xi_1}(\partial_{\xi_2}x_3\partial_{\xi_3}x_3)\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-1-k}v \\
& +\partial_{\xi_1}\partial_{\xi_2}\partial_{\xi_3}x_1\partial_{x_1}^{j+1}\partial_{x_2}^{k-j}\partial_{x_3}^{r-3-k}v \\
& +\partial_{\xi_1}(\partial_{\xi_2}x_1\partial_{\xi_3}x_2 + \partial_{\xi_3}x_1\partial_{\xi_2}x_2)\partial_{x_1}^{j+1}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-3-k}v \\
& +\partial_{\xi_1}\partial_{\xi_2}\partial_{\xi_3}x_2\partial_{x_1}^{j}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-3-k}v \\
& +\partial_{\xi_1}(\partial_{\xi_2}x_1\partial_{\xi_3}x_3 + \partial_{\xi_3}x_1\partial_{\xi_2}x_3)\partial_{x_1}^{j+1}\partial_{x_2}^{k-j}\partial_{x_3}^{r-2-k}v \\
& +\partial_{\xi_1}\partial_{\xi_2}\partial_{\xi_3}x_3\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-2-k}v \\
& +\partial_{\xi_1}(\partial_{\xi_2}x_2\partial_{\xi_3}x_3 + \partial_{\xi_3}x_2\partial_{\xi_2}x_3)\partial_{x_1}^{j}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-2-k}v) \\
& +C_{r-2}^{2}\sum_{k=0}^{r-4}\sum_{j=0}^{k} C_{r-4}^{k}C_{k}^{j}(\partial_{\xi_1}x_1)^j(\partial_{\xi_1}x_2)^{k-j}(\partial_{\xi_1}x_3)^{r-4-k} \\
& \times(\partial_{\xi_1}^2(\partial_{\xi_2}x_1\partial_{\xi_3}x_1)\partial_{x_1}^{j+2}\partial_{x_2}^{k-j}\partial_{x_3}^{r-4-k}v \\
& +\partial_{\xi_1}^2(\partial_{\xi_2}x_2\partial_{\xi_3}x_2)\partial_{x_1}^{j}\partial_{x_2}^{k+2-j}\partial_{x_3}^{r-4-k}v \\
& +\partial_{\xi_1}^2(\partial_{\xi_2}x_1\partial_{\xi_3}x_2 + \partial_{\xi_3}x_1\partial_{\xi_2}x_2)\partial_{x_1}^{j+1}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-4-k}v \\
& +\partial_{\xi_1}^2(\partial_{\xi_2}x_3\partial_{\xi_3}x_3)\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-2-k}v \\
& +\partial_{\xi_1}^2(\partial_{\xi_2}x_1\partial_{\xi_3}x_3 + \partial_{\xi_3}x_1\partial_{\xi_2}x_3)\partial_{x_1}^{j+1}\partial_{x_2}^{k-j}\partial_{x_3}^{r-3-k}v \\
& +\partial_{\xi_1}^2(\partial_{\xi_2}x_2\partial_{\xi_3}x_3 + \partial_{\xi_3}x_2\partial_{\xi_2}x_3)\partial_{x_1}^{j}\partial_{x_2}^{k+1-j}\partial_{x_3}^{r-3-k}v).
\end{aligned}
$$

Therefore, for $r \geq 4$,

(37)

$$
\begin{aligned}
& \int\int\int_K (1-\xi_1^2)^{r-3}(\partial_{\xi_1}^{r-2}\partial_{\xi_2}\partial_{\xi_3}u)^2 d\xi_1 d\xi_2 d\xi_3 \\
& \leq c\delta_\Omega^{-1}d_\Omega^{2r}\sum_{i=1}^{3}\sum_{k=0}^{r-2}\sum_{j=0}^{k}(\|(1-\xi_1^2)^{\frac{r-3}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-2}\partial_{x_i}\partial_{x_{i+1}}v\|_\Omega^2 \\
& +\|(1-\xi_1^2)^{\frac{r-3}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-2}\partial_{x_i}^2 v\|_\Omega^2 + d_\Omega^{-2}\|(1-\xi_1^2)^{\frac{r-3}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-2}\partial_{x_i}v\|_\Omega^2) \\
& +c\delta_\Omega^{-1}d_\Omega^{2r-2}\sum_{i=1}^{3}\sum_{k=0}^{r-3}\sum_{j=0}^{k}(\|(1-\xi_1^2)^{\frac{r-3}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-3}\partial_{x_i}\partial_{x_{i+1}}v\|_\Omega^2 \\
& +\|(1-\xi_1^2)^{\frac{r-3}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-3}\partial_{x_i}^2 v\|_\Omega^2 + d_\Omega^{-2}\|(1-\xi_1^2)^{\frac{r-3}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-3}\partial_{x_i}v\|_\Omega^2) \\
& +c\delta_\Omega^{-1}d_\Omega^{2r-4}\sum_{i=1}^{3}\sum_{k=0}^{r-4}\sum_{j=0}^{k}(\|(1-\xi_1^2)^{\frac{r-3}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-4}\partial_{x_i}\partial_{x_{i+1}}v\|_\Omega^2 \\
& +\|(1-\xi_1^2)^{\frac{r-3}{2}}\partial_{x_1}^{j}\partial_{x_2}^{k-j}\partial_{x_3}^{r-k-4}\partial_{x_i}^2 v\|_\Omega^2).
\end{aligned}
$$

We can estimate the other two terms involved in (5) in the same manner, and obtain their upper-bounds similar to (37). But, the weight $(1-\xi_1^2)^{r-3}$ in (5) is now replaced by $(1-\xi_2^2)^{r-3}$ or $(1-\xi_3^2)^{r-3}$, respectively. Consequently, we obtain

$$\mathbb{B}^{(3)}_{r,K}(u) \le c\mathbb{B}^{(3)}_{r,\Omega}(v), \qquad r \ge 4. \tag{38}$$

Moreover, a direct calculation yields

$$\mathbb{B}^{(3)}_{3,K}(u) \le c\delta_\Omega^{-1}\sum_{\lambda=1}^{3} d_\Omega^{2\lambda}|v|^2_{H^\lambda(\Omega)} = c\mathbb{B}^{(3)}_{3,\Omega}(v). \tag{39}$$

A combination of (31), (35), (38) and (39) leads to

$$\mathbb{B}_{r,K}(u) \le c\mathbb{B}_{r,\Omega}(v), \qquad r \ge 3. \tag{40}$$

This, together with (29) and (30), implies the first result (28) with $r \ge 3$.

On the other hand, with the aid of (2), (10), and Poincaré inequality, a direct calculation shows that

$$\begin{aligned} \mathbb{B}_{1,K}(u) &\le c\delta_\Omega^{-1} d_\Omega^2 |v|^2_{H^1(\Omega)} = c\mathbb{B}_{1,\Omega}(v), \\ \mathbb{B}_{2,K}(u) &\le c\delta_\Omega^{-1}(d_\Omega^2|v|^2_{H^1(\Omega)} + d_\Omega^4|v|^2_{H^2(\Omega)}) = c\mathbb{B}_{2,\Omega}(v). \end{aligned} \tag{41}$$

The above two inequalities, together with (29) and (30), lead to the first result (28) with $r = 1, 2$.

We now prove the second result of (28). Let $g \in L^2(\Omega)$ and consider an auxiliary problem. It is to find $w \in H_0^1(\Omega)$ such that

$$(\nabla w, \nabla z)_\Omega = (g, z)_\Omega, \qquad \forall z \in H_0^1(\Omega). \tag{42}$$

Taking $z = w$ in (42) and using (21), we obtain $\|\nabla w\|_\Omega \le c_\Omega \|g\|_\Omega$. Moreover, by the property of elliptic equation with the homogeneous boundary condition, there exists a positive constant $\bar{c}_\Omega$ such that

$$\|w\|_{H^2(\Omega)} \le \bar{c}_\Omega(\|w\|_\Omega + \|g\|_\Omega) \le \bar{c}_\Omega(c_\Omega\|\nabla w\|_\Omega + \|g\|_\Omega) \le \bar{c}_\Omega(c_\Omega^2+1)\|g\|_\Omega. \tag{43}$$

We now take $z = P^{1,0}_{N,\Omega}v - v$ in (42). Then, we use (22) and the first result of (28) to verify that for $1 \le r \le N+1$,

$$\begin{aligned} |(P^{1,0}_{N,\Omega}v - v, g)_\Omega| &= |(\nabla w, \nabla(P^{1,0}_{N,\Omega}v - v))_\Omega| = |(\nabla(P^{1,0}_{N,\Omega}w - w), \nabla(P^{1,0}_{N,\Omega}v - v))_\Omega| \\ &\le \|\nabla(P^{1,0}_{N,\Omega}w - w)\|_\Omega \|\nabla(P^{1,0}_{N,\Omega}v - v)\|_\Omega \le c d_\Omega^4 \delta_\Omega^{-1} N^{-r}(\mathbb{B}_{r,\Omega}(v))^{\frac12}(\mathbb{B}_{2,\Omega}(w))^{\frac12}. \end{aligned} \tag{44}$$

Moreover, a calculation shows that we have $(\mathbb{B}_{2,\Omega}(w))^{\frac12} \le \delta_\Omega^{-\frac12} d_\Omega(d_\Omega+1)\|w\|_{H^2(\Omega)}$. Finally, we use (43) and (44) to deduce that for $1 \le r \le N+1$,

$$\begin{aligned} \|\nabla(P^{1,0}_{N,\Omega}v - v)\|_\Omega &= \sup_{g\in L^2(\Omega), g\ne 0} \frac{|(P^{1,0}_{N,\Omega}v - v, g)_\Omega|}{\|g\|_\Omega} \\ &\le c d_\Omega^4 \delta_\Omega^{-1} N^{-r} \frac{(\mathbb{B}_{r,\Omega}(v))^{\frac12}(\mathbb{B}_{2,\Omega}(w))^{\frac12}}{\|g\|_\Omega} \\ &\le c d_\Omega^5 (d_\Omega+1)\delta_\Omega^{-\frac32} N^{-r} \frac{(\mathbb{B}_{r,\Omega}(v))^{\frac12}\|w\|_{H^2(\Omega)}}{\|g\|_\Omega} \\ &\le c\bar{c}_\Omega(c_\Omega^2+1) d_\Omega^5(d_\Omega+1)\delta_\Omega^{-\frac32} N^{-r}(\mathbb{B}_{r,\Omega}(v))^{\frac12}. \end{aligned}$$

This ends the proof of this theorem. ■

Remark 3.3. *In the case with $\Omega = K_{a_1,a_2,a_3}$ as in Remark 3.2, we could improve the results in Theorem 3.2. To do this, let*

$$\begin{aligned}
\tilde{\mathbb{B}}_{1,\Omega}(v) = \quad & (\sum_{i=1}^{3} \frac{1}{a_i^2})(\sum_{i=1}^{3} a_i^2 \|\partial_{x_i} v\|_\Omega^2 + ||v||_\Omega^2), \\
\tilde{\mathbb{B}}_{2,\Omega}(v) = \quad & \tilde{\mathbb{B}}_{1,\Omega}(v) + (\sum_{i=1}^{3} \frac{1}{a_i^2}) \sum_{i=1}^{3} \sum_{j=1}^{3} a_i^2 a_j^2 \|\partial_{x_i} \partial_{x_j} v\|_\Omega^2,
\end{aligned}$$

and $\tilde{\mathbb{B}}_{r,\Omega}(v) = \sum_{j=1}^{3} \tilde{\mathbb{B}}_{r,\Omega}^{(j)}(v)$ *for* $r \geq 3$, *with*

$$\begin{aligned}
\tilde{\mathbb{B}}_{r,\Omega}^{(1)}(v) = & (\sum_{i=1}^{3} \frac{1}{a_i^2}) \int\int\int_\Omega (a_1^2(a_1^2 - x_1^2)^{r-1}(\partial_{x_1}^r v)^2 + a_2^2(a_2^2 - x_2^2)^{r-1}(\partial_{x_2}^r v)^2 \\
& + a_3^2(a_3^2 - x_3^2)^{r-1}(\partial_{x_3}^r v)^2) dx_1 dx_2 dx_3, \\
\tilde{\mathbb{B}}_{r,\Omega}^{(2)}(v) = & (\sum_{i=1}^{3} \frac{1}{a_i^2})(a_1^2 \int\int\int_\Omega (a_1^2 - x_1^2)^{r-2}(a_2^2(\partial_{x_1}^{r-1}\partial_{x_2} v)^2 + a_3^2(\partial_{x_1}^{r-1}\partial_{x_3} v)^2) dx_1 dx_2 dx_3 \\
& + a_2^2 \int\int\int_\Omega (a_2^2 - x_2^2)^{r-2}(a_1^2(\partial_{x_1}\partial_{x_2}^{r-1} v)^2 + a_3^2(\partial_{x_2}^{r-1}\partial_{x_3} v)^2) dx_1 dx_2 dx_3 \\
& + a_3^2 \int\int\int_\Omega (a_3^2 - x_3^2)^{r-2}(a_1^2(\partial_{x_1}\partial_{x_3}^{r-1} v)^2 + a_2^2(\partial_{x_2}\partial_{x_3}^{r-1} v)^2) dx_1 dx_2 dx_3), \\
\tilde{\mathbb{B}}_{r,\Omega}^{(3)}(v) = & (\sum_{i=1}^{3} \frac{1}{a_i^2}) a_1^2 a_2^2 a_3^2 \int\int\int_\Omega ((a_1^2 - x_1^2)^{r-3}(\partial_{x_1}^{r-2}\partial_{x_2}\partial_{x_3} v)^2 \\
& + (a_2^2 - x_2^2)^{r-3}(\partial_{x_1}\partial_{x_2}^{r-2}\partial_{x_3} v)^2 + (a_3^2 - x_3^2)^{r-3}(\partial_{x_1}\partial_{x_2}\partial_{x_3}^{r-2} v)^2) dx_1 dx_2 dx_3.
\end{aligned}$$

By (2) and an argument similar to the derivation of (30), we verify that for $r \geq 1$,

$$\|\nabla(P_{N,\Omega}^{1,0} v - v)\|_\Omega^2 \leq cN^{2-2r} \tilde{\mathbb{B}}_{r,\Omega}(v). \tag{45}$$

Next, like (44), we have that for $1 \leq r \leq N+1$,

$$|(P_{N,\Omega}^{1,0} v - v, g)_\Omega| \leq cN^{-r} (\tilde{\mathbb{B}}_{r,\Omega}(v))^{\frac{1}{2}} (\tilde{\mathbb{B}}_{2,\Omega}(w))^{\frac{1}{2}}.$$

Moreover, we obtain from (42) that $|w|_{H^2(\Omega)} \leq c\|g\|_\Omega$. *Finally, by an argument as in the last part of the proof of Theorem 3.2, we derive that for* $1 \leq r \leq N+1$,

$$\|P_{N,\Omega}^{1,0} v - v\|_\Omega \leq cN^{-r} (\tilde{\mathbb{B}}_{r,\Omega}(u))^{\frac{1}{2}}. \tag{46}$$

3.4. Other irrational orthogonal approximations. For spectral method of problems with mixed boundary conditions, we need other irrational orthogonal approximations. For instance, we denote the boundary of the reference cube K by $\partial K = \cup_{j=1}^6 S_j$, with

$$\begin{aligned}
& S_1 = \{\boldsymbol{\xi} \in K, \xi_1 = -1\}, \quad S_2 = \{\boldsymbol{\xi} \in K, \xi_2 = -1\}, \quad S_3 = \{\boldsymbol{\xi} \in K, \xi_3 = -1\}, \\
& S_4 = \{\boldsymbol{\xi} \in K, \xi_1 = 1\}, \qquad S_5 = \{\boldsymbol{\xi} \in K, \xi_2 = 1\}, \qquad S_6 = \{\boldsymbol{\xi} \in K, \xi_3 = 1\}.
\end{aligned}$$

Meanwhile, let the boundary $\partial\Omega = \cup_{j=1}^6 F_j$ and $F_j = \{\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{\xi}), \boldsymbol{\xi} \in S_j\}, 1 \leq j \leq 6$.

Now, let $\partial^{**}\Omega = \cup_{j=1}^3 F_j$, $\partial^*\Omega = \cup_{j=4}^6 F_j$, and

$${}^0H^1(\Omega) = \{ \ v \mid v \in H^1(\Omega) \text{ and } v = 0 \text{ on } \partial^*\Omega \ \}, \qquad {}^0V_N(\Omega) = {}^0H^1(\Omega) \cap V_N(\Omega).$$

The ${}^0H^1(\Omega)$-irrational orthogonal projection ${}^0P^1_{N,\Omega} : {}^0H^1(\Omega) \to {}^0V_N(\Omega)$ is defined by

$$(\nabla({}^0P^1_{N,\Omega}v - v), \nabla\phi)_\Omega = 0, \qquad \forall \phi \in {}^0V_N(\Omega). \tag{47}$$

Following the same line as in the proof of the last theorem, we use (7) to obtain the following result.

Theorem 3.3. If $v \in {}^0H^1(\Omega)$ and $\mathbb{B}_{r,\Omega}(v)$ is finite for integers $1 \le r \le N+1$, then

$$\begin{aligned} &\|\nabla({}^0P^1_{N,\Omega}v - v)\|^2_\Omega \le c d^4_\Omega \delta^{-1}_\Omega N^{2-2r}\mathbb{B}_{r,\Omega}(v), \\ &\|{}^0P^1_{N,\Omega}v - v\|^2_\Omega \le c\bar{c}^2_{\Omega,*}(c^2_{\Omega,*}+1)^2 d^{10}_\Omega (d_\Omega+1)^2\delta^{-3}_\Omega N^{-2r}\mathbb{B}_{r,\Omega}(v), \end{aligned} \tag{48}$$

where $c_{\Omega,*}$ and $\bar{c}_{\Omega,*}$ are certain positive constants, which are similar to c_Ω and $\bar{c}_\Omega$, respectively.

4. Spectral method for problems defined on hexahedrons

In this section, we propose the spectral method for boundary value problems defined on hexahedrons.

4.1. A steady problem with Dirichlet boundary condition. We consider the following Dirichlet boundary value problem,

$$\begin{cases} -\Delta W(\boldsymbol{x}) = G(\boldsymbol{x}), & \text{in } \Omega, \\ W(\boldsymbol{x}) = g(\boldsymbol{x}), & \text{on } \partial\Omega, \end{cases} \tag{49}$$

where $G(\boldsymbol{x})$ and $g(\boldsymbol{x})$ are given functions. Let $g(\boldsymbol{x}) = g_j(\boldsymbol{x})$ on the faces $F_j, 1 \le j \le 6$. If $\bar{F}_j \cap \bar{F}_k \ne \emptyset$, then we denote their common edge by $E_{jk}, 1 \le j,k \le 6$. Assume that the boundary value $g(\boldsymbol{x})$ satisfies the consistent condition, namely, $g_j(\boldsymbol{x}) = g_k(\boldsymbol{x})$ at the common edge $E_{jk}, 1 \le j,k \le 6$. In other words, $g(\boldsymbol{x})$ is continuous on $\partial\Omega$.

We shall reformulate problem (49) to a homogeneous boundary value problem. To do this, we set $\hat{g}(\boldsymbol{\xi}) = g(\boldsymbol{x}(\boldsymbol{\xi}))$, and introduce the following functions,

$$\begin{aligned}
\hat{W}_S(\boldsymbol{\xi}) = \frac{1}{2}&((1-\xi_1)\hat{g}(-1,\xi_2,\xi_3) + (1-\xi_2)\hat{g}(\xi_1,-1,\xi_3) + (1-\xi_3)\hat{g}(\xi_1,\xi_2,-1) \\
&+(1+\xi_1)\hat{g}(1,\xi_2,\xi_3) + (1+\xi_2)\hat{g}(\xi_1,1,\xi_3) + (1+\xi_3)\hat{g}(\xi_1,\xi_2,1)), \\
\hat{W}_L(\boldsymbol{\xi}) = -\frac{1}{4}&((1-\xi_1)(1-\xi_2)\hat{g}(-1,-1,\xi_3) + (1-\xi_1)(1+\xi_2)\hat{g}(-1,1,\xi_3) \\
&+(1+\xi_1)(1-\xi_2)\hat{g}(1,-1,\xi_3) + (1+\xi_1)(1+\xi_2)\hat{g}(1,1,\xi_3) \\
&+(1-\xi_1)(1-\xi_3)\hat{g}(-1,\xi_2,-1) + (1-\xi_1)(1+\xi_3)\hat{g}(-1,\xi_2,1) \\
&+(1+\xi_1)(1-\xi_3)\hat{g}(1,\xi_2,-1) + (1+\xi_1)(1+\xi_3)\hat{g}(1,\xi_2,1) \\
&+(1-\xi_2)(1-\xi_3)\hat{g}(\xi_1,-1,-1) + (1-\xi_2)(1+\xi_3)\hat{g}(\xi_1,-1,1) \\
&+(1+\xi_2)(1-\xi_3)\hat{g}(\xi_1,1,-1) + (1+\xi_2)(1+\xi_3)\hat{g}(\xi_1,1,1)), \\
\hat{W}_V(\boldsymbol{\xi}) = \frac{1}{8}&((1+\xi_1)(1+\xi_2)(1+\xi_3)\hat{g}(1,1,1) \\
&+(1-\xi_1)(1-\xi_2)(1-\xi_3)\hat{g}(-1,-1,-1) \\
&+(1-\xi_1)(1-\xi_2)(1+\xi_3)\hat{g}(-1,-1,1) \\
&+(1+\xi_1)(1-\xi_2)(1+\xi_3)\hat{g}(1,-1,1) \\
&+(1+\xi_1)(1+\xi_2)(1-\xi_3)\hat{g}(1,1,-1) \\
&+(1-\xi_1)(1+\xi_2)(1-\xi_3)\hat{g}(-1,1,-1) \\
&+(1-\xi_1)(1+\xi_2)(1+\xi_3)\hat{g}(-1,1,1) \\
&+(1+\xi_1)(1-\xi_2)(1-\xi_3)\hat{g}(1,-1,-1)).
\end{aligned}$$

Furthermore,

$$\hat{W}_{\partial K}(\boldsymbol{\xi}) = \hat{W}_S(\boldsymbol{\xi}) + \hat{W}_L(\boldsymbol{\xi}) + \hat{W}_V(\boldsymbol{\xi}).$$

Next, we let $W_{\partial\Omega}(\boldsymbol{x}) = \hat{W}_{\partial K}(\boldsymbol{\xi}(\boldsymbol{x}))$, which only depends on $g(\boldsymbol{x})$. It can be checked that $W(\boldsymbol{x}) = W_{\partial\Omega}(\boldsymbol{x})$ on $\partial\Omega$.

We now make the variable transformation

$$W(\boldsymbol{x}) = U(\boldsymbol{x}) + W_{\partial\Omega}(\boldsymbol{x}), \qquad f(\boldsymbol{x}) = G(\boldsymbol{x}) + \Delta W_{\partial\Omega}(\boldsymbol{x}).$$

Then, (49) is changed to

$$\begin{cases} -\Delta U(\boldsymbol{x}) = f(\boldsymbol{x}), & \text{in } \Omega, \\ U(\boldsymbol{x}) = 0, & \text{on } \partial\Omega. \end{cases} \tag{50}$$

A weak formulation of (50) is to seek solution $U \in H_0^1(\Omega)$ such that

$$(\nabla U, \nabla v)_\Omega = (f, v)_\Omega, \qquad \forall v \in H_0^1(\Omega). \tag{51}$$

The irrational spectral scheme for (51) is to find $u_N \in V_N^0(\Omega)$ such that

$$(\nabla u_N, \nabla \phi)_\Omega = (f, \phi)_\Omega, \qquad \forall \phi \in V_N^0(\Omega). \tag{52}$$

The numerical solution of problem (49) is given by

$$w_N(\boldsymbol{x}) = u_N(\boldsymbol{x}) + W_{\partial\Omega}(\boldsymbol{x}). \tag{53}$$

We now deal with the convergence of scheme (52). Let $U_N = P^{1,0}_{N,\Omega}U$. We have from (22) and (51) that

$$(\nabla U_N, \nabla \phi)_\Omega = (f, \phi)_\Omega, \qquad \forall \phi \in V_N^0(\Omega). \tag{54}$$

Let $\widetilde{u}_N = u_N - U_N$. By subtracting (54) from (52), we obtain

$$(\nabla \widetilde{u}_N, \nabla \phi)_\Omega = 0, \qquad \forall \phi \in V_N^0(\Omega).$$

Taking $\phi = \widetilde{u}_N$ in the above equation, we obtain $||\nabla \widetilde{u}_N||^2_\Omega = 0$. It follows from Pocar$\acute{e}$ inequality that $\widetilde{u}_N(\mathbf{x}) \equiv 0$, and so $u_N = P^{1,0}_{N,\Omega}U$. Finally, we use (28) to conclude that for integers $1 \le r \le N+1$,

$$\begin{aligned} &\|\nabla(U - u_N)\|^2_\Omega \le c d^4_\Omega \delta^{-1}_\Omega N^{2-2r} \mathbb{B}_{r,\Omega}(U), \\ &\|U - u_N\|^2_\Omega \le c\bar{c}^2_\Omega (c^2_\Omega + 1)^2 d^{10}_\Omega (d_\Omega + 1)^2 \delta^{-3}_\Omega N^{-2r} \mathbb{B}_{r,\Omega}(U). \end{aligned} \tag{55}$$

This, together with (53), implies that for $1 \le r \le N+1$,

$$\begin{aligned} &\|\nabla(W - w_N)\|^2_\Omega \le c d^4_\Omega \delta^{-1}_\Omega N^{2-2r} (\mathbb{B}_{r,\Omega}(W) + \mathbb{B}_{r,\Omega}(W_{\partial_\Omega})), \\ &\|W - w_N\|^2_\Omega \le c\bar{c}^2_\Omega (c^2_\Omega + 1)^2 d^{10}_\Omega (d_\Omega + 1)^2 \delta^{-3}_\Omega N^{-2r} (\mathbb{B}_{r,\Omega}(W) + \mathbb{B}_{r,\Omega}(W_{\partial\Omega})), \end{aligned} \tag{56}$$

provided that $\mathbb{B}_{r,\Omega}(W)$ and $\mathbb{B}_{r,\Omega}(W_{\partial\Omega})$ are finite.

4.2. A mixed boundary value problem. In this subsection, we propose the spectral method for a mixed boundary value problem. Let $\partial^{**}\Omega = F_1 \cup F_2 \cup F_3$, $\partial^*\Omega = F_4 \cup F_5 \cup F_6$, and $\alpha(\boldsymbol{x})$ be a non-negative and uniformly bounded function. We consider the following problem,

$$\begin{cases} -\Delta W(\boldsymbol{x}) = G(\boldsymbol{x}), & \text{in } \Omega, \\ W(\boldsymbol{x}) = g(\boldsymbol{x}), & \text{on } \partial^*\Omega, \\ \partial_n W(\boldsymbol{x}) + \alpha(\boldsymbol{x}) W(\boldsymbol{x}) = H(\boldsymbol{x}), & \text{on } \partial^{**}\Omega. \end{cases} \tag{57}$$

where G, g and H are given functions. Let $g_j(\boldsymbol{x}) = g(\boldsymbol{x})|_{F_j}, j = 4, 5, 6$. Assume that the boundary value $g(\boldsymbol{x})$ satisfies the consistent condition, namely, $g_j(\boldsymbol{x}) = g_k(\boldsymbol{x})$ at the common edges E_{jk}, $4 \le j, k \le 6$.

We shall change the inhomogeneous boundary value problem (57) to a boundary value problem with homogeneous Dirichlet boundary condition on $\partial^*\Omega$. To do this, we set $\partial^* K = S_4 \cup S_5 \cup S_6$ and $\hat{g}(\boldsymbol{\xi}) = g(\boldsymbol{x}(\boldsymbol{\xi}))$. We also introduce the following auxiliary function,

$$
\begin{aligned}
\hat{W}_S(\boldsymbol{\xi}) &= \frac{1}{2}((1+\xi_1)\hat{g}(1,\xi_2,\xi_3) + (1+\xi_2)\hat{g}(\xi_1,1,\xi_3) + (1+\xi_3)\hat{g}(\xi_1,\xi_2,1)),\\
\hat{W}_L(\boldsymbol{\xi}) &= -\frac{1}{4}((1+\xi_1)(1+\xi_2)\hat{g}(1,1,\xi_3) + (1+\xi_1)(1+\xi_3)\hat{g}(1,\xi_2,1)\\
&\quad + (1+\xi_2)(1+\xi_3)\hat{g}(\xi_1,1,1)),\\
\hat{W}_V(\boldsymbol{\xi}) &= \frac{1}{8}(1+\xi_1)(1+\xi_2)(1+\xi_3)\hat{g}(1,1,1).
\end{aligned}
$$

Furthermore,

$$\hat{W}_{\partial^* K}(\boldsymbol{\xi}) = \hat{W}_S(\boldsymbol{\xi}) + \hat{W}_L(\boldsymbol{\xi}) + \hat{W}_V(\boldsymbol{\xi}).$$

Next, we let $W_{\partial^*\Omega}(\boldsymbol{x}) = \hat{W}_{\partial^* K}(\boldsymbol{\xi}(\boldsymbol{x}))$, which only depends on $g(\boldsymbol{x})$. It can be shown that $W(\boldsymbol{x}) = W_{\partial^*\Omega}(\boldsymbol{x})$ on $\partial^*\Omega$.

We now make a change of the variables:

$$
\begin{gathered}
W(\boldsymbol{x}) = U(\boldsymbol{x}) + W_{\partial^*\Omega}(\boldsymbol{x}), \quad f(\boldsymbol{x}) = G(\boldsymbol{x}) + \Delta W_{\partial^*\Omega}(\boldsymbol{x}),\\
h(\boldsymbol{x}) = H(\boldsymbol{x}) - \partial_n W_{\partial^*\Omega}(\boldsymbol{x}) - \alpha W_{\partial^*\Omega}(\boldsymbol{x}).
\end{gathered}
$$

Then, (57) is reformulated as

$$
\left\{
\begin{array}{ll}
-\Delta U(\boldsymbol{x}) = f(\boldsymbol{x}), & \text{in } \Omega,\\
U(\boldsymbol{x}) = 0, & \text{on } \partial^*\Omega,\\
\partial_n U(\boldsymbol{x}) + \alpha U(\boldsymbol{x}) = h(\boldsymbol{x}), & \text{on } \partial\Omega \setminus \partial^*\Omega.
\end{array}
\right. \tag{58}
$$

Let

$$a_\alpha(u,v) = (\nabla u, \nabla v)_\Omega + \int\int_{\partial\Omega\setminus\partial^*\Omega} \alpha(\boldsymbol{x}) uv dS, \qquad \forall\ u,v \in {}^0H^1(\Omega).$$

A weak formulation of (58) is to seek the solution $U \in {}^0H^1(\Omega)$ such that

$$a_\alpha(U,v) = (f,v)_\Omega + \int\int_{\partial\Omega\setminus\partial^*\Omega} hv dS, \qquad \forall v \in {}^0H^1(\Omega). \tag{59}$$

The irrational spectral scheme for solving (59) is to find $u_N \in {}^0V_N(\Omega)$ such that

$$a_\alpha(u_N,\phi) = (f,\phi)_\Omega + \int\int_{\partial\Omega\setminus\partial^*\Omega} h\phi dS, \qquad \forall \phi \in {}^0V_N(\Omega). \tag{60}$$

The numerical solution of the original problem (57) is given by

$$w_N(\boldsymbol{x}) = u_N(\boldsymbol{x}) + W_{\partial^*\Omega}(\boldsymbol{x}). \tag{61}$$

For analyzing the convergence of scheme (60), we introduce the auxiliary projection $P_N^* v : {}^0H^1(\Omega) \to {}^0V_N(\Omega)$, such that

$$a_\alpha(P_N^* v - v, \phi) = 0, \qquad \forall \phi \in {}^0V_N(\Omega). \tag{62}$$

With the aid of (62), a direct calculation shows that for any $v \in {}^0H^1(\Omega)$ and $z \in {}^0V_N(\Omega)$,

$$
\begin{aligned}
a_\alpha(v-z, v-z) &= a_\alpha(v - P_N^* v, v - P_N^* v) + a_\alpha(z - P_N^* v, z - P_N^* v)\\
&\quad + 2a_\alpha(v - P_N^* v, P_N^* v - z)\\
&\geq a_\alpha(v - P_N^* v, v - P_N^* v).
\end{aligned} \tag{63}
$$

It follows from (59) and (62) that

$$a_\alpha(P_N^* U, \phi) = (f,\phi)_\Omega + \int\int_{\partial\Omega\setminus\partial^*\Omega} h\phi dS, \qquad \forall \phi \in {}^0V_N(\Omega).$$

Subtracting the above equality from (60), we have

$$a_\alpha(u_N - P_N^* U, \phi) = 0, \qquad \forall \phi \in {}^0V_N(\Omega).$$

By taking $\phi = u_N - P_N^* U$ in the above equation, we find that $||\nabla(u_N - P_N^* U)||_\Omega = 0$ and $u_N - P_N^* U = 0$ on $\partial\Omega \setminus \partial^*\Omega$. This fact, together with the Poincaré inequality, leads to $u_N = P_N^* U$.

Next, let ${}^0P^1_{N,\Omega}v$ be the projection defined by (47). By using (63) with $v = U$ and $z = {}^0P^1_{N,\Omega}U$, the trace theorem, the Poincaré inequality and (48) successively, we derive that

$$\begin{aligned}
||\nabla(u_N - U)||^2_\Omega &\le a_\alpha(u_N - U, u_N - U)\\
&= a_\alpha(P_N^* U - U, P_N^* U - U)\\
&\le a_\alpha({}^0P^1_{N,\Omega}U - U, {}^0P^1_{N,\Omega}U - U)\\
&\le c(1+\alpha)||{}^0P^1_{N,\Omega}U - U||^2_{1,\Omega}\\
&\le c(1+\alpha)(1+c^2_{\Omega,*})||\nabla({}^0P^1_{N,\Omega}U - U)||^2_\Omega\\
&\le c(1+\alpha)(1+c^2_{\Omega,*})d^4_\Omega \delta^{-1}_\Omega N^{2-2r}\mathbb{B}_{r,\Omega}(U),
\end{aligned} \tag{64}$$

whence

$$||u_N - U||^2_{1,\Omega} \le c(1+\alpha)(1+c^2_{\Omega,*})^2 d^4_\Omega \delta^{-1}_\Omega N^{2-2r}\mathbb{B}_{r,\Omega}(U). \tag{65}$$

We next use a duality argument to derive the optimal estimate of $\|u_N - U\|_\Omega$. Let $g \in L^2(\Omega)$. We consider an auxiliary problem. It is to find $\eta \in {}^0H^1(\Omega)$ such that

$$a_\alpha(\eta, z) = (g, z)_\Omega, \qquad \forall z \in {}^0H^1(\Omega). \tag{66}$$

By taking $z = \eta$ in (66), we use Poincaré inequality to assert that $||\eta||_{1,\Omega} \le c_{\Omega,*}(1 + c_{\Omega,*})||g||_\Omega$. Furthermore, by taking $z = u_N - U$ in (66), we obtain

$$a_\alpha(\eta, u_N - U) = (g, u_N - U)_\Omega.$$

Since $u_N = P_N^* U \in {}^0V_N(\Omega)$, we use (62) with $v = U$ and $\phi = P_N^*\eta$ to deduce that

$$a_\alpha(P_N^*\eta, u_N - U) = 0.$$

A combination of the above two equalities leads to

$$a_\alpha(\eta - P_N^*\eta, u_N - U) = (g, u_N - U)_\Omega.$$

Therefore, it follows from the trace theorem that

$$|(g, u_N - U)_\Omega| \le c\|\eta - P_N^*\eta\|_{1,\Omega}\|u_N - U\|_{1,\Omega}. \tag{67}$$

Furthermore, by taking $v = \eta$ and $z = {}^0P^1_{N,\Omega}\eta$ in (63), we find that

$$a_\alpha(\eta - P_N^*\eta, \eta - P_N^*\eta) \le a_\alpha(\eta - {}^0P^1_{N,\Omega}\eta, \eta - {}^0P^1_{N,\Omega}\eta).$$

Thus, an argument as in the derivation of (65) leads to

$$\begin{aligned}
||\eta - P_N^*\eta||^2_{1,\Omega} &\le c(1+\alpha)(1+c^2_{\Omega,*})^2 d^4_\Omega \delta^{-1}_\Omega N^{-2}\mathbb{B}_{2,\Omega}(\eta)\\
&\le c(1+\alpha)(1+c^2_{\Omega,*})^2 d^4_\Omega \delta^{-1}_\Omega N^{-2}||\eta||^2_{2,\Omega}.
\end{aligned} \tag{68}$$

Accordingly, we use (65), (67) and (68) to reach that

$$|(g, u_N - U)_\Omega| \le c(1+\alpha)(1+c^2_{\Omega,*})^2 d^4_\Omega \delta^{-1}_\Omega N^{-r}||\eta||_{2,\Omega}\mathbb{B}^{\frac{1}{2}}_{r,\Omega}(U).$$

By virtue of the property of elliptic equation, there exists $\zeta_\Omega > 0$, such that $\|\eta\|_{2,\Omega} \le \zeta_\Omega\|g\|_\Omega$ (cf. [5]). Consequently, we verify that

$$\|u_N - U\|_\Omega = \sup_{g\in L^2(\Omega), g\ne 0}\frac{|(g, u_N - U)_\Omega|}{\|g\|_\Omega} \le c\zeta_\Omega(1+\alpha)(1+c^2_{\Omega,*})^2 d^4_\Omega \delta^{-1}_\Omega N^{-r}\mathbb{B}^{\frac{1}{2}}_{r,\Omega}(U). \tag{69}$$

Finally, we obtain from (61), (64) and (69) that for $1 \le r \le N+1$,

(70)

$$\begin{aligned} ||\nabla(w_N - W)||^2_\Omega &\le c(1+\alpha)(1+c^2_{\Omega,*})d^4_\Omega \delta^{-1}_\Omega N^{2-2r}(\mathbb{B}_{r,\Omega}(W) + \mathbb{B}_{r,\Omega}(W_{\partial^*\Omega})), \\ \|w_N - W\|^2_\Omega &\le c\zeta^2_\Omega(1+\alpha)^2(1+c^2_{\Omega,*})^4 d^8_\Omega \delta^{-2}_\Omega N^{-2r}(\mathbb{B}_{r,\Omega}(W) + \mathbb{B}_{r,\Omega}(W_{\partial^*\Omega})), \end{aligned}$$

provided that $\mathbb{B}_{r,\Omega}(W)$ and $\mathbb{B}_{r,\Omega}(W_{\partial\Omega})$ are finite.

5. Numerical results

In this section, we describe the numerical implementations and present some numerical results.

5.1. Dirichlet boundary value problem. We first consider the spectral scheme (52). Let $L_l(\xi)$ be the Legendre polynomial of degree l, and

$$\chi_l(\xi) = \frac{L_l(\xi) - L_{l+2}(\xi)}{\sqrt{4l+6}}, \qquad 0 \le l \le N-2.$$

The basis functions are given by

$$\psi_{l_1,l_2,l_3}(\boldsymbol{x}) = \chi_{l_1}(\xi_1(\boldsymbol{x}))\chi_{l_2}(\xi_2(\boldsymbol{x}))\chi_{l_3}(\xi_3(\boldsymbol{x})).$$

We expand the numerical solution as

$$u_N(\boldsymbol{x}) = \sum_{l_3=0}^{N-2}\sum_{l_2=0}^{N-2}\sum_{l_1=0}^{N-2} u_{l_1,l_2,l_3}\psi_{l_1,l_2,l_3}(\boldsymbol{x}). \tag{71}$$

Inserting (71) into (52) and taking the previous basis functions $\phi = \psi_{l_1',l_2',l_3'}(\boldsymbol{x})$ as the test functions, we obtain a symmetrical discrete system with the unknown coefficients a_{l_1,l_2,l_3} as follows,

$$\sum_{l_3=0}^{N-2}\sum_{l_2=0}^{N-2}\sum_{l_1=0}^{N-2}(\nabla\psi_{l_1,l_2,l_3}, \nabla\psi_{\Omega,l_1',l_2',l_3'})_\Omega u_{l_1,l_2,l_3} = (f, \psi_{\Omega,l_1',l_2',l_3'})_\Omega. \tag{72}$$

Let $\mathbf{X}$ be the vectors of unknown coefficients u_{l_1,l_2,l_3}, namely,

$\mathbf{X} =$

$(u_{0,0,0}, u_{1,0,0}, \cdots, u_{N-2,0,0}, u_{0,1,0}, u_{1,1,0}, \cdots, u_{N-2,1,0}, \cdots, u_{0,N-2,0}, u_{1,N-2,0}, \cdots, u_{N-2,N-2,0},$

$u_{0,0,1}, u_{1,0,1}, \cdots, u_{N-2,0,1}, u_{0,1,1}, u_{1,1,1}, \cdots, u_{N-2,1,1}, \cdots, u_{0,N-2,1}, u_{1,N-2,1}, \cdots, u_{N-2,N-2,1},$

$\cdots, \cdots, \cdots,$

$u_{0,0,N-2}, u_{1,0,N-2}, \cdots, u_{N-2,0,N-2}, u_{0,1,N-2}, u_{1,1,N-2}, \cdots, u_{N-2,1,N-2}, \cdots, u_{0,N-2,N-2},$

$u_{1,N-2,N-2}, \cdots, u_{N-2,N-2,N-2})^T.$

Also, we put

$\mathbf{F} =$

$(f_{0,0,0}, f_{1,0,0}, \cdots, f_{N-2,0,0}, f_{0,1,0}, f_{1,1,0}, \cdots, f_{N-2,1,0}, \cdots, f_{0,N-2,0}, f_{1,N-2,0}, \cdots, f_{N-1,N-2,0},$

$f_{0,0,1}, f_{1,0,1}, \cdots, f_{N-2,0,1}, f_{0,1,1}, f_{1,1,1}, \cdots, f_{N-2,1,1}, \cdots, f_{0,N-2,1}, f_{1,N-1,1}, \cdots, f_{N-2,N-2,1},$

$\cdots, \cdots, \cdots,$

$f_{0,0,N-2}, f_{1,0,N-2}, \cdots, f_{N-2,0,N-2}, f_{0,1,N-2}, f_{1,1,N-2}, \cdots, f_{N-2,1,N-2}, \cdots, f_{0,N-2,N-2},$

$f_{1,N-2,N-2}, \cdots, f_{N-2,N-2,N-2})^T,$

with the components

$$f_{l_1',l_2',l_3'} = (f, \psi_{\Omega,l_1',l_2',l_3'})_\Omega, \qquad 0 \le l_1', l_2', l_3' \le N-2.$$

Then, we obtain the following compact matrix form of (72),

$$AX = F, \tag{73}$$

where $A = (a_{l'_1,l'_2,l'_3,l_1,l_2,l_3})$ with the following entries,

$$a_{l'_1,l'_2,l'_3,l_1,l_2,l_3} = (\nabla\psi_{\Omega,l_1,l_2,l_3}, \nabla\psi_{\Omega,l'_1,l'_2,l'_3})_\Omega. \tag{74}$$

We now calculate the entries $a_{l'_1,l'_2,l'_3,l_1,l_2,l_3}$. The hexahedron Ω is transformed to the reference cube K by the coordinate transformation $x_i = x_i(\boldsymbol{\xi})$. Similar to the derivation of (30), we have

$$(\nabla v, \nabla\phi)_\Omega = (J_\Omega^{-1} M_\Omega^* \nabla_K u, M_\Omega^* \nabla_K \psi)_K.$$

More precisely, we denote the entries of the matric M_Ω^* by $m_{ij}(1 \le i, j \le 3)$. Then

$$\begin{aligned}
(\nabla v, \nabla\phi)_\Omega &= \int\int\int_K J_\Omega^{-1} M_\Omega^* \nabla_K u \cdot M_\Omega^* \nabla_K \psi d\xi_1\xi_2\xi_3 \\
&= \int\int\int_K J_\Omega^{-1}((m_{11}\partial_{\xi_1}u + m_{12}\partial_{\xi_2}u + m_{13}\partial_{\xi_3}u)(m_{11}\partial_{\xi_1}\psi + m_{12}\partial_{\xi_2}\psi + m_{13}\partial_{\xi_3}\psi) \\
&+(m_{21}\partial_{\xi_1}u + m_{22}\partial_{\xi_2}u + m_{23}\partial_{\xi_3}u)(m_{21}\partial_{\xi_1}\psi + m_{22}\partial_{\xi_2}\psi + m_{23}\partial_{\xi_3}\psi) \\
&+(m_{31}\partial_{\xi_1}u + m_{32}\partial_{\xi_2}u + m_{33}\partial_{\xi_3}u)(m_{31}\partial_{\xi_1}\psi + m_{32}\partial_{\xi_2}\psi + m_{33}\partial_{\xi_3}\psi))d\xi_1\xi_2\xi_3.
\end{aligned}$$

Accordingly, we obtain from (74) that

$$\begin{aligned}
a_{l'_1,l'_2,l'_3,l_1,l_2,l_3} &= (\nabla\psi_{\Omega,l_1,l_2,l_3}, \nabla\psi_{\Omega,l'_1,l'_2,l'_3})_\Omega \\
&= \int\int\int_K J_\Omega^{-1}(\sum_{j=1}^{3} m_{1j}\partial_{\xi_j}(\phi_{l_1}(\xi_1)\phi_{l_2}(\xi_2)\phi_{l_3}(\xi_3))\sum_{j=1}^{3} m_{1j}\partial_{\xi_j}(\phi_{l'_1}(\xi_1)\phi_{l'_2}(\xi_2)\phi_{l'_3}(\xi_3)) \\
&+\sum_{j=1}^{3} m_{2j}\partial_{\xi_j}(\phi_{l_1}(\xi_1)\phi_{l_2}(\xi_2)\phi_{l_3}(\xi_3))\sum_{j=1}^{3} m_{2j}\partial_{\xi_j}(\phi_{l'_1}(\xi_1)\phi_{l'_2}(\xi_2)\phi_{l'_3}(\xi_3)) \\
&+\sum_{j=1}^{3} m_{3j}\partial_{\xi_j}(\phi_{l_1}(\xi_1)\phi_{l_2}(\xi_2)\phi_{l_3}(\xi_3))\sum_{j=1}^{3} m_{3j}\partial_{\xi_j}(\phi_{l'_1}(\xi_1)\phi_{l'_2}(\xi_2)\phi_{l'_3}(\xi_3)))d\xi_1 d\xi_2 d\xi_3.
\end{aligned}$$

Besides,

$$f_{l'_1,l'_2,l'_3} = (f, \psi_{\Omega,l'_1,l'_2,l'_3})_\Omega = (f, \chi_{l'_1}(\xi_1)\chi_{l'_2}(\xi_2)\chi_{l'_3}(\xi_3)J_\Omega)_K, \qquad 0 \le l'_1, l'_2, l'_3 \le N-2.$$

For description of numerical errors, let $\zeta_{N,i}$ and $\rho_{N,i}(1 \le i \le N)$ be the nodes and the weights of the one-dimensional Legendre-Gauss-Lobatto quadrature. We measure the errors of numerical solution of (49) by

$$\begin{aligned}
E_N &= (\sum_{l_1=0}^{N}\sum_{l_2=0}^{N}\sum_{l_3=0}^{N}(W(\boldsymbol{x}(\zeta_{N,l_1}, \zeta_{N,l_2}, \zeta_{N,l_3})) - w_N(\boldsymbol{x}(\zeta_{N,l_1}, \zeta_{N,l_2}, \zeta_{N,l_3})))^2 \\
&\quad\times J_\Omega(\boldsymbol{\xi})\rho_{N,l_1}\rho_{N,l_2}\rho_{N,l_3})^{\frac{1}{2}} \\
&\simeq (\int\int\int_K (W(\boldsymbol{x}(\boldsymbol{\xi})) - w_N(\boldsymbol{x}(\boldsymbol{\xi})))^2 J_\Omega(\boldsymbol{\xi})d\xi_1 d\xi_2 d\xi_3)^{\frac{1}{2}} = \|W - w_N\|_\Omega.
\end{aligned}$$

Our first example is for the Dirichlet problem of (49) posed on a hexahedron domain with the following vertices:

$$\begin{aligned}
&Q_1 = (0,0,0), \quad Q_2 = (2,0,0), \quad Q_3 = (\tfrac{4}{3}, \tfrac{4}{3}, 0), \quad Q_4 = (0,2,0), \\
&Q_5 = (0,0,\tfrac{3}{2}), \quad Q_6 = (\tfrac{4}{3}, 0, 1), \quad Q_7 = (1,1,\tfrac{3}{4}), \quad Q_8 = (0,\tfrac{4}{3},1).
\end{aligned} \tag{75}$$

We assume that the right hand side f and the boundary value g are suitably defined so that (49) admits the following exact solution

$$W(x_1, x_2, x_3) = (x_1 + 2x_2 + 3_3)\sin(x_1 + x_2 + x_3). \tag{76}$$

In Table 1, we present the values of $\log_{10} E_N$ vs. the mode N. As is predicted by (56), the numerical errors decay faster than any power of N^{-1} since the exact solution $W(x_1, x_2, x_3)$ is analytic.

TABLE 1. Numerical errors of problem (49).

$N=5$	$N=10$	$N=15$	$N=20$
8.27E-05	1.48E-10	1.89E-15	1.87E-15

5.2. Mixed boundary value problem. We next consider spectral scheme (60). Let

$$\phi_l(\xi) = \frac{L_l(\xi) - L_{l+1}(\xi)}{2\sqrt{l+1}}.$$

The base functions are given by

$$\psi_{l,m,k}(\boldsymbol{x}) = \phi_l(\xi_1(\boldsymbol{x}))\phi_m(\xi_2(\boldsymbol{x}))\phi_k(\xi_3(\boldsymbol{x})).$$

We expand the numerical solution as

$$u_N(\boldsymbol{x}) = \sum_{l_3=0}^{N-1}\sum_{l_2=0}^{N-1}\sum_{l_1=0}^{N-1} u_{l_1,l_2,l_3}\psi_{l_1,l_2,l_3}(\boldsymbol{x}). \tag{77}$$

Inserting (77) into (60) and taking the previous basis functions $\phi = \psi_{\Omega,l_1',l_2',l_3'}(\boldsymbol{x})$ as the test functions, we obtain a symmetrical discrete system with the unknown coefficients u_{l_1,l_2,l_3} as follow,

$$A\mathbf{X} = \mathbf{F}^*,$$

where $\mathbf{X}$ and $\mathbf{F}^*$ are similar to $\mathbf{X}$ and $\mathbf{F}$ in (73),

$$f^*_{l_1',l_2',l_3'} = (f, \psi_{\Omega,l_1',l_2',l_3})_\Omega + \int_{\partial\Omega\backslash\partial^*\Omega} h(\boldsymbol{x})\psi_{\Omega,l_1',l_2',l_3}dS, \qquad 0 \le l_1', l_2', l_3' \le N-1.$$

The matrix $A = (a_{l_1',l_2',l_3',l_1,l_2,l_3})$ with the following entries,

$$a_{l_1',l_2',l_3',l_1,l_2,l_3} = (\nabla\psi_{\Omega,l_1,l_2,l_3}, \nabla\psi_{\Omega,l_1',l_2',l_3'})_\Omega + \int_{\partial\Omega\backslash\partial^*\Omega} \alpha(\boldsymbol{x})\psi_{l_1,l_2,l_3}\psi_{\Omega,l_1',l_2',l_3}dS.$$

As the second example of our numerical experiment, we consider the Neumann and mixed problem (57) with the same domain Ω as in (75) and the same solution as in (76). The boundary value g and H in (57) are slected according to the exact solution for two different cases of $\alpha = 0$ and $\alpha = 1$. In Table 2, we list the values of $\log_{10} E_N$ vs. the mode N. As is predicted by (70), the numerical errors decay again faster than any power of N^{-1}.

TABLE 2. Numerical errors of problem (57).

	$N=5$	$N=10$	$N=15$	$N=20$
$\alpha=0$	3.56E-05	8.50E-11	1.63E-14	8.04E-15
$\alpha=1$	3.50E-05	8.43E-11	1.16E-14	6.99E-15

Concluding remarks

In this paper, we proposed a spectral method for mixed boundary value problems on hexahedrons and prove its spectral accuracy. As examples of applications, the spectral schemes were applied to two model problems. The numerical results demonstrated the high efficiency of the proposed schemes, which is consistent with our theoretical analysis well. Although we only considered two model problems, the main idea and techniques developed in this work are also applicable to other mixed boundary value problems. In particular, the proposed irrational orthogonal approximation may serve as the mathematical foundation of spectral method for partial differential equations defined on hexahedrons.

An more important problem is how to design spectral element method for problems on polyhedrons. In fact, we may generalize the basic results of this paper to the composite irrational quasi-orthogonal approximation on polyhedrons, which in turn leads to the spectral element method for polyhedrons. We shall report the related work in the future. On the other hand, some authors also considered pseudospectral method for non-rectangular domains, which are also called as spectral element method oftentimes, see [4, 6, 17] and the references therein.

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